USE OF COVARIANCE MATRICES IN A CONSISTENT (MULTISCALE) DATA ASSIMILATION FOR IMPROVEMENT OF BASIC NUCLEAR PARAMETERS IN NUCLEAR REACTOR APPLICATIONS: FROM METERS TO FEMTOMETERS

PIs: G. Palmiotti[1], M. W. Herman[2]

Collaborators: M. Salvatores[1,3], H. Hiruta[1], P. Oblozinsky[2], M. T. Pigni[2]

[1] Idaho National Laboratory USA
[2] Brookhaven National Laboratory USA
[3] Commissariat à l'Energie Atomique, Cadarache France

DOE-NP ANS&T Exchange Meeting

August 22-23, 2011

Hilton Hotel & Executive Meeting Center, Rockville, MD

www.inl.gov

Introduction

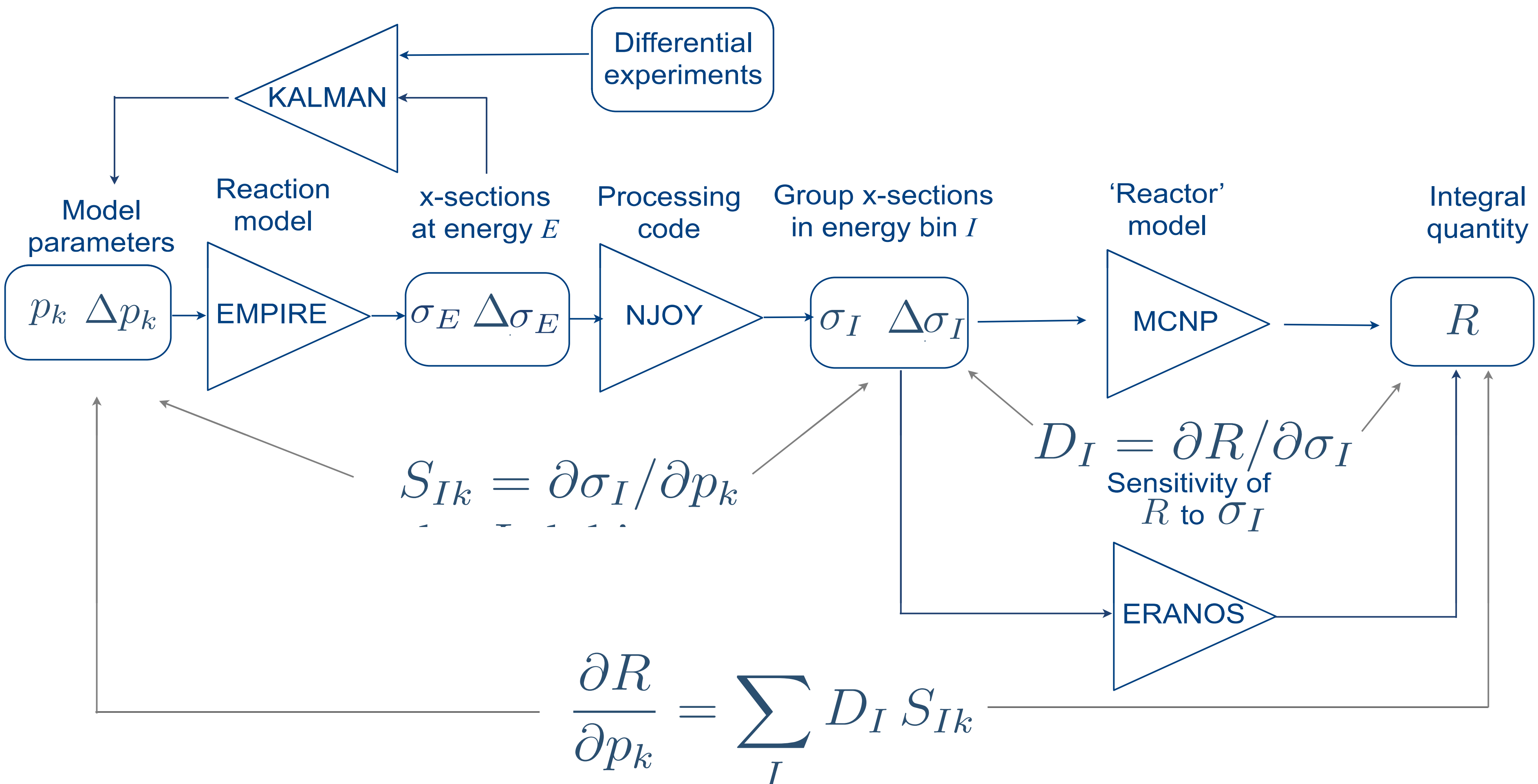
- One of the major requirement needed in order to make nuclear energy economical viable, safe proof, and gain a wide acceptance is related to the reduction of uncertainty associated to the design and operation of nuclear reactors and fuel cycles.
- Industry and utilities want reduced uncertainty for economical reasons (design and operation), while safety authorities want "guaranteed margins" that they can trust. As nuclear reactors are perceived as safe proof, acceptance becomes more widespread.
- The neutron cross section uncertainty are classified as epistemic ones. These are uncertainties related to lack of knowledge. Reduction of the epistemic uncertainty can be performed when useful and relevant experimental information is available through an adjustment (also called: calibration, tuning, assimilation) process.
- The major drawbacks of the classical adjustment method are related to the multigroup cross section approach. This implies several constraints:
  - potential limitation of the domain of application of the adjusted data
  - fixed energy multigroup structure
  - dependence on the neutron spectrum used as weighting function and the code used to process the basic data file

Consistent Data Assimilation

- A new approach has been developed in order to adjust physical parameters and not multigroup nuclear data, the objective being now to correlate the uncertainties of some basic parameters that characterize the neutron cross section description, to the discrepancy between calculation and experimental value for a large number of clean, high accuracy integral experiments.
- This new approach is the first attempt to build up a link between the wealth of precise integral experiments and basic theory of nuclear reactions. By using integral reactor physics experiments (meter scale), information is propagated back to the nuclear physics level (femtometers). In this way, the worlds of reactor nuclear physicists and that of nuclear physicists are bridged together.
- The classical statistical adjustment method can be improved by "adjusting" reaction model parameters rather than multigroup nuclear data. The objective is to associate uncertainties of certain model parameters (such as those determining neutron resonances, optical model potentials, level densities, strength functions, etc.) and the uncertainties of theoretical nuclear reaction models themselves (such as optical model, compound nucleus, pre-equilibrium and fission models) with observed discrepancies between calculations and experimental values for a large number of integral experiments.

Consistent Data Assimilation

Linking integral experiments with reaction model parameters



S_{Ik} **contains all restrictions imposed by differential data**

Requisites for assimilation

- Adequate set of reaction models
- Entire evaluation expressed in terms of model parameters
- Reaction model and its parameterization flexible enough to reproduce differential and integral data
- Clean, well defined, integral experiments predominantly sensitive to a single material.

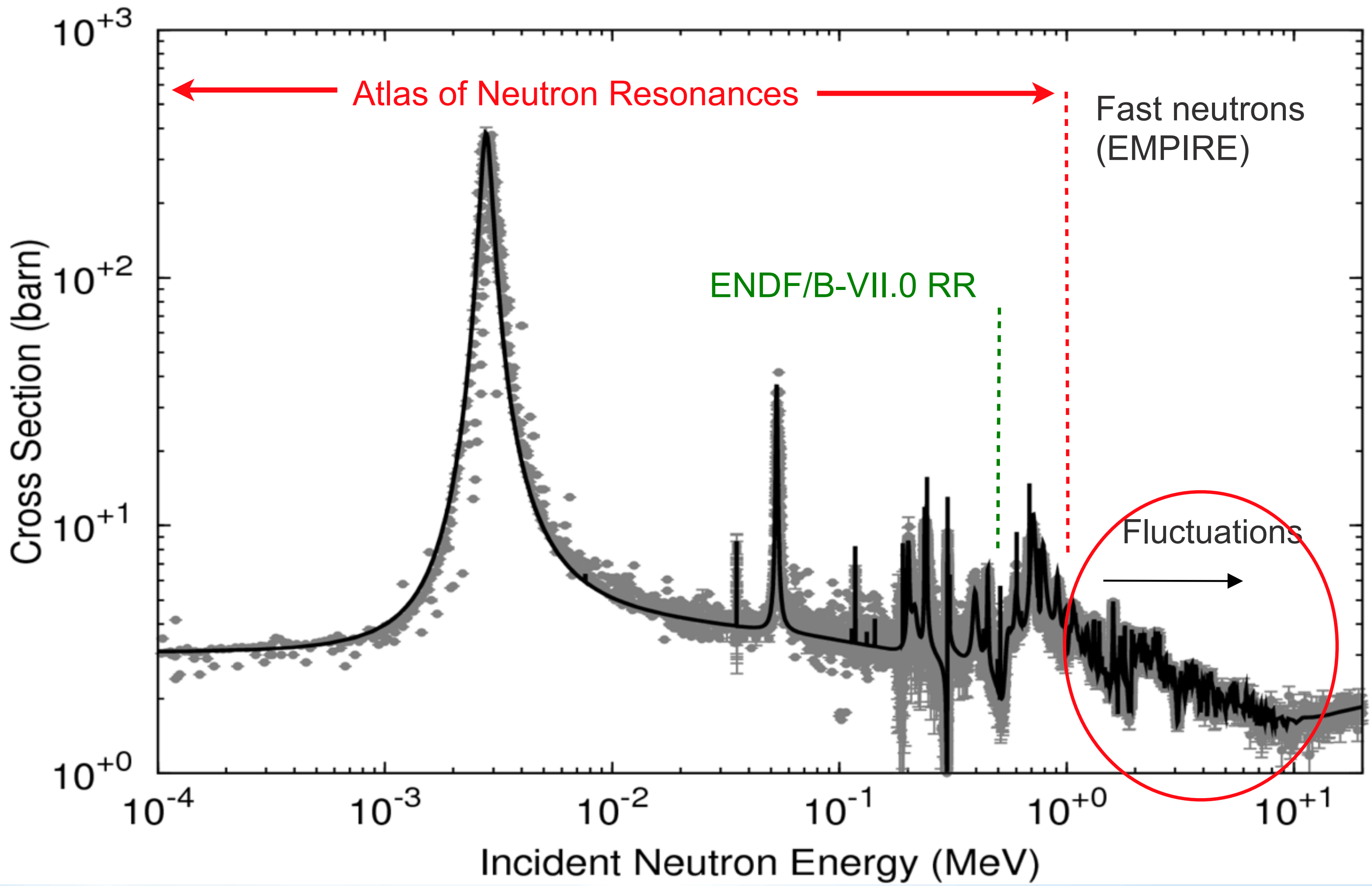
^{23}Na Consistent Data Assimilation

- As first practical example we have considered the case of the ^{23}Na isotope. A set of 136 nuclear parameters were selected and sensitivities to them in terms of multigroup cross section were calculated. The selected parameters include:
  - nuclear scattering radius
  - bound level and 33 resonances (for each one: E_n resonance peak energy, Γ_n neutron width, Γ_g radiative width, for a total of 102 parameters).
  - 21 Optical model parameters
  - 7 Statistical Hauser-Feshbach model parameters
  - 5 Preequilibrium Exciton model parameters
- We have used propagation experiments of neutrons in a medium dominated by sodium. These kinds of experiments were specifically intended for improving the data used in the shielding design of fast reactors. Two experimental campaigns taken from the SINBAD database have been used in this practical application:
  - the EURACOS campaign
  - the JANUS-8 campaign

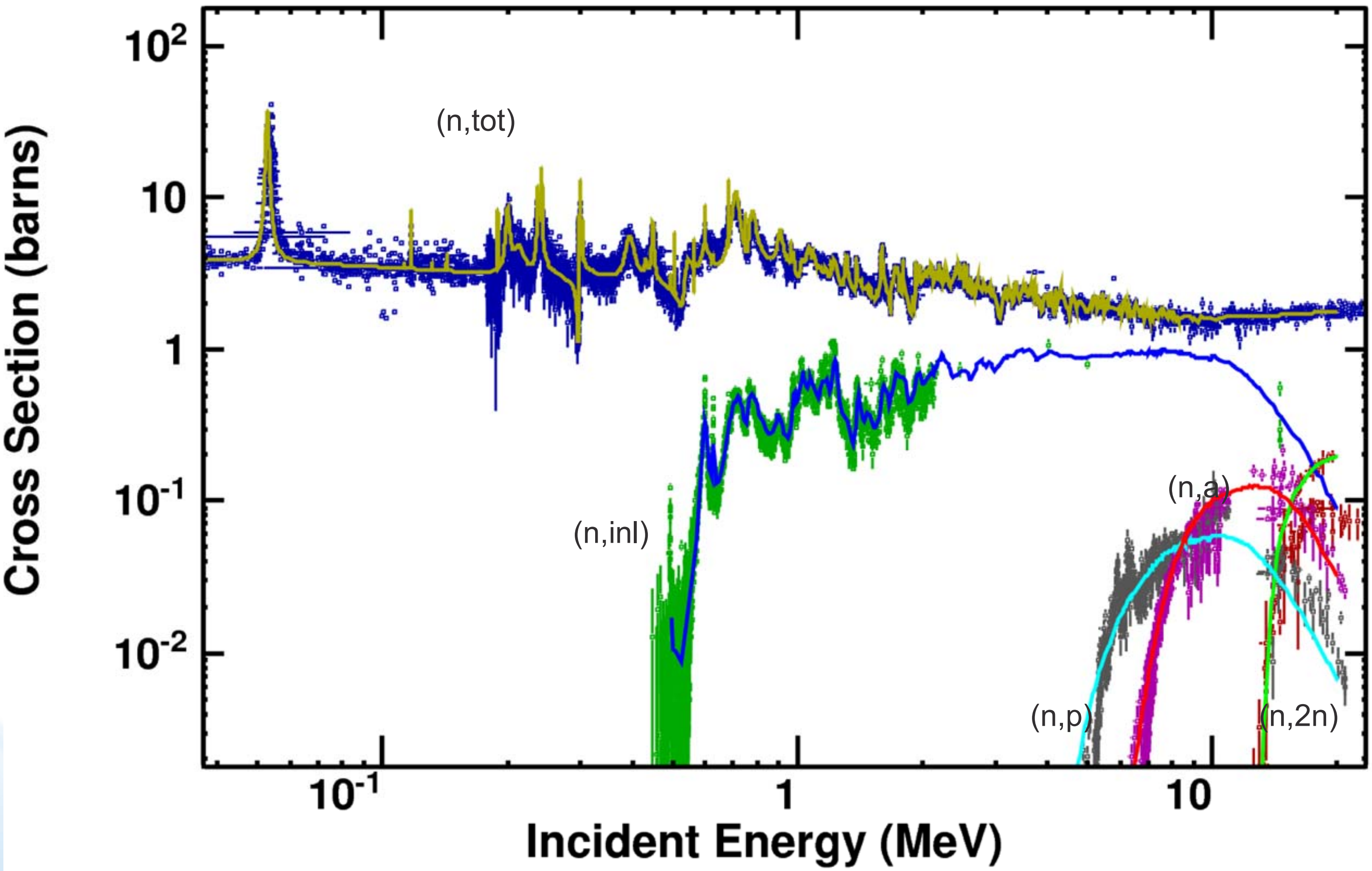
^{23}Na evaluation methodology

- Atlas of Neutron Resonances => Resonance Region
- EMPIRE => Fast Neutron Region
  - Spherical optical model (Coupled-Channel potential prepared)
  - EMPIRE-specific level densities
  - Modified Lorentzian (MLO1) gamma-ray strength functions
  - Exciton model with cluster emission
  - Cross section fluctuations accounted for through energy dependent tuning of total and absorption

^{23}Na(n,tot)
Atlas RR up to ~1 MeV; fluctuations in fast region



^{23}Na(n,*) cross sections



Uncertainties of model parameters

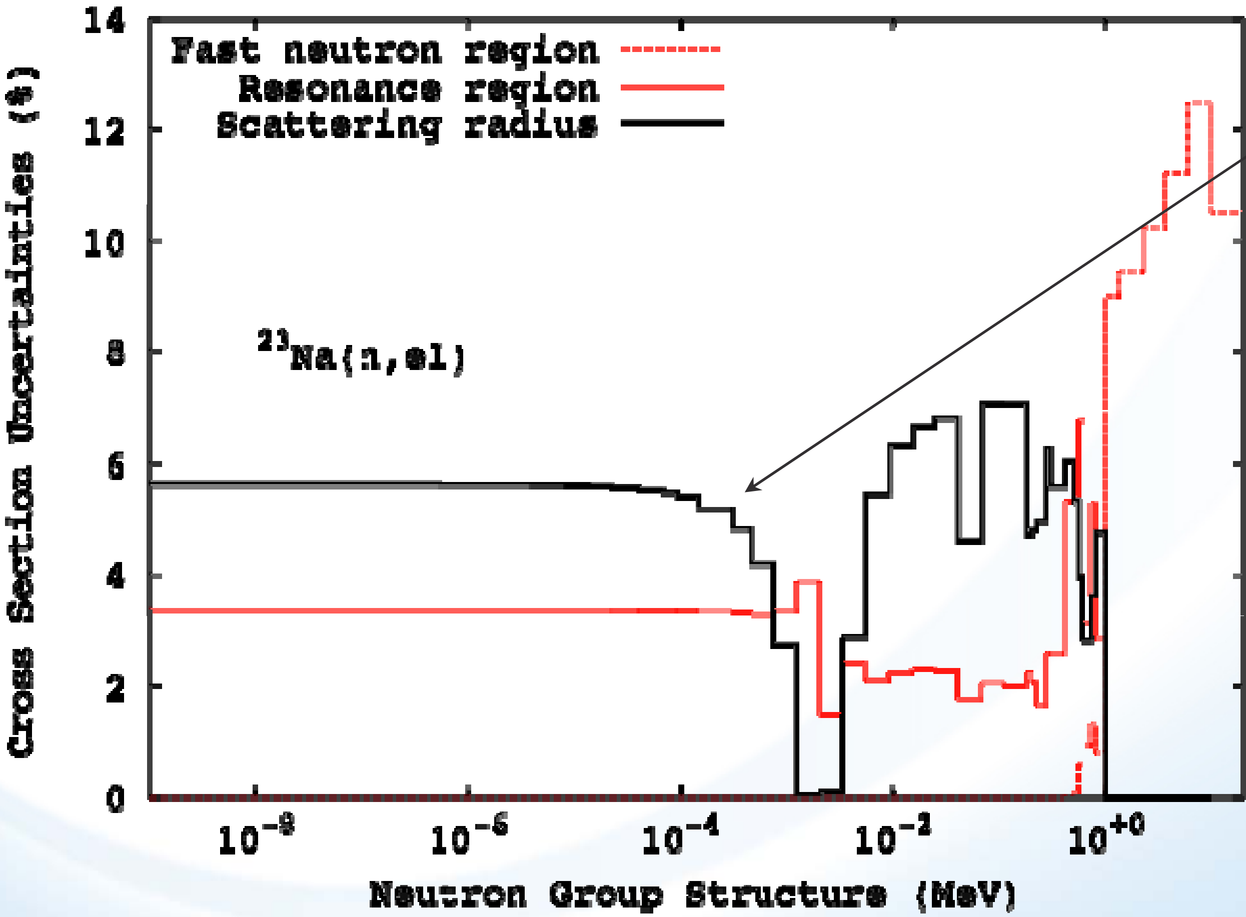
Table 1. *Optical-model parameter uncertainties (in %): r radius, a diffuseness, V real depth, W imaginary depth. The subscripts v, s, and w, respectively, denote real volume, real surface, and imaginary surface. The superscripts, tg=n+A(Z), np=p+A(Z-1), and na=a+A-3(Z-2) identify nucleon-nucleus* interaction.

Δr_v^{tg}	Δr_s^{tg}	Δr_w^{tg}	ΔV_v^{tg}	ΔW_s^{tg}	ΔW_v^{tg}	Δa_s^{tg}	Δa_v^{tg}
2	0.8	3.5	0.7	1.7	3.5	1.1	1.5
Δr_s^{np}	Δr_w^{np}	ΔV_v^{np}	ΔW_s^{np}	ΔW_v^{np}	Δa_s^{np}	Δa_v^{np}	Δr_v^{na}
1.5	3.6	0.5	1	3.5	1	1	1
ΔV_v^{na}	ΔW_v^{na}	Δa_v^{na}					
1	3.5	1					

Table 2. *Parameter uncertainties (in %) used for the Hauser-Feshbach and exciton models: ã-total level density, ḡ single-particle level density, f_γ, f_p, f_α, emission width for gammas, protons, alphas, mfp nucleon mean-free path, tpe scaling of pre-equilibrium gamma-ray strength function. The superscripts refer to cn=compound, tg=target, np=(n,p) residue, na=(n,a) residue.*

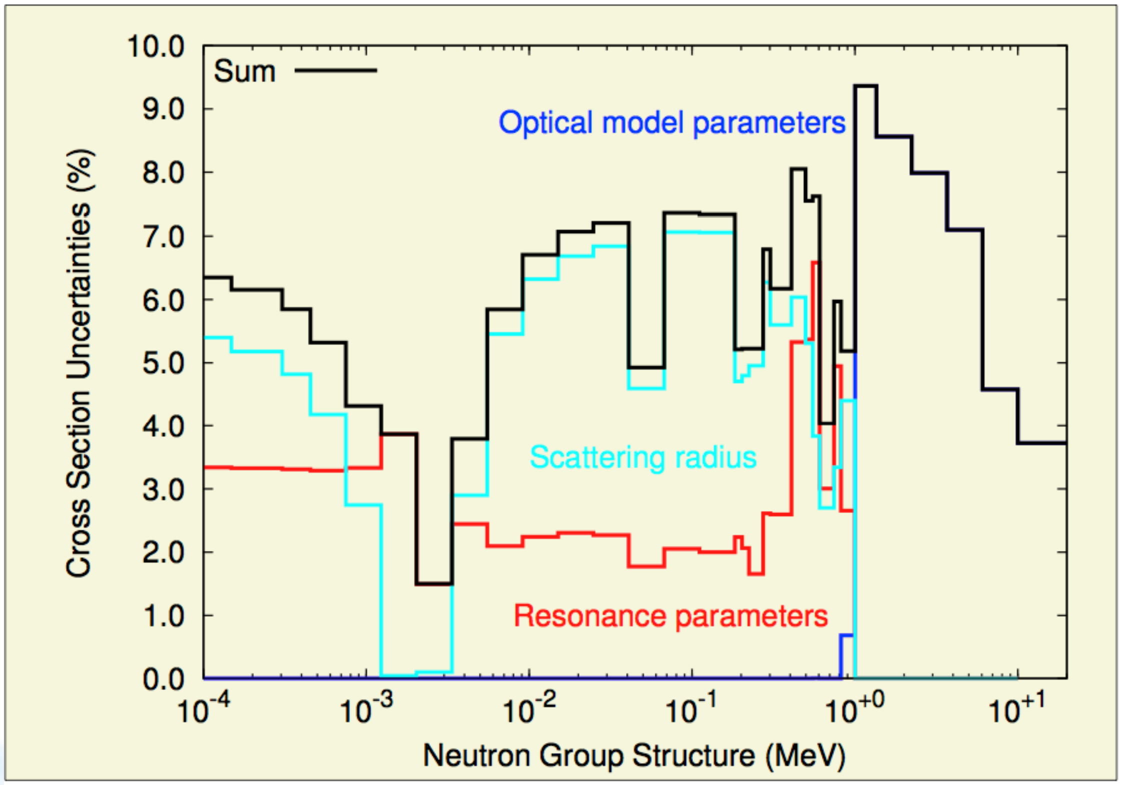
$\Delta\tilde{a}^{cn}$	$\Delta\tilde{a}^{tg}$	$\Delta\tilde{a}^{np}$	$\Delta\tilde{a}^{na}$	$\Delta\bar{g}^{tg}$	$\Delta\bar{g}^{np}$	$\Delta\bar{g}^{na}$	Δf_γ
2.5	1.1	3	7	6	8	7.9	10
Δf_p	Δf_α	Δmfp	Δtpe				
14	12	11	25				

23Na(n,el)
Uncertainty components



Essential contribution of scattering radius uncertainty

23Na(n,tot)
Uncertainty components

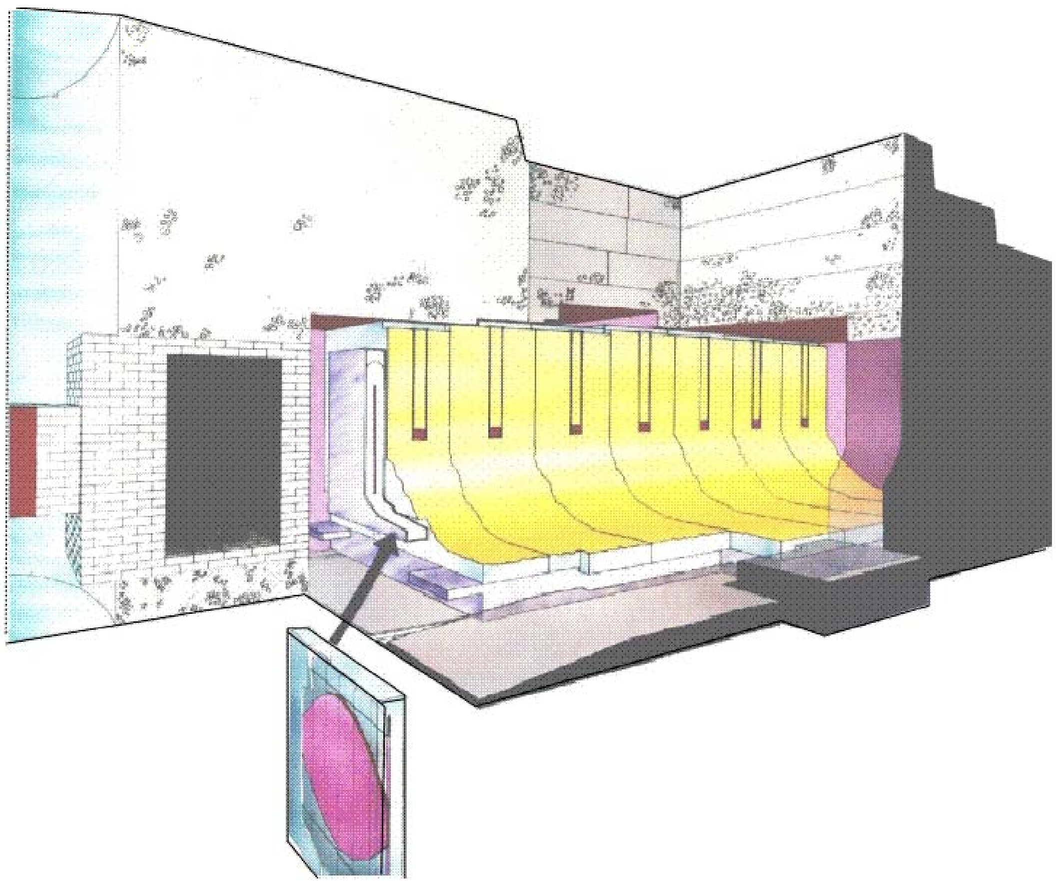


- Multi-group ^{23}Na(n,tot) cross-section uncertainties obtained from scattering radius (light blue line), resonance (dotted red line) and optical model parameter (dashed blue line) uncertainties. Solid black line is the sum of the three contributions. Fast neutron region from EMPIRE/KALMAN

BROOKHAVEN NATIONAL LABORATORY

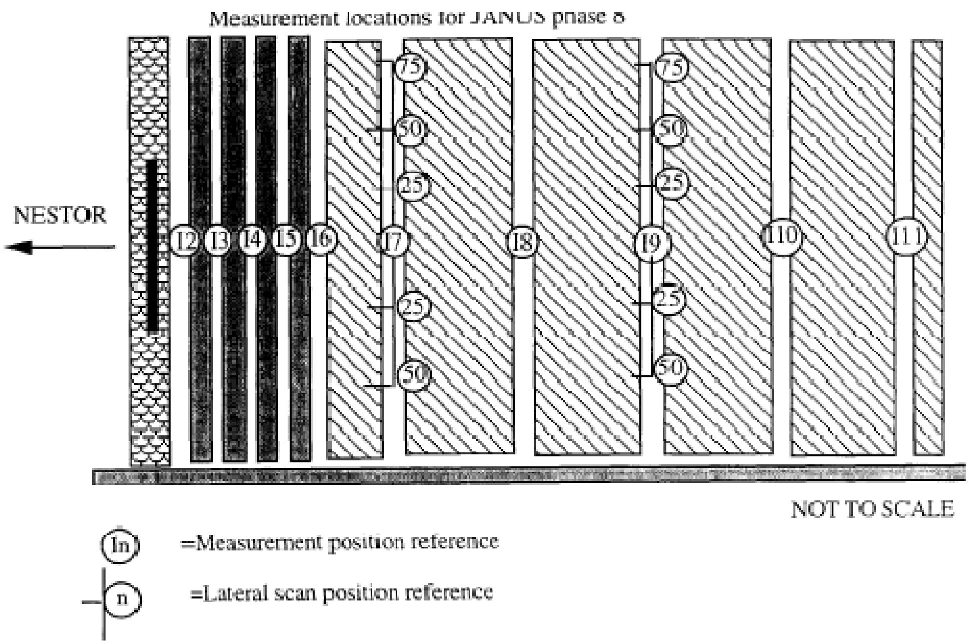
EURACOS

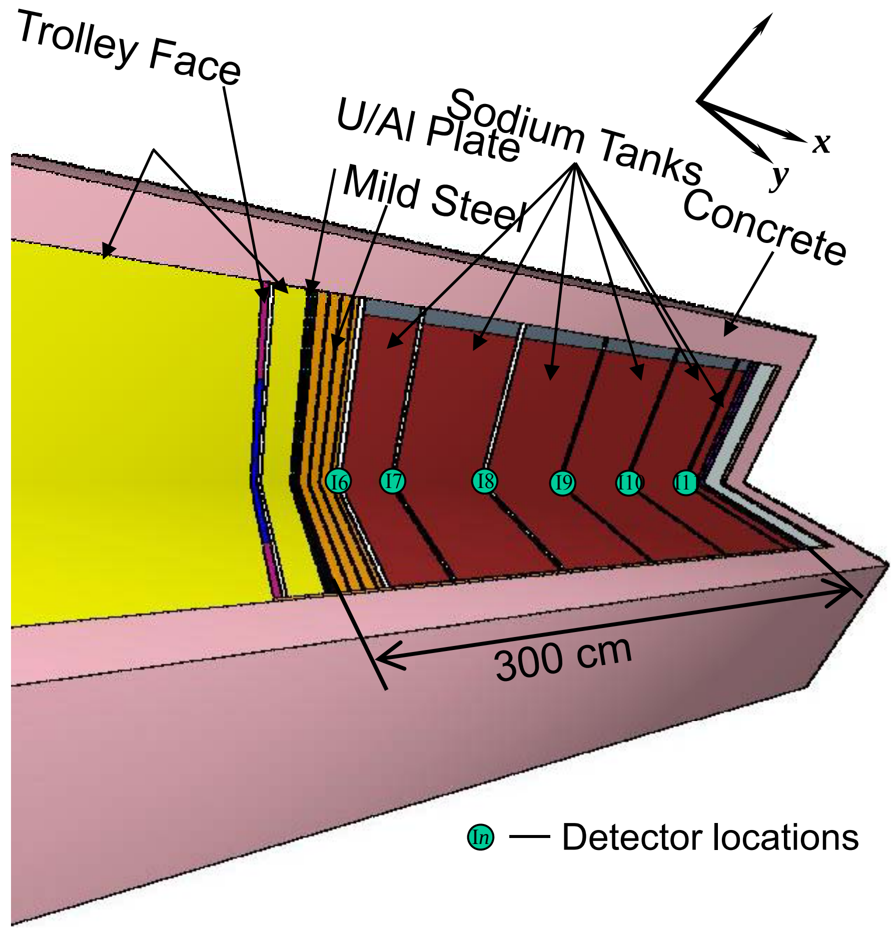
- The Ispra sodium benchmark project was performed under the EURACOS (Enriched URAnium COnverter Source) irradiation facility.
- Measurements with activation detectors were carried out at distances from the source for $^{32}S(n,p)$ and $^{197}Au\ (n,\gamma)$ in order to analyze fast and epithermal neutron attenuations.



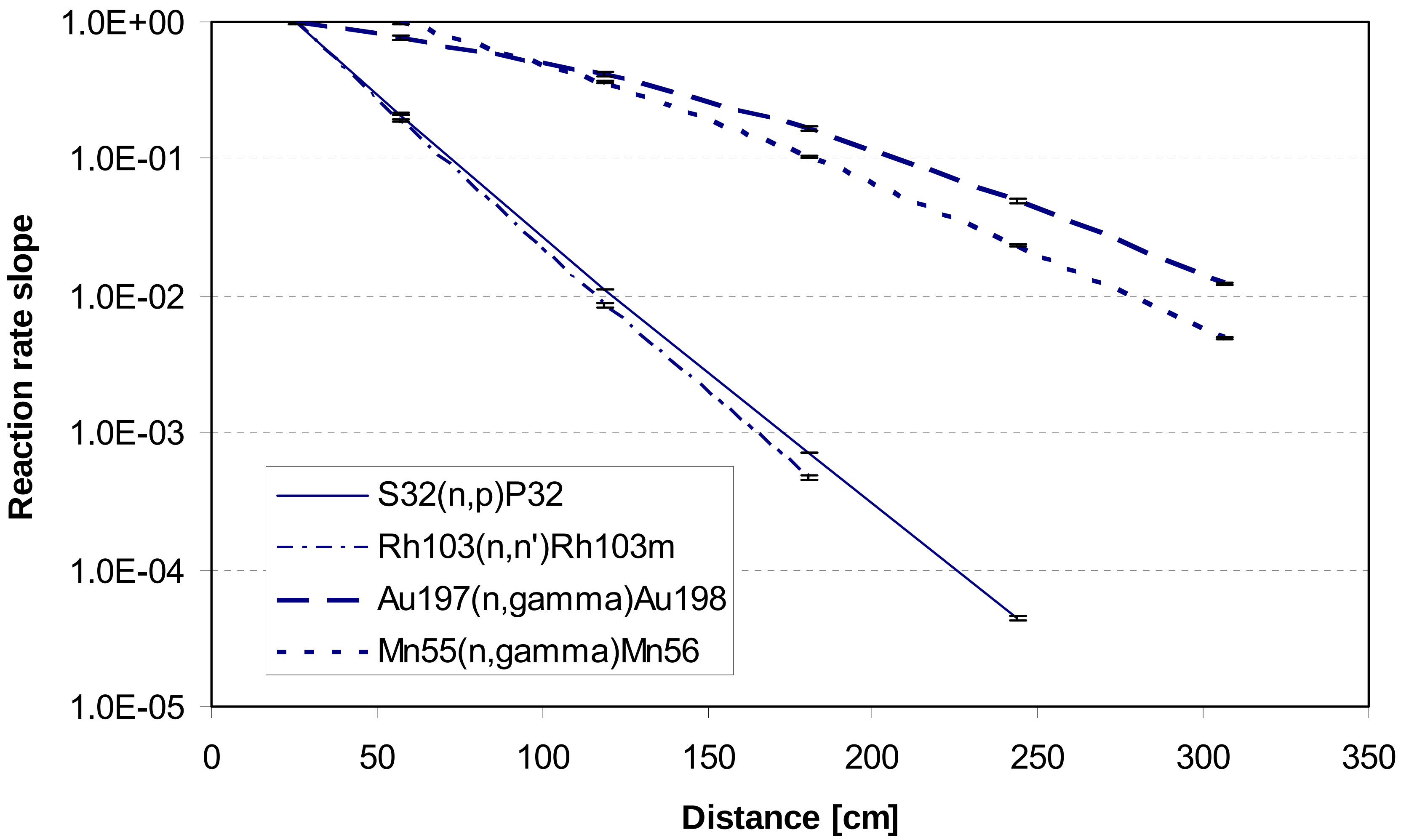
JANUS-8 Sodium Propagation Experiment

- The JANUS Phase 8 experiments were performed at the ASPIS facility.
- The neutron attenuations of several different detectors were analyzed and in particular for the following reaction rates: $^{32}S(n,p)^{32}P$, $^{103}Rh(n,n')^{103m}Rh$, $^{197}Au(n,\gamma)^{198}Au$, and $^{55}Mn(n,\gamma)^{56}Mn$.





JANUS-8 Calculated (MCNP5 and EMPIRE σ) Attenuations



Selection of Reaction Rate Slopes

- A set of reaction rate slopes (one for each detector in the two experiment campaigns) was selected.
- The selection was based, on:
  - low experimental and calculation uncertainty,
  - good depiction of the neutron attenuation for the energy range to be characterized by the corresponding detector,
  - complement of information (obtained by correlation calculations using the sensitivity coefficients)
  - good consistency among the C/E on the selected slopes
- The selected slopes were the ratios of the fourth position to the first one for both detectors in the EURACOS experiment, while for the JANUS-8 experiment we selected the fourth to first position ratio for the ^{32}S and ^{197}Au detectors, fourth to second position for the ^{55}Mn (there was no measurement in the first position), and third to first for the ^{103}Rh (the fourth position has a very large experimental uncertainty)

Statistical Adjustment Method

The method makes use of:

- “a priori” nuclear data covariance information,
- integral experiments analysis to define C/E values
- integral experiment uncertainties
- sensitivity coefficients

If we define: $\mathbf{y_j=(p_j^{adj}-p_j)/p_j}$ and $\mathbf{y_{Qi}^{exp}=(Q_i^{exp}-Q_i)/Q_i}$, the $\mathbf{y_i}$ are given by:

$$\mathbf{y_i} = \left(\mathbf{S^T D_Q^{-1} S} + \mathbf{D}^{-1}\right)^{-1} \mathbf{S^T D_Q^{-1}\, y_{Qi}^{exp}}$$

where $\mathbf{D_Q}$ is the covariance matrix of the experiments, **D** the covariance matrix of the nuclear parameters $\mathbf{p_j}$, and **S** is the sensitivity vector. It will also result an adjusted covariance matrix for the nuclear data:

$$\left(\mathbf{D^{adj}}\right)^{-1} = \mathbf{D}^{-1} + \mathbf{S^T D_Q^{-1}\, S}$$

Data Assimilation

Detector	C/E before assim.	C/E after assim.
EURACOS ^{32}S	**0.770 ± 0.085**	**0.997 ± 0.057**
EURACOS ^{197}Au	**0.954 ± 0.102**	**0.946 ± 0.010**
JANUS-8 ^{32}S	**0.538 ± 0.022**	**1.000 ± 0.022**
JANUS-8^{197}Au	**1.010 ± 0.033**	**0.959± 0.028**
JANUS-8 ^{55}Mn	**1.158 ± 0.025**	**1.028 ± 0.023**
JANUS-8 ^{103}Rh	**0.960 ± 0.106**	**0.976 ± 0.047**

^{23}Na consistent data assimilation

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
Scat. Rad.[a)]	1.9	4.1	1.7
Γ_n Bou. Lev.[b)]	-6.4	8.0	6.4
Γ_n 2.8 Kev[c)]	0.6	1.9	1.9
Γ_g 2.8 Kev[c)]	10.5	11.8	10.5
Γ_n 538 Kev[c)]	-57.2	65.9	58.4
R. Vol. Rad.[d)]	-1.8	2.8	1.6
R. Surf. Dif.[e)]	-0.8	5.0	4.7
R. Vol. Dif.[f)]	-0.4	2.1	2.1
TOTRED[g)]	-1.1	3.5	3.2
FUSRED[h)]	-0.8	5.0	4.0

[a)] Nuclear Scattering Radius, [b)] Bound Level resonance, [c)] Resonance Peak Energy
[d)] Optical model real volume radius for target nucleus, [e)] Optical model real surface ,
[g)] Optical model scaling of total cross sections due to intrinsic model uncertainty,
[h)] Optical model scaling of absorption cross sections due to intrinsic model uncertainty

- Apparently excellent result of assimilation. χ^2 was close to 1 with relative small changes of model parameters
- Later found that assimilation was affected by non-linear effects. Improvements are under way by computing sensitivity coefficients of nuclear parameters by direct numerical differentiation.

^{56}Fe consistent data assimilation

Parameter	Variation (%)	Init. Stand. Dev. (%)	Final Stand. Dev. (%)
Scat. Rad.[a)]	**-13.25**	**5.1**	**2.1**
Γ_n Bou. Lev.[b)]	**1.9**	**4.0**	**3.7**
Γ_g Bou. Lev.[b)]	**-2.1**	**5.0**	**4.8**
Γ_n 277 Kev[c)]	**-1.1**	**8.0**	**8.0**
Γ_n 317 Kev[c)]	**-2.2**	**8.0**	**8.0**
Γ_n 361 Kev[c)]	**-2.9**	**8.0**	**8.0**
Γ_n 381 Kev[c)]	**-3.0**	**8.0**	**8.0**
Γ_n 665.6 Kev[c)]	**1.3**	**8.0**	**8.0**
R. Well. Vol.[d)]	**15.1**	**3.0**	**2.2**
Nuc. Rad. R. Surf.[e)]	**10.5**	**3.0**	**2.9**
Im. R. Surf.[f)]	**10.8**	**5.0**	**4.9**
TOTRED[g)]	**-0.9**	**1.0**	**1.0**
FUSRED[h)]	**-2.0**	**1.3**	**1.2**

- Performance of the assimilated file inferior to the ENDF/B-VII.0 evaluation
  - strong cross section fluctuations ignored (too dense for tuning used in ^{23}Na)
  - model calculations not flexible enough (too few parameters)
  - soft-rotor o.m. potential needed
- Addressing these issues would be beyond allocated resources

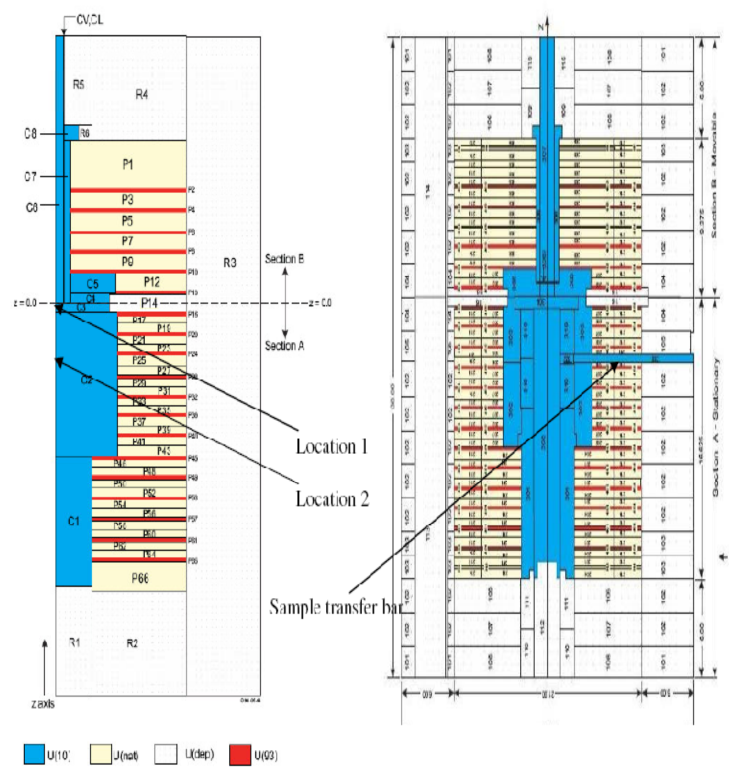
a) Nuclear Scattering Radius, b) Bound Level resonance, c) Resonance Peak Energy
d) Optical model real well depth and real volume of target nucleus, e) Optical model nuclear radius and real surface of target nucleus, f) Optical model imaginary and real surface of target nucleus, g) Optical model scaling of total cross sections due to intrinsic model uncertainty, h) Optical model scaling of absorption cross sections due to intrinsic model uncertainty

FY11: ^{235}U, ^{238}U, ^{239}Pu Nuclear Data Assimilation

- ***^{235}*U, *^{238}*U, and *^{239}*Pu** have been evaluated by EMPIRE.
- MCNP calculations with these cross sections were performed for **JEZEBEL, GODIVA, BIG TEN, ZPR6-6A, and ZPR6-7** on K_{eff} and spectral indices.

Comparison of K_{eff}

Experiment	EMPIRE	ENDF/B-VII.0
JEZEBEL 240	0.98699±13pcm	0.99981±9pcm
JEZEBEL 239	0.98547±8pcm	0.99986±9pcm
GODIVA	0.99086±9pcm	0.99983±9pcm
FLATTOPS 235U	1.00182±17pcm	1.00217±17pcm
FLATTOPS Pu	0.98838±18pcm	1.00097±18pcm
BIG TEN	1.00705±8pcm	1.00452±7pcm
ZPR6-6A	1.00092±7pcm	1.0005±10pcm
ZPR6-7	1.00839±7pcm	1.00094±7pcm
ZPR6-7 High 240Pu	1.00725±11pcm	1.00017±11pcm



MCNP detailed model

Big Ten detailed schematic

Summary of BNL expenditures (Q3 2011)

WBS or ID #	Item/Activity	Baseline Total Cost (AY$)	Costed & Committed (AY$)	Estimate To Complete (AY$)	Estimated Total Cost (AY$)
1	Development of methodology for creating sensitivity matrices for assimilation procedure	41k	41k	0k	41k
2	Calculation of sensitivity matrices for 23Na, 56Fe and two fission products	170k	140k	30k	170k
3	Extending methodology to account for fission	60k	60k	0k	60k
4	Calculation of sensitivity matrices for 235U, 239Pu and minor actinide	137k	58k	79k	137k
Totals:		**408k**	**299k**	**109k**	**408k**

Note: the expenditures were adjusted according to the project exigencies by moving $30k from ID#4 to ID#2 (see 'red' colored numbers)

INL Summary of total expenditures (Q3 FY11)

WBS or ID #	Item/Activity	Baseline Total Cost (AY$)	Costed & Committed (AY$)	Estimate To Complete (AY$)	Estimated Total Cost (AY$)
CE031100	Use Covariance Matrices – Yr. 1	$216,930	$187,404	$29,526	$216,930
CE031105	Domestic Travel – 1st Qtr. – Yr. 1	$2,690	$0	$0	$0
CE031110	Domestic Travel – 3rd Qtr. – Yr. 1	$2,690	$7,703	$0	$7,703
CE031115	Domestic Travel – 4th Qtr. – Yr. 1	$2,690	$1,368	$0	$1,368
CE031200	Use Covariance Matrices – Yr. 2	$216,930	$208,433	$8,497	$216,930
CE031205	Domestic Travel – Oct thru Mar – Yr. 2	$5,368	$4,233	$0	$4,233
CE031210	Domestic Travel – Apr thru Sept – Yr. 2	$5,368	$0	$5,368	$5,368
CE031300	Use Covariance Matrices – Yr. 3	$223,880			
CE031305	Domestic Travel – 1st Qtr. – Yr. 3	$2,707			
CE031310	Domestic Travel – 3rd Qtr. – Yr. 3	$2,707			
CE031315	Domestic Travel – 4th Qtr. – Yr. 3	$2,706			
Totals:		**$682,000**	**$409,141**	**$43,391**	**$452,532**

Summary of BNL expenditures by FY

	FY 2010	FY 2011 (Q3)	FY 2012
Funds allocated	181k	189k	38k
Costs accrued	178k	124k	0
Uncosted commitments	0	0	0
Uncommitted funds (d=a-b-c)	**3k**	**65k**	**38k**

INL Summary of expenditures by fiscal year (FY):

	FY 2010	FY 2011	FY 2012
a) Funds allocated	$225,000	$225,000	$232,000
b) Costs accrued	$196,475	$212,666	$0
c) Uncosted commitments	$0	$0	$0
d) Uncommitted funds (d=a-b-c)	$28,525	$12,334	$232,000

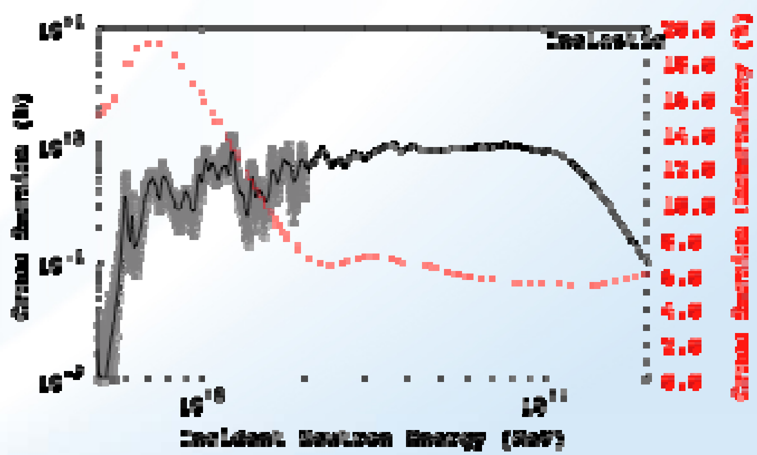
INL Summary of schedule:

	Baseline Start Date mo/year	Actual/ Forecast Start Date mo/year	Baseline Complete Date mo/year	Actual/ Forecast Completion Date mo/year	% Complete Baseline	% Complete Actual
Design	October 2009	October 2009	Sept. 2012		58.0%	60.0%
Procurement						
Construction						
Operation						

FY2010 milestone (BNL)

- **Milestone**: Perform consistent data assimilation on structural isotopes relevant to AFCI reactor systems using neutron propagation experiments
  - Two versions of EMPIRE based **23Na** evaluations along with sensitivity matrices developed and provided to INL
  - EMPIRE based evaluation and sensitivity matrices for **56Fe** developed and provided to INL

- **Achievements**
  - Good reproduction of exp. data for 23Na
  - Fluctuations accounted for with the energy-dependent tuning factor
  - Reducing number of parameters from over 100 to 10 most important ones
- **Challenges**
  - Fluctuations can’t be modeled
  - 56Fe would need more effort (soft-rotor optical potential)



INL Milestones FY10

- **First Quarter Milestone:** Perform analysis of EURACOS experiment for improvement of basic nuclear parameters of ^{23}Na.
- **Second Quarter Milestone:** Perform analysis of JANUS-8 experiment for improvement of basic nuclear parameters of ^{23}Na.
- **Third Quarter Milestone:** Perform ^{23}Na data assimilation using neutron propagation experiments EURACOS and JANUS-8. Analyze iron neutron propagation experiments.
- **Fourth Quarter Milestone**: Perform ^{56}Fe data assimilation using neutron propagation experiments.

- **Yearly Milestone:** Perform consistent data assimilation on structural isotopes relevant to AFCI reactor systems using neutron propagation experiments.

  Document on this milestone delivered to DOE NP by September 30, 2010.

FY2011 milestone (BNL)

- **Milestone**: Extend assimilation procedure to fissile isotopes. Perform proof of principle by applying the procedure to 235U and 239Pu
  - EMPIRE based evaluations produced for ^{235}**U and** ^{238}**U** (Godiva reproduced within 1% - much worse than ENDF/B-VII.0 but good enough as the starting point for assimilation)
  - EMPIRE based evaluations, with energy dependent tuning, produced for ^{239}**Pu**
  - 33-energy group sensitivity matrices for ^{235,238}**U** and ^{239}**Pu** to be calculated in Q4 FY2011.

INL Milestones FY11

- **First Quarter Milestone:** Perform analysis of LANL GODIVA and JEZEBEL experiments for improvement of ^{235}U and ^{239}Pu cross sections.
- **Second Quarter Milestone:** Perform analysis of FLATTOP and BIGTEN experiments for improvement of ^{235}U and ^{239}Pu cross sections.
- **Third Quarter Milestone:** Perform analysis of ZPR6 Assembly 6A and Assembly 7 experiments for improvement of ^{235}U and ^{239}Pu cross sections.
- **Fourth Quarter Milestone**: Perform data assimilation of ^{235}U and ^{239}Pu using the experiments analyzed during the current fiscal year.

- **Yearly Milestone:** Extend assimilation procedure to allow consistent data assimilation on fissile isotopes, relevant to AFCI reactor systems. Perform proof of principle by applying the procedure to ^{235}U and ^{239}Pu using default cross sections calculated by the EMPIRE code and simple, very well characterized fast neutron assemblies.

  Document on this milestone will be delivered to DOE NP by September 30, 2011

Conclusions

- Innovative approach to nuclear data evaluation and validation is being developed
  - consistent account for differential and integral experimental data
  - more reliable, application independent, adjusted nuclear data (‘good results for good reason’)
  - deeper insight into adjustment procedure
  - integral experiments’ feedback onto reaction model parameters
  - nuclear physics will directly impact energy production by improving margins and reducing uncertainties
- Newly trained evaluators and nuclear engineers:
  - Marco Pigni (currently at ORNL)
  - Caleb Mattoon (currently at LLNL)
  - Samuel Hoblit (BNL)
  - Hikaru Hiruta (INL)
  - Andrea Alfonsi (INL)
  - Gustavo Nobre (postdoc, new trainee, BNL)
  - Annalia Palumbo (postdoc, new trainee, BNL)

Conclusions

- Challenges
  - controlling non-linearity effects
  - reducing statistical uncertainties in Monte Carlo calculations of sensitivity matrices (computing power)
  - ensuring enough model flexibility to allow effective adjustment keeping model parameters within accepted range
- Future challenges
  - include physical quantities beyond cross sections (angular distributions, nu-bars, prompt fission neutron spectra)
  - including cross-correlations among reactions
  - including cross-correlations among materials
  - including cross-correlations among experiments
- Future work
  - Perform consistent data assimilation on minor actinides and fission products of interest of the AFCI program using irradiation experiments

FY2012 milestone (BNL)

- **Milestone**: Perform consistent data assimilation on fission products isotopes and minor actinide
  - assimilation to be performed on ^{105}Pd (fission product) and ^{237}Np (minor actinide)

INL Milestones FY12

- **First Quarter Milestone:** Perform analysis of the irradiation experiments PROFIL 1 for improvement of fission products and minor actinide cross sections.
- **Second Quarter Milestone:** Perform analysis of the irradiation experiments PROFIL 2 for improvement of fission products and minor actinide cross sections.
- **Third Quarter Milestone:** Perform analysis of the irradiation experiments TRAPU for improvement of minor actinide cross sections.
- **Fourth Quarter Milestone**: Perform data assimilation on fission product and minor actinide nuclei using analyzed irradiation experiments.
- **Yearly Milestone:** Perform consistent data assimilation on fission products isotopes and minor actinide relevant to AFCI reactor systems using irradiation experiments and clean representative integral experiments.

  Document on this milestone will be delivered to DOE NP by September 30, 2012