The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific
and Cultural Organization

International Atomic
Energy Agency

Workshop on
"Technology and Applications of Accelerator Driven Systems (ADS)"

17 - 28 October 2005

1677/4

Nuclear Data and Methods for ADS Design

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LECTURES OUTLINE

- ✓ LECTURE 1: Physics of Spallation and Sub-critical Cores, Fundamentals
  (Monday 17/10/05, 16:00 – 17:30)
- ✓ **LECTURE 2: Nuclear Data & Methods for ADS Design I**
  (Tuesday 18/10/03, 08:30 – 10:00)
- ✓ LECTURE 3: Nuclear Data & Methods for ADS Design II
  (Tuesday 18/10/03, 10:30 – 12:00)
- ✓ LECTURE 4: ADS Design Exercises I & II
  (Tuesday 18/10/03, 14:00 – 17:30)
- ✓ LECTURE 5: Examples of ADS Design I
  (Thursday 20/10/03, 08:30 – 10:00)
- ✓ LECTURE 6: Examples of ADS Design II
  (Thursday 20/10/03, 10:30 – 12:00)
- ✓ LECTURE 7: ADS Design Exercises III & IV
  (Thursday 20/10/03, 14:00 – 17:30)

Nuclear Data & Methods for ADS Design I : Nuclear Data Processing

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18 October 2005, ICTP, Trieste, Italy

LECTURE OUTLINE

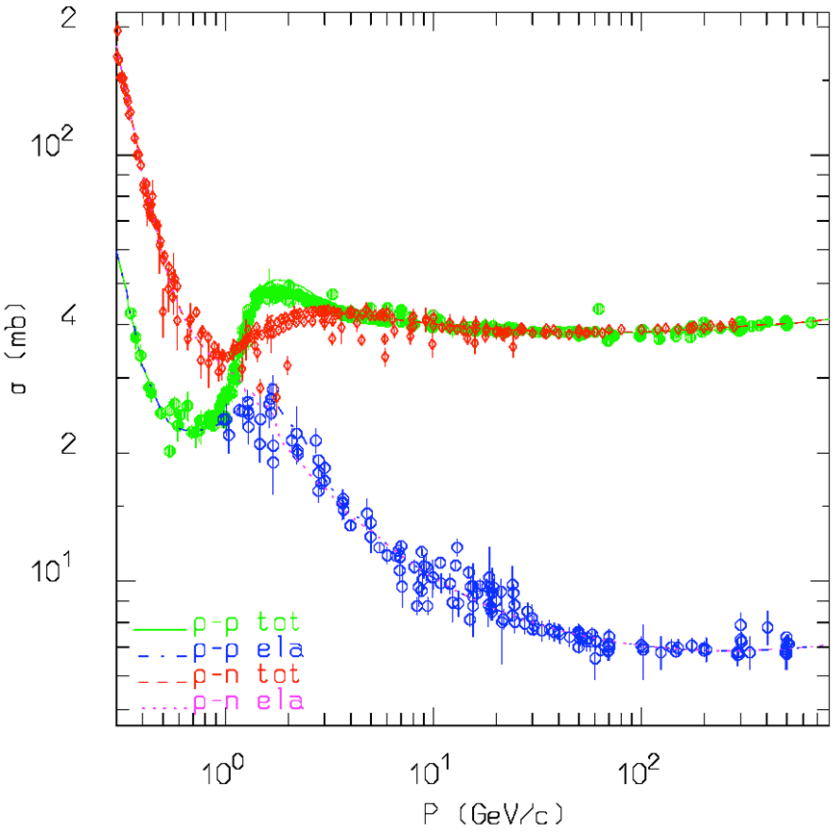
I – LIMITATIONS IN THE HIGH-ENERGY PARTICLE TRANSPORT

- Cross section data
- Neutron Yield
- Spallation Product Distribution

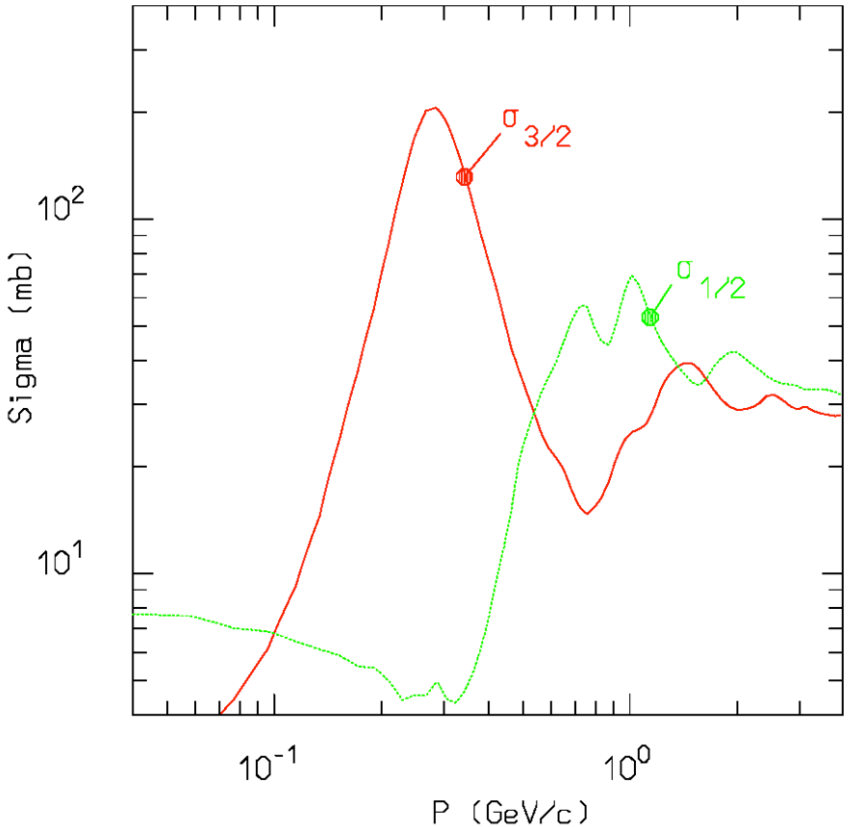
II – LIMITATIONS IN THE LOW-ENERGY NEUTRON TRANSPORT

- Nuclear Data Below 20 MeV

Hadron-Nucleon Cross Section



Total and elastic cross section for p-p and p-n scattering, together with experimental data



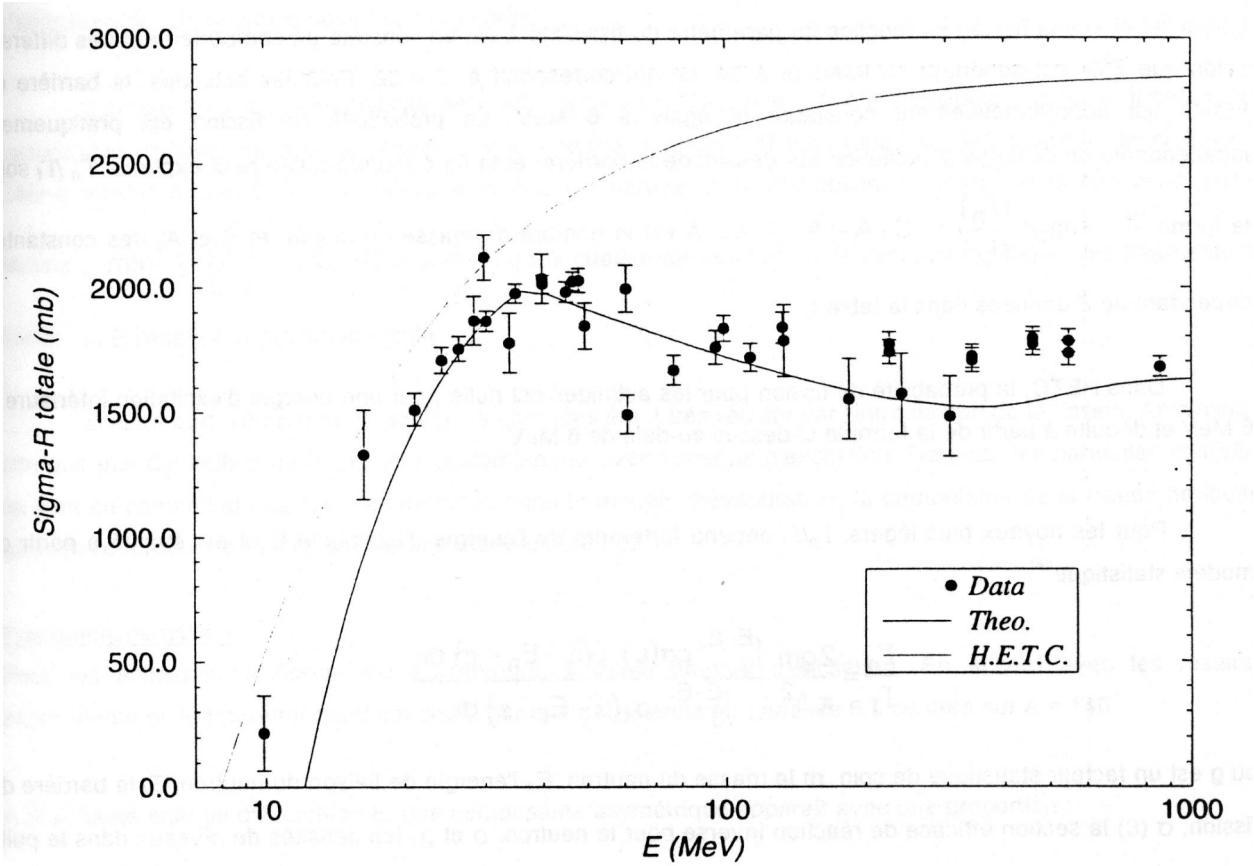
Isospin decomposition of p-nucleon cross section in the T=3/2 and T=1/2 components

Hadronic interactions are mostly surface effects ⇒ hadron nucleus cross section scale with the target atomic mass $A^{2/3}$

Total Reaction Cross Section

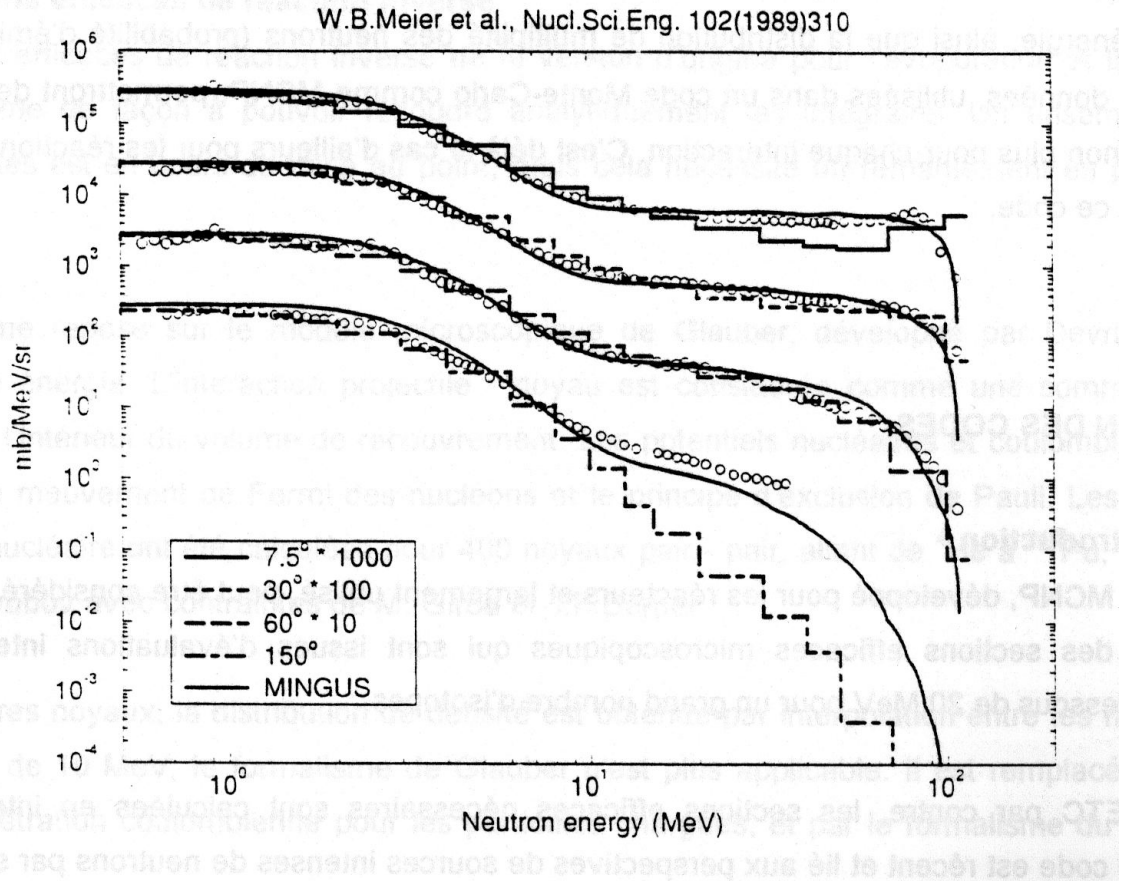
^{208}Pb reaction cross section. Comparison between experimental results and calculations based on the Glauber Model. The upper curve represents the reaction cross as calculated by HETC

- ✓ *We note that the maximum differences in reaction cross sections are of the order of 50% above a few MeV in Pb for instance.*
- ✓ *Clearly there is room for improvement in this most basic reaction value.*



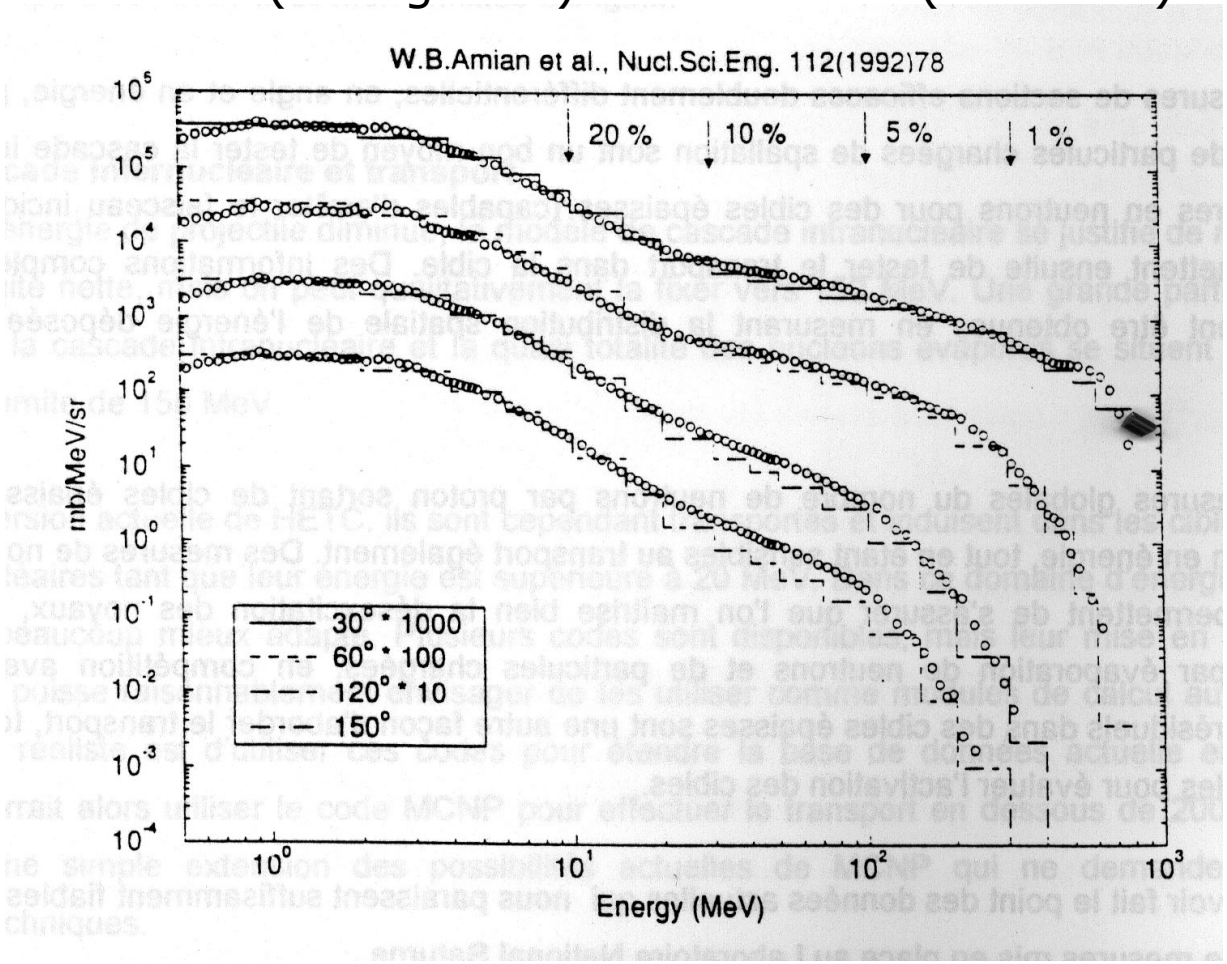
Neutron Multiplicity

Neutron production differential cross section for thin Pb target bombarded by 113 MeV protons. Comparison of experimental results with standard HETC (histograms) and MINGUS (solid line) calculations



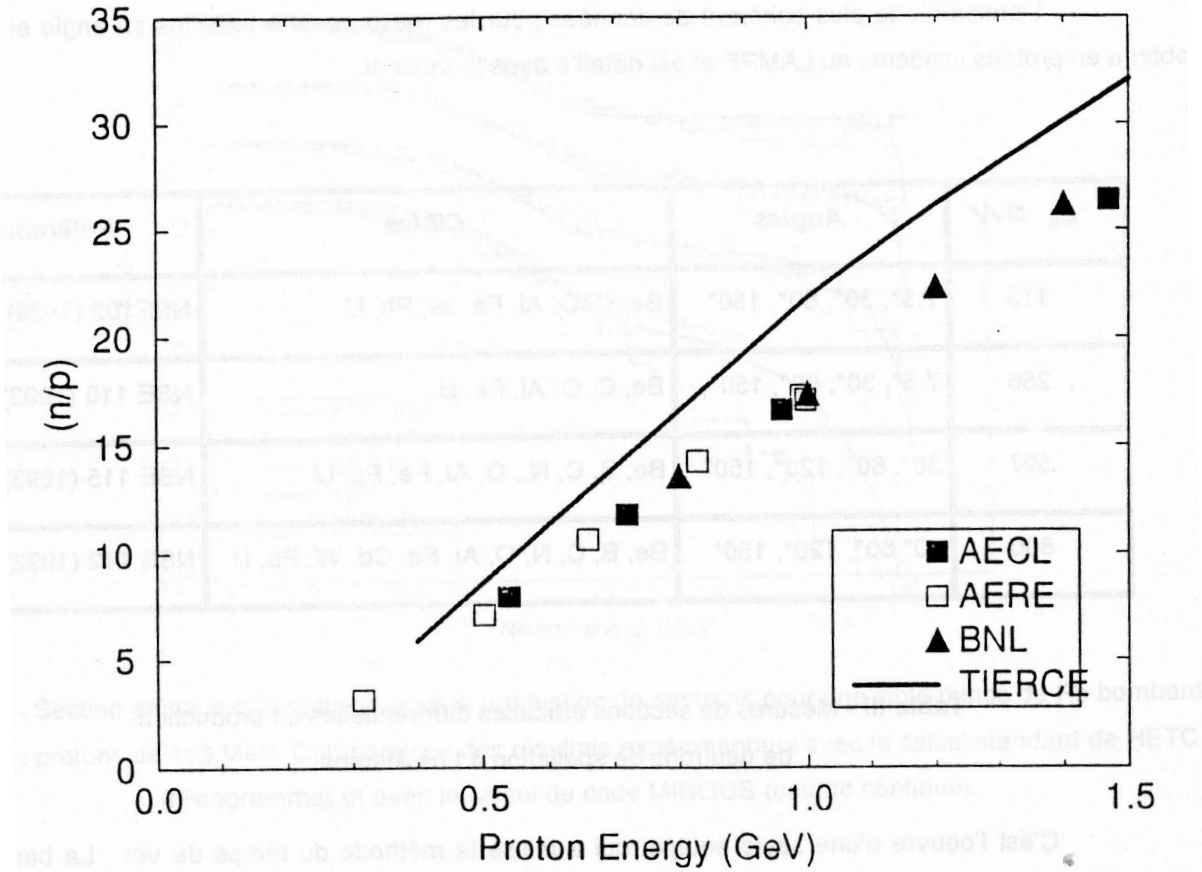
Neutron Multiplicity (2)

Neutron production differential cross section for thin Pb target bombarded by 800 MeV protons. Comparison of experimental results with standard HETC (histograms) and MINGUS (solid line) calculations



Neutron Multiplicity (3)

Number of neutrons produced per proton as a function of proton incident energy for a thick Pb target. Comparison of experimental results with standard TIERCE calculations



Neutron Multiplicity: summary

✓ *The uncertainties due to reaction cross sections are removed when comparing the neutron and proton multiplicities.*

✓ *Nevertheless, large differences between different codes may be seen.*

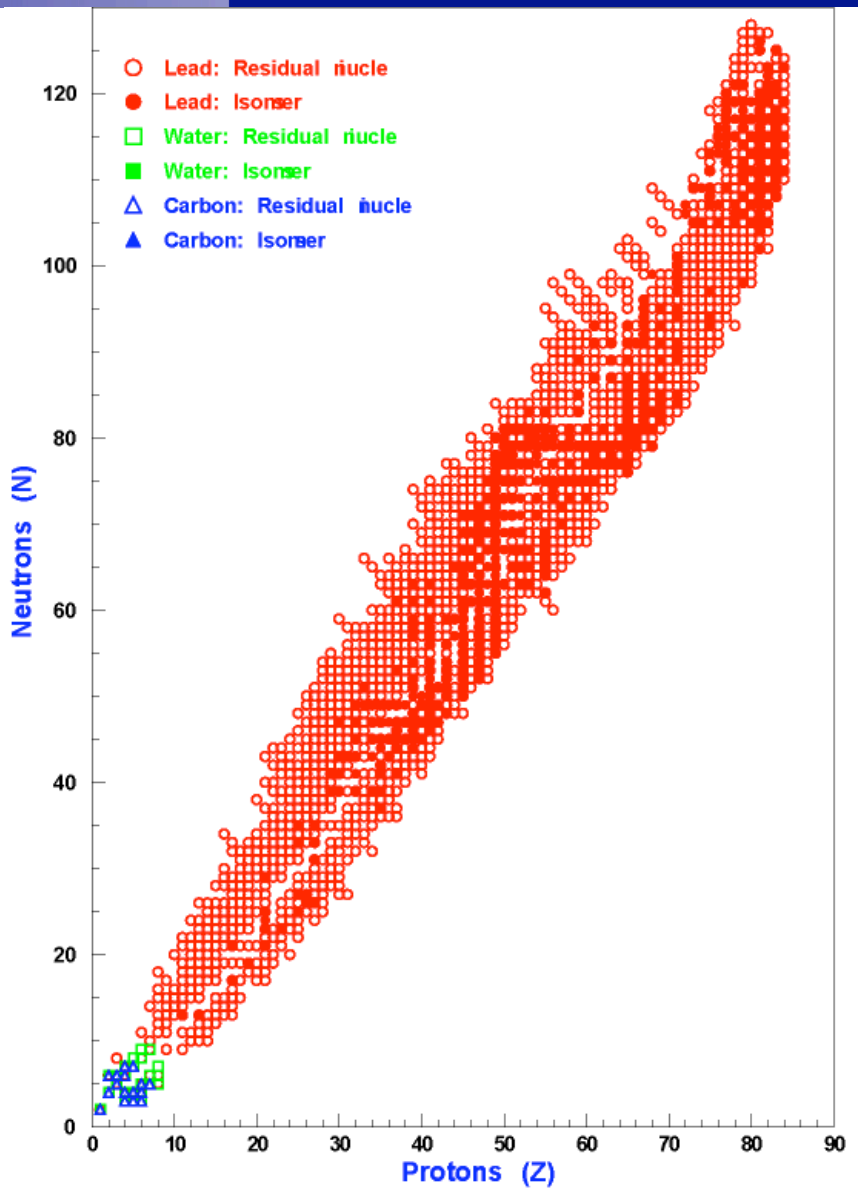
✓*Proton multiplicities show the broadest excursions reflecting different treatments of barrier penetrability.*

✓ *Neutron multiplicities reach nearly a factor two difference, and this would be a serious consideration when using codes for calculating the efficiency of ADS facilities.*

✓ *This difference may be somewhat mitigated in the thick target transport calculations since results show lower microscopic multiplicities may have higher average emission energies. These in turn will give higher secondary emission multiplicities, partially compensating differences in the primary spectra.*

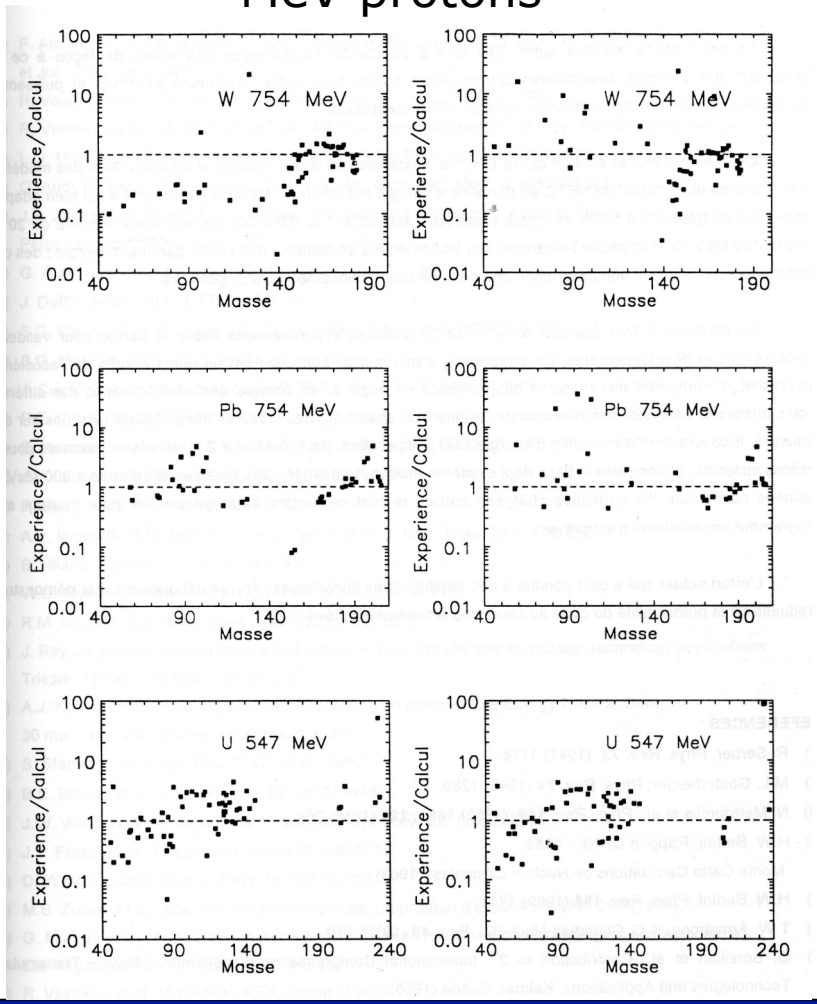
Residual Nuclei

- The production of residuals is the result of the last step of the nuclear reaction, thus it is influenced by all the previous stages
- Residual mass distributions are very well reproduced
- Residuals near to the compound mass are usually well reproduced
- However, the production of specific isotopes may be influenced by additional problems which have little or no impact on the emitted particle spectra (Sensitive to details of evaporation, Nuclear structure effects, Lack of spin-parity dependent calculations in most MC models)

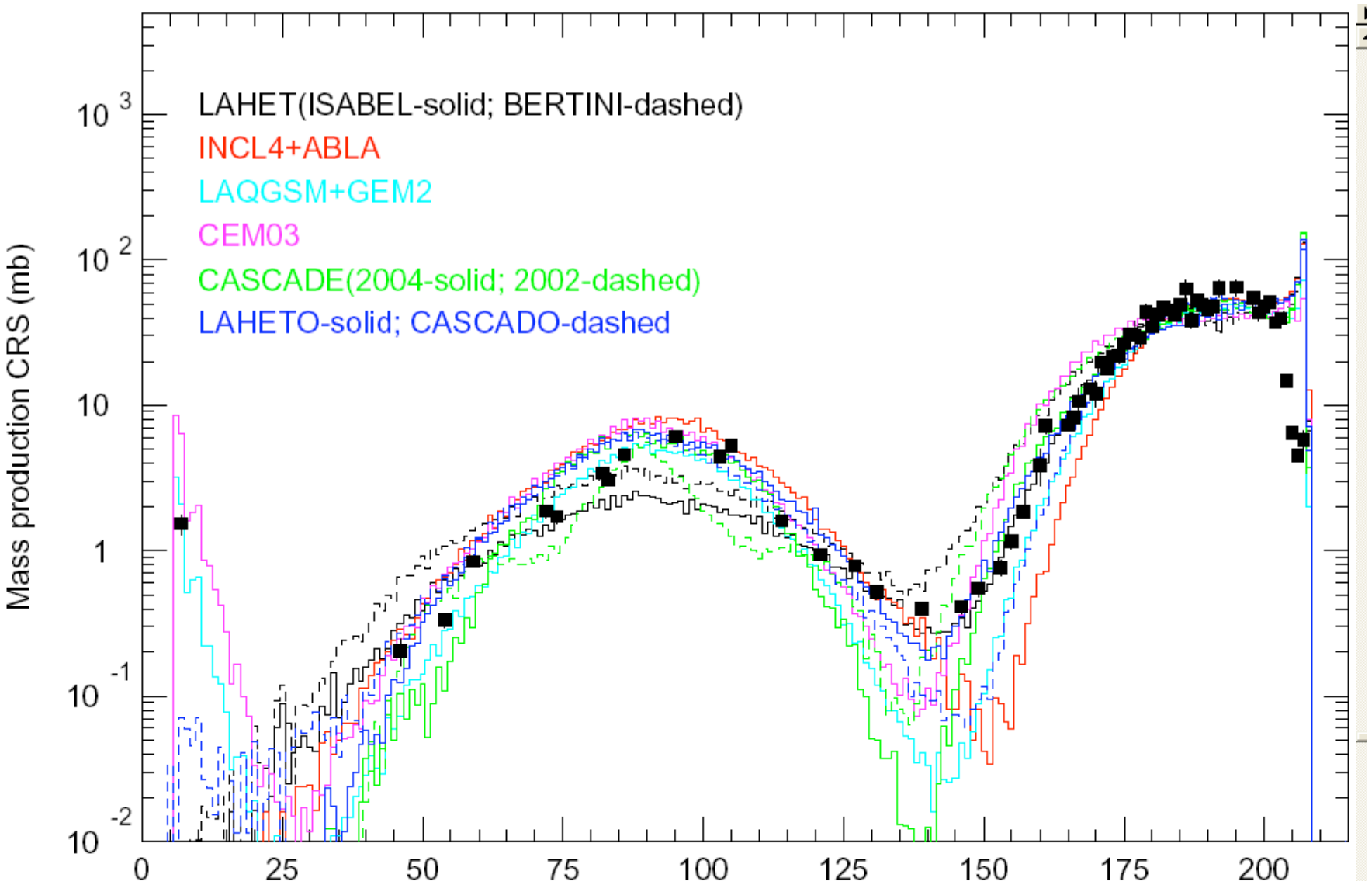


Residual Nuclei (2)

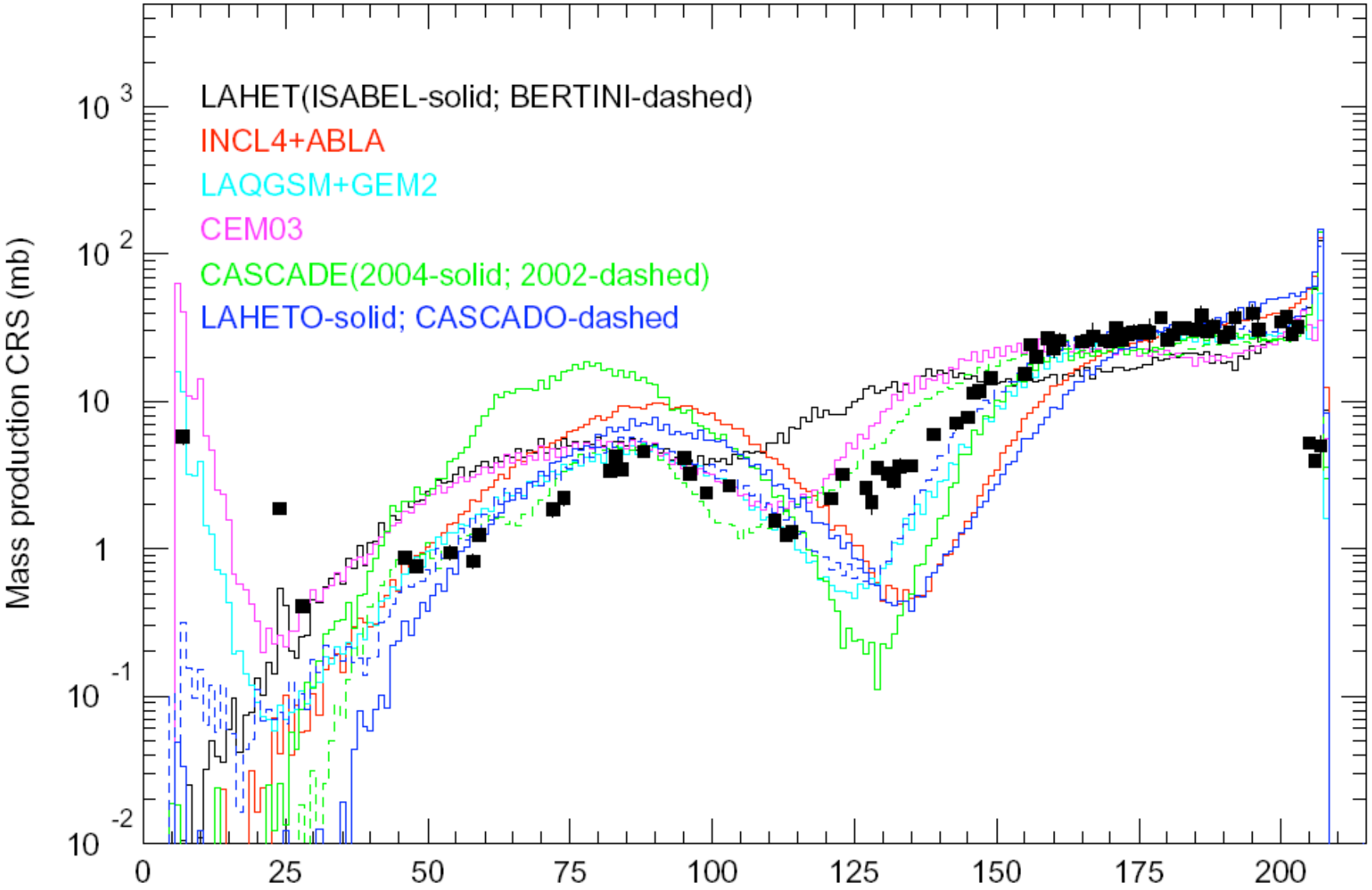
Ratio Exp./Calc. relative to the production of spallation residues for W and Pb targets irradiated by 754 MeV protons and for U target irradiated by 547 MeV protons



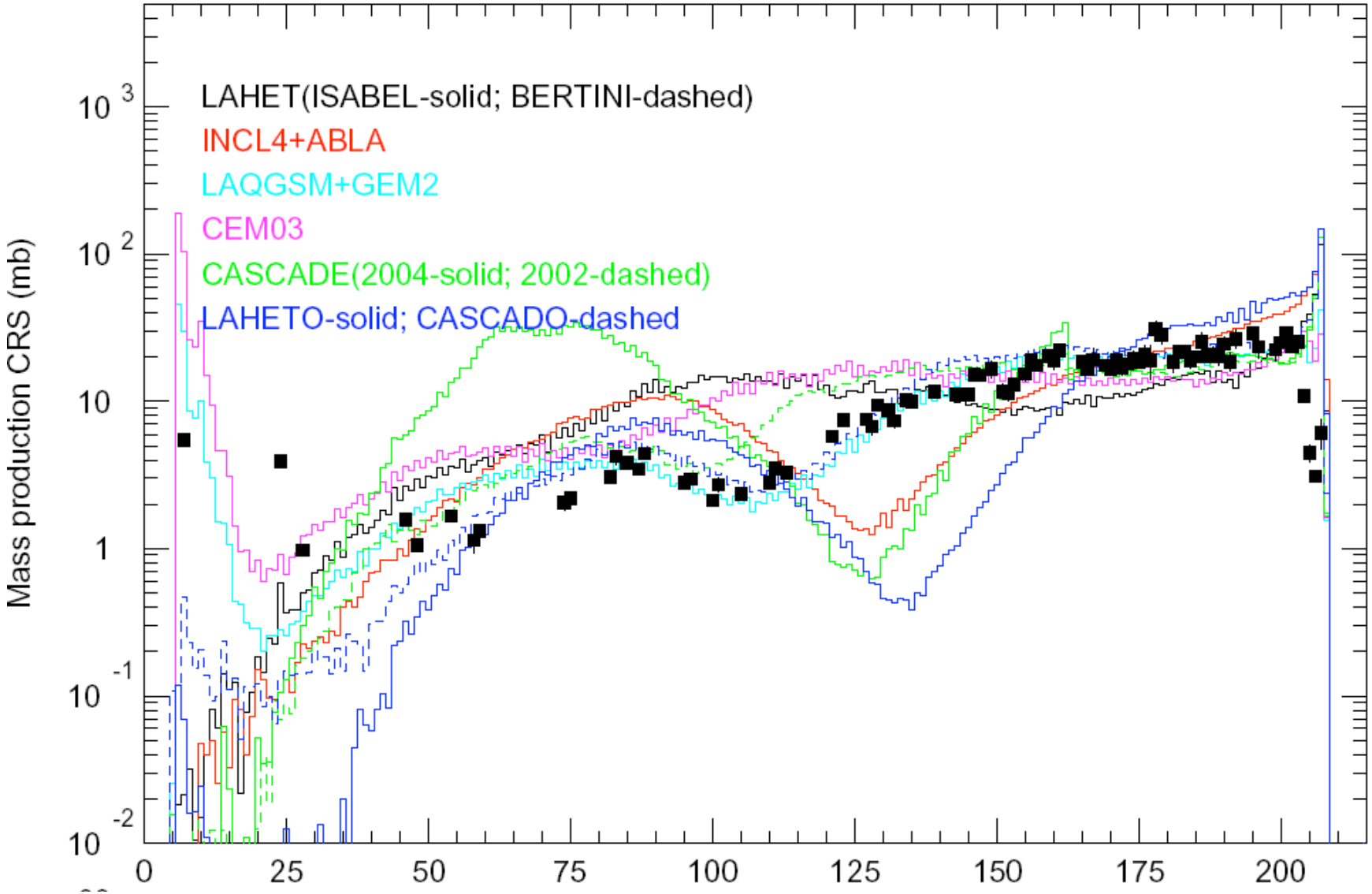
Mass distribution for ^{208}Pb 800MeV



Mass distribution for ^{208}PB 1600MeV

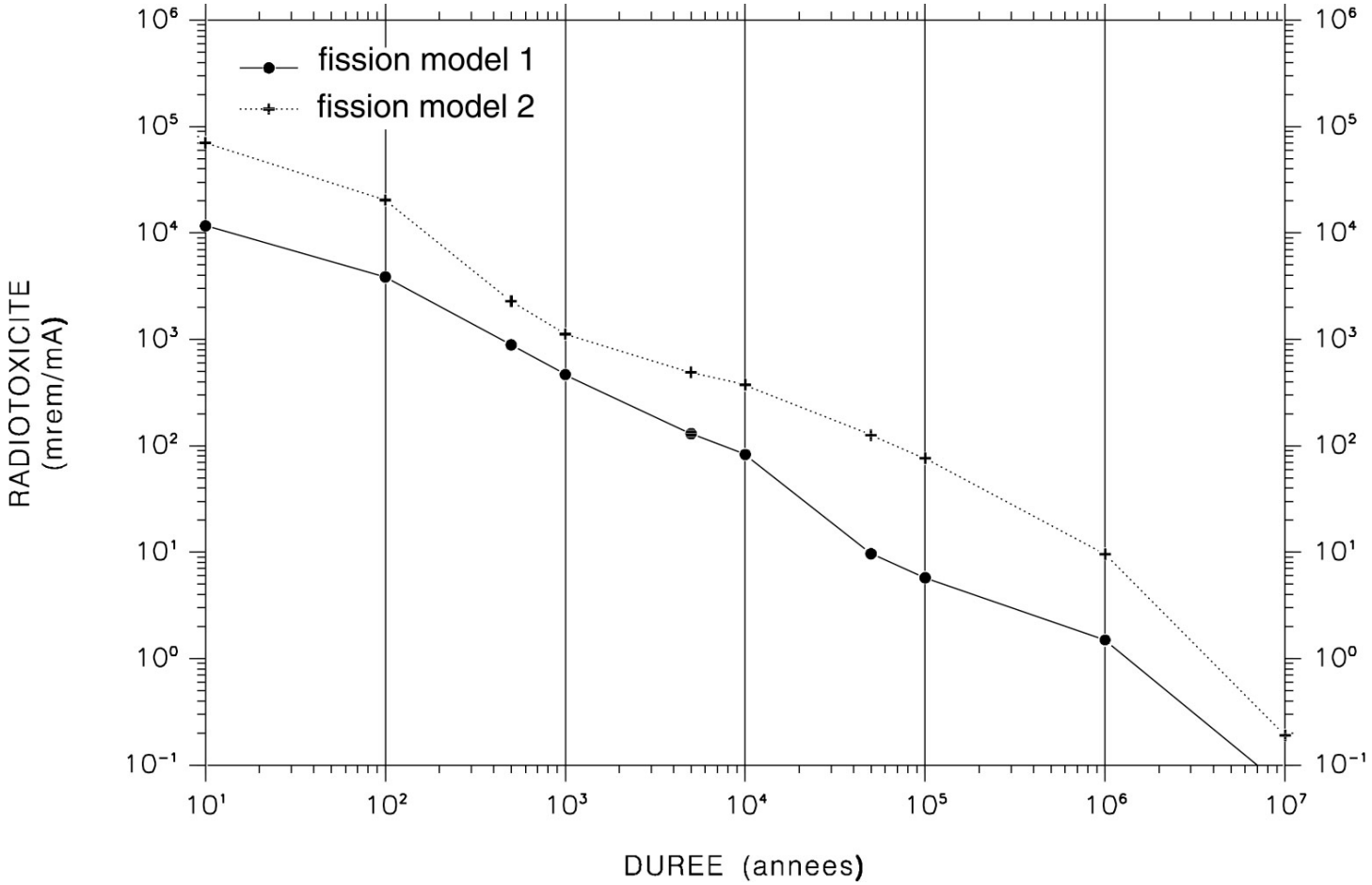


Mass distribution for ^{208}Pb 2600MeV



Radio-toxicity

Evolution of the spallation product radiological impact as a function of time.
Comparison between different high-energy fission models



Advantages and Limitations of GINC

Advantages

- No other model available for energies above the pion threshold production (except QMD models)
- No other model for projectiles other than nucleons
- Easily available for on-line integration into transport codes
- Every target-projectile combination without any extra information
- Particle-to-particle correlations preserved
- Valid on light and on heavy nuclei
- Capability of computing cross sections, even when it is unknown

Limitations

- **Low projectile energies E<200MeV are badly described**
- Quasi electric peaks above 100MeV are usually too sharp
- Coherent effect as well as direct transitions to discrete states are not included
- Nuclear medium effects, which can alter interaction properties are not taken into account
- Multibody processes (i.e. interaction on nucleon clusters) are not included
- Composite particle emissions (d,t,^{3}He,α) cannot be easily accommodated into INC, but for the evaporation stage.
- Backward angle emission poorly described (Corrected for FLUKA)

LECTURE OUTLINE

I – LIMITATIONS IN THE HIGH-ENERGY PARTICLE TRANSPORT

- Cross section data
- Neutron Yield
- Spallation Product Distribution

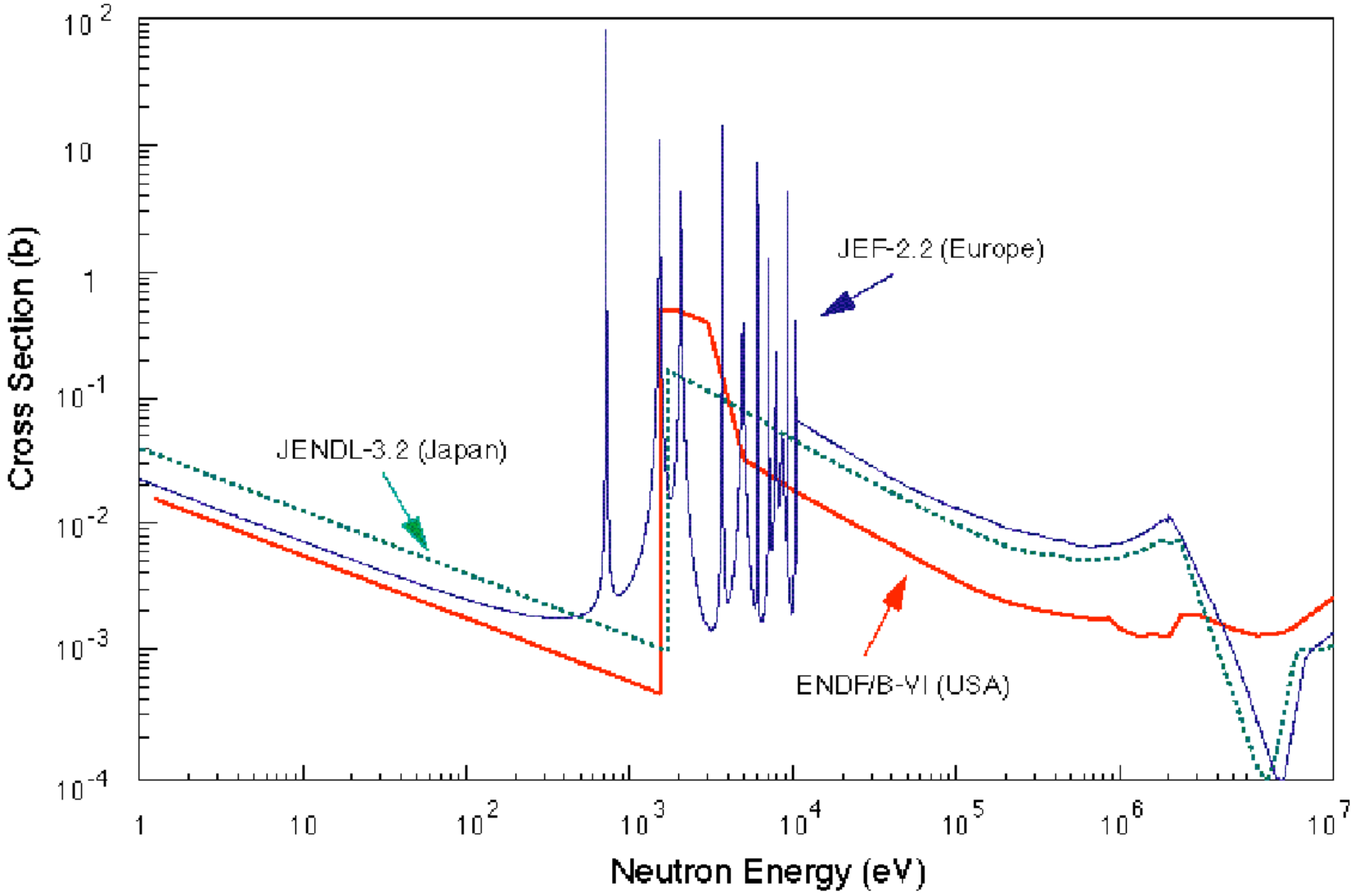
II – LIMITATIONS IN THE LOW-ENERGY NEUTRON TRANSPORT

- Nuclear Data Processing
- Uncertainties: sensitivity study on a fast ADS
- Status of the nuclear data: MA & LLFP

Low-Energy Neutron Data

- The nuclear data files are taken from the latest compilations available : ENDF/B-VI 8, JEFF3.0, JENDL-3.3, BROND-2, CENDL-2.1 and EFF-2.4
- Only original data files are used, not derived ones
- For each nuclide we have selected one evaluation out of those available on the basis of a systematic comparison :
  - We have ≈ 800 nuclides with reaction cross sections out of which ≈ 400 have also the elastic cross section;
- Activation/Transmutation data for unstable nuclides are from the EAF-4.2 compilation that we have converted in ENDF-6 format (including files 8, 9 and 10)
- All cross sections habe been checked for inconsistencies

^{137}Cs neutron capture cross section



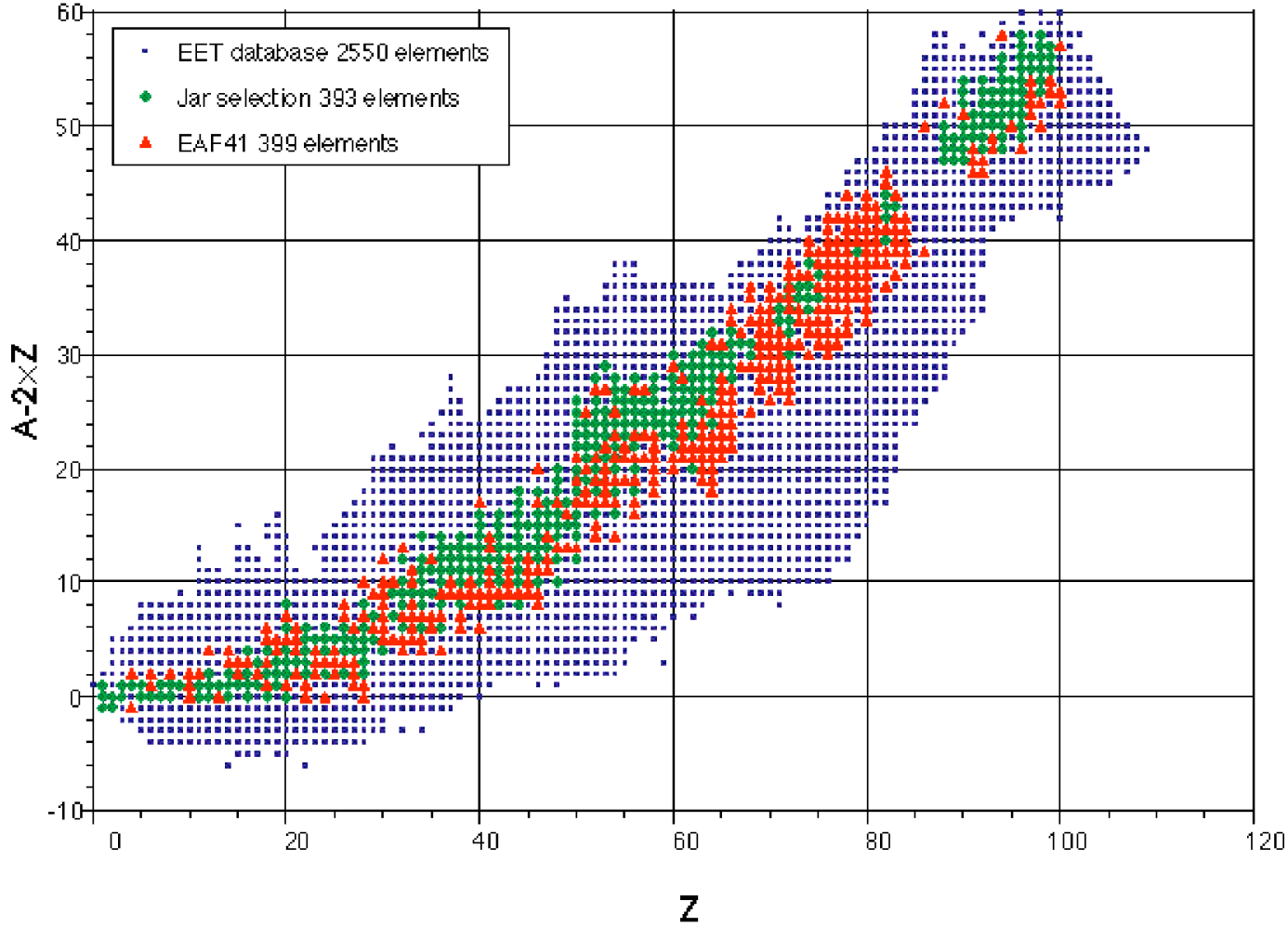
Nuclear Data Processing

- The files are :
  - Processed with the standard PREPRO-2000 code suite (LINEAR, RECENT, SIGMA1 and FIXUP), including the EAF-4.2 files;
  - Processed with a home-grown code package PROCESS to create a direct access library with : Cross sections, Cumulative secondary energy distributions and Cumulative angular distributions;
- Different temperatures can be present at the same time in memory for the same isotope
- Auxillary routines have been developed to sample :
  - The products of a reaction, including the isomeric state of the residual nuclei (information extracted from ENDF files);
  - The (correlated) fission fragments (based on the European, American, Japanese and Russian evaluations);
  - The energy dependent number of neutrons produced in neutron-nucleus reactions

Nuclear Data Processing (2)

- The EA-MC nuclear database contains 3154 isomers and has been developed from :
  - Brookhaven Nuclear Database;
  - NUBASE by Audi et al.;
  - National Radiological Protection Board (NRPB) database;
  - ICRP database;
  - Nuclear information from ENDF-6 files;
- For each isomer we list : A, Sym, Z, Is, Level, ΔM, Half-life, J^p, Decay mode, ΔIs, Branching ratio, reaction Q, nat. abundance, inhalation toxicity, and the ingestion toxicity
- Nuclear Data are extensively checked for consistencies :
  - All decay paths are closed (i.e. terminate in a nuclide present in the database);
  - All branching ratios are consistent (i.e. sum = 100%);
  - All nuclei produced by neutron reactions of which we have cross sections are present in the database;
  - All nuclear masses are consistent between cross sections, isomer yield and nuclear database;

The EA-MC Nuclear Database



Sensitivity Study for a fast ADS

- Better knowledge of nuclear data to validate calculational models ⇒ insight on uncertainties associated with integral parameters that characterize a particular core

- For ADS, minimization of uncertainty in $\Delta\rho$ /cycle essential ⇒ determines margins
  - at $k \approx 0.98$, ± 2% uncertainty in $\Delta\rho$/cycle has serious consequences on safety analysis and accelerator current requirements

Requested Precisions

- Also need to validate:
  - Neutron flux distributions and competition of different modes (source and higher harmonics)
  - Importance of source neutrons with respect to fission neutrons
  - Effect of buffer medium around spallation source
  - Kinematics of sub-critical cores

- Between k ≈ 0.9 and k ≈ 0.99

⇒ Aim for same precisions as required for critical cores:

± 100 pcm for UO2
± 40 pcm for MOX

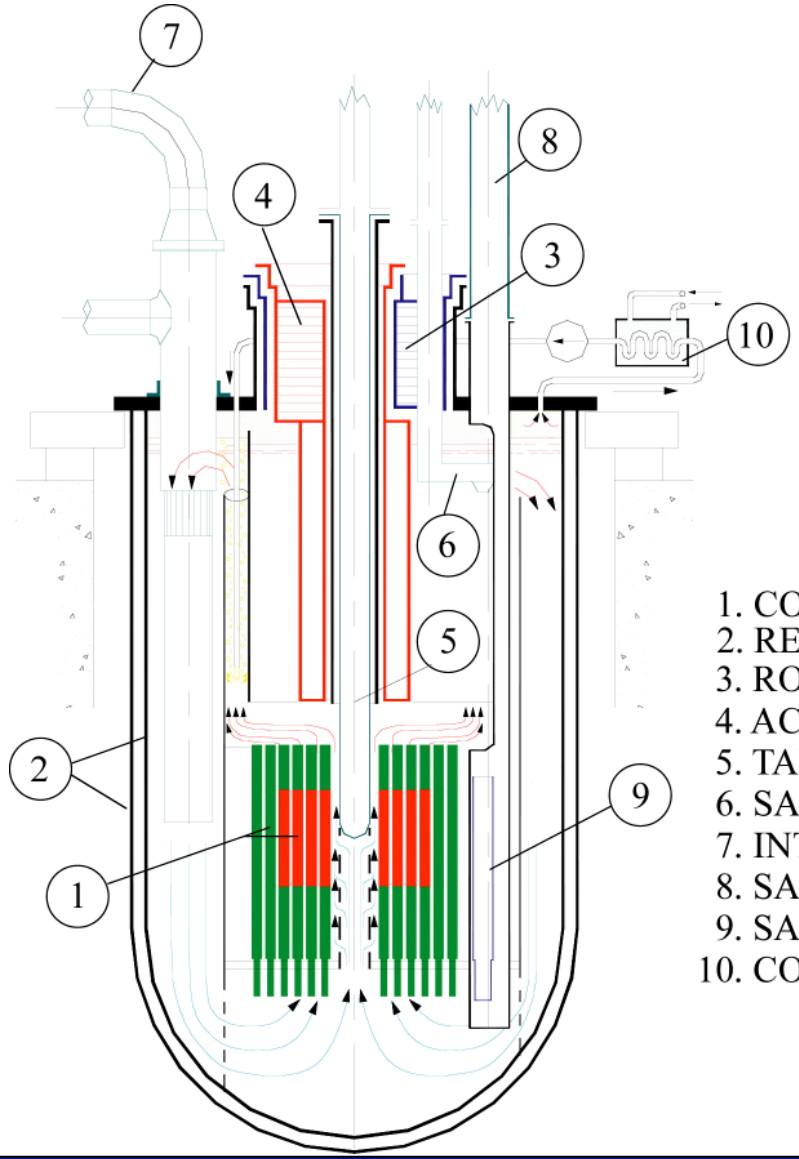
Principal Requirements for ADS Technology

- Structural materials and coolant:
  - Inelastic scattering and (n,xn) in Fe, Cr, Ni, Pb, Bi and W (± 5% to ± 10%)
- Fission products:
  - Capture XS of Tc-99, I-129, Xe-131, Cs-133, Cs-135, Sm-149, Sm-151 (typically ± 10%)
- Primary actinides:
  - Capture XS of Th-232, U-233, U-235, Pu-isotopes in the energy range 1 eV to 500 keV (typically ± 10%)
  - Inelastic scattering of Th-232 and U-238 (± 5%), Pu-239 (± 10%), Pu-240 (± 20%)

Principal Requirements for ADS Technology

- Primary actinides (continued):
  - Fission XS of Th-232 and U-238 above 500 keV (typically ± 10%), U-233, U-235, Pu-239, Pu-241 in the energy range 1 eV to a few MeV (± 1% to ± 5%)
  - Fission product yields for mass chains 92 to 140 in U-233, U-235 and Pu-239
  - Delayed neutron yields for Th-232 and U-238 (± 3%), Pu-isotopes (± 3% to ± 7%), Np-237 and Am-241 (± 5%)
- Minor actinides:
  - Capture, fission, inelastic scattering, (n,2n), fission neutron spectra, delayed neutron yields, fission product yields and spontaneous fission half-lives for Np-237, Pu-238, Am-241, Am-243, Cm-244 (typically ± 10%)

Energy Amplifier Demonstration Facility

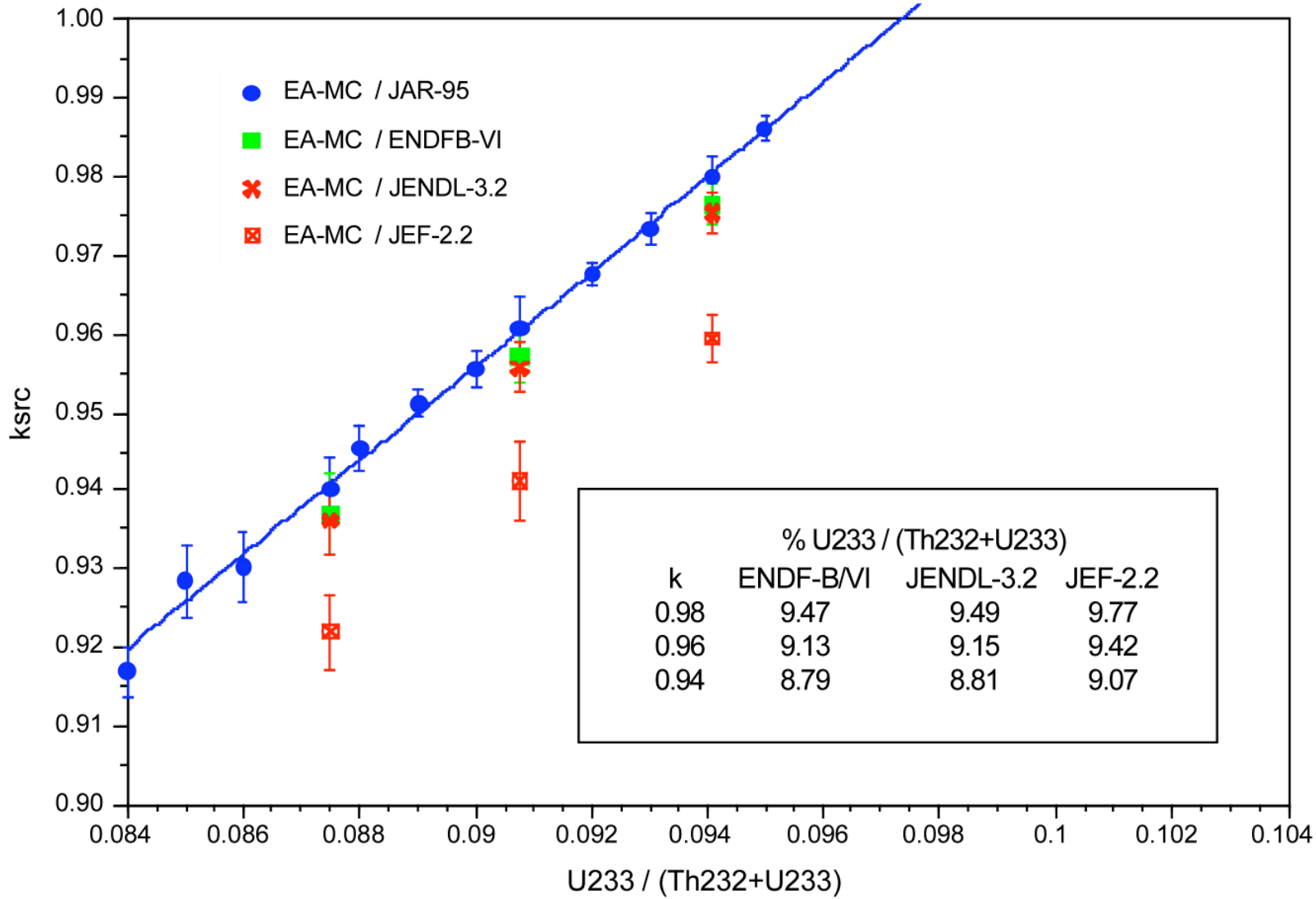


1. CORE
2. REACTOR VESSELS
3. ROTATING PLUGS
4. ACS
5. TARGET UNIT
6. SA TRANSFER MACHINE
7. INT. HEAT EXCH.
8. SA HANDLING CHANNEL
9. SA BASKET
10. COVER GAS COOLER

EADF Main Parameters

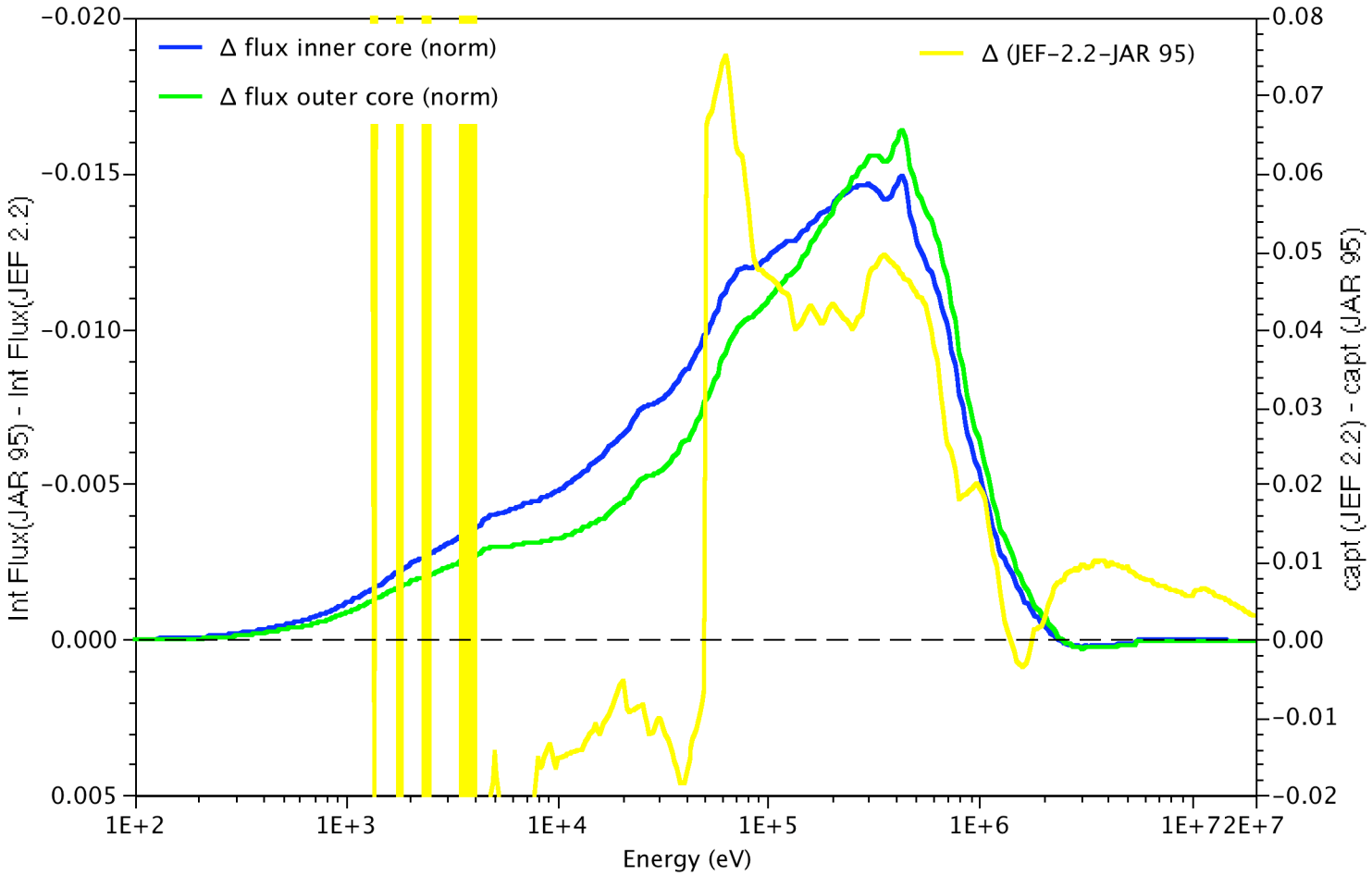
Global Parameters	Symbol	EADF	EADF	Units
Initial fuel mixture	MOX	$(U\text{-}Pu)O_2$	$(Th\text{-}Pu)O_2$	
Initial fuel mass	m_{fuel}	3.793	3.793	ton
Initial Pu concentration	m_{Pu}/m_{fuel}	17.7	20.2	wt.%
Initial Fissile enrichment	$Pu^{39,41}$	14.7	16.9	wt.%
Thermal Power Output	P_{th}	80	80	MWatt
Proton Beam Energy	E_p	600	600	MeV
Spallation Neutron Yield	$N_{(n/p)}$	14.51 ± 0.10	14.51 ± 0.10	n/p
Net neutron multiplication	M	27.80 ± 0.56	26.74 ± 0.75	
Multiplication Coefficient	k=(M-1)/M	0.9640 ± 0.0007	0.9626 ± 0.0010	
Energetic Gain	G	42.73 ± 0.88	40.64 ± 1.19	
Gain coefficient	G_0	1.54	1.52	
Accelerator Current	I_p	3.20 ± 0.07	3.36 ± 0.10	mA

IAEA ADS Neutronic Benchmark (IAEA-TC-903.3)



	% U233 / (Th232+U233)		
k	ENDF-B/VI	JENDL-3.2	JEF-2.2
0.98	9.47	9.49	9.77
0.96	9.13	9.15	9.42
0.94	8.79	8.81	9.07

IAEA ADS Neutronic Benchmark (IAEA-TC-903.3)



20% deviation in $^{232}Th(n,\gamma)$ between 50 and 800 keV

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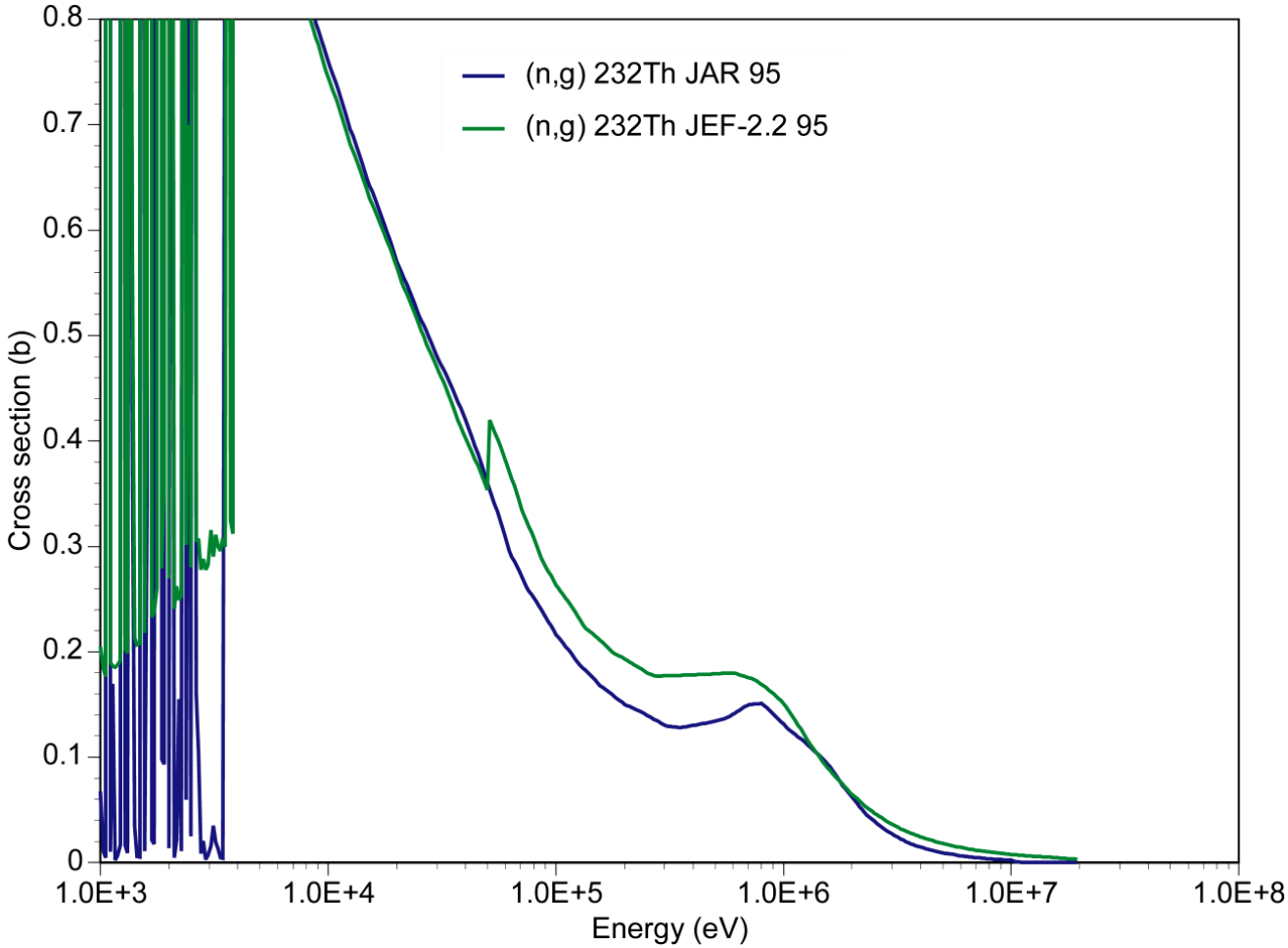
2000 pcm deviation in Keff



XS Data Effect on K

Neutron cross section data effect in k_{src}

	JAR-95	ENDF/B-VI	JENDL-3.2
$UPuO_2$	0.96403	0.95883	0.93937
error	±0.00070	±0.00094	±0.00106
$\Delta k/k$ [pcm]		–539	–2558
$ThPuO_2$	0.96260	0.94945	0.94526
error	±0.00102	±0.00109	±0.00088
$\Delta k/k$ [pcm]		–1366	–1801

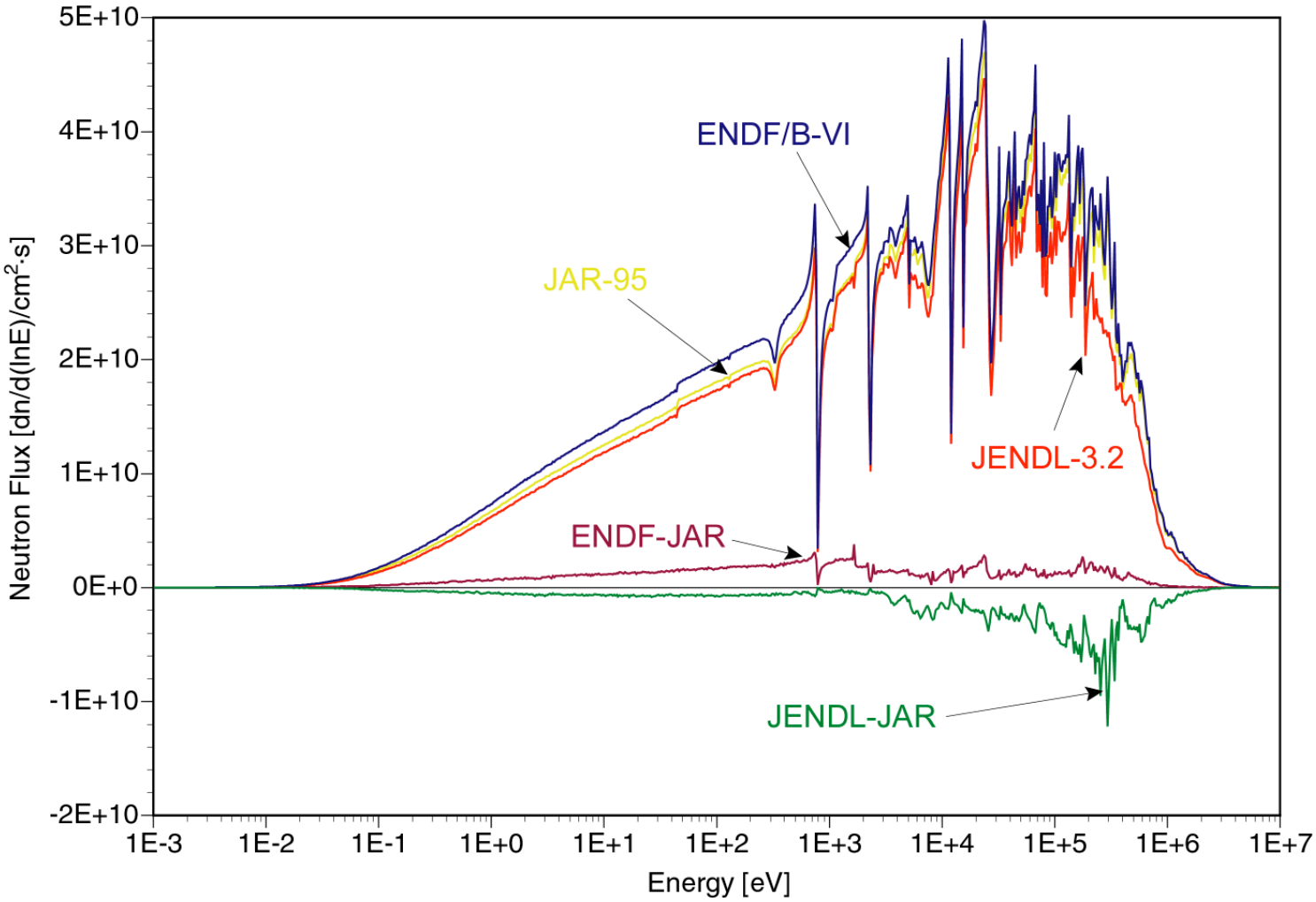
Neutron Balance (Device)

- U-Pu and Th-Pu fuel types show similar trends in library differences
- JAR-95 compilation taken as reference
- Differences for JENDL-3.2:
  - 2-4% excess for capture in fuels, coolant and cladding
  - 2-4% deficit for fission in fuels, (n,xn) in coolant
  - 25-30% deficit for (n,xn) in cladding
- Differences for ENDF/B-VI:
  - 0.5-2% excess for capture in fuels and cladding
  - Around 4% deficit for capture in coolant
  - 0.5-2% deficit for fission in fuels
  - Around 6% excess for (n,xn) in coolant
  - 1.5-2.5% excess for (n,xn) in cladding

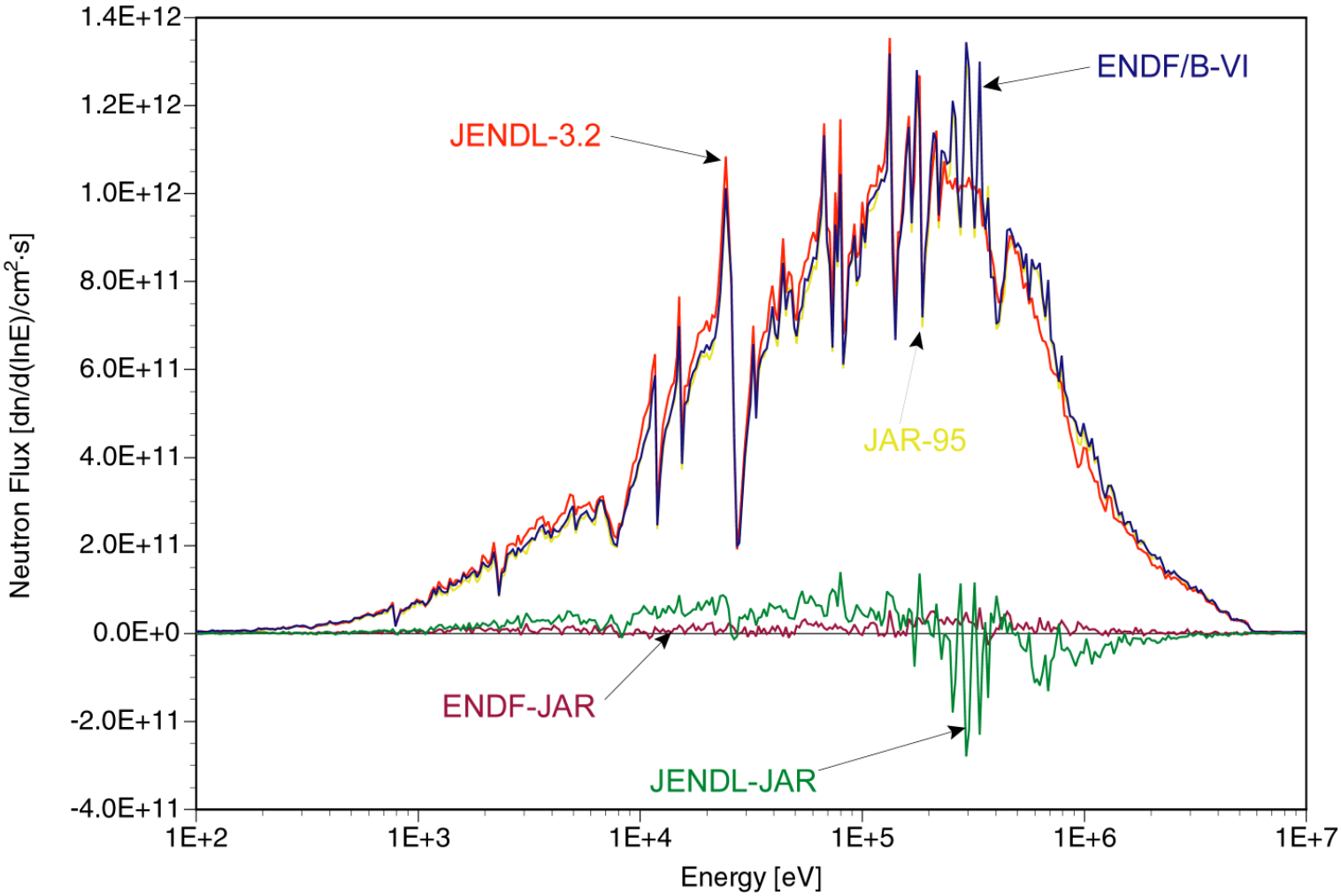
Neutron Balance (Fuel)

- Fission to capture ratio:
  - U fuel: JAR 0.92, JENDL 0.85, ENDF 0.91
  - Th fuel: JAR 0.88, JENDL 0.83, ENDF 0.84
- Differences for JENDL-3.2:
  - Capture:
    - 1.5% excess in ^{235}U, ^{238}U
    - 4% excess in ^{239}Pu
    - 10% excess in ^{240}Pu
    - 15-25% excess in ^{241}Pu
  - Fission:
    - 11% deficit in ^{238}U
    - 9% deficit in ^{232}Th
    - 12-16% deficit in ^{240}Pu
    - 2.5-4% deficit in ^{241}Pu

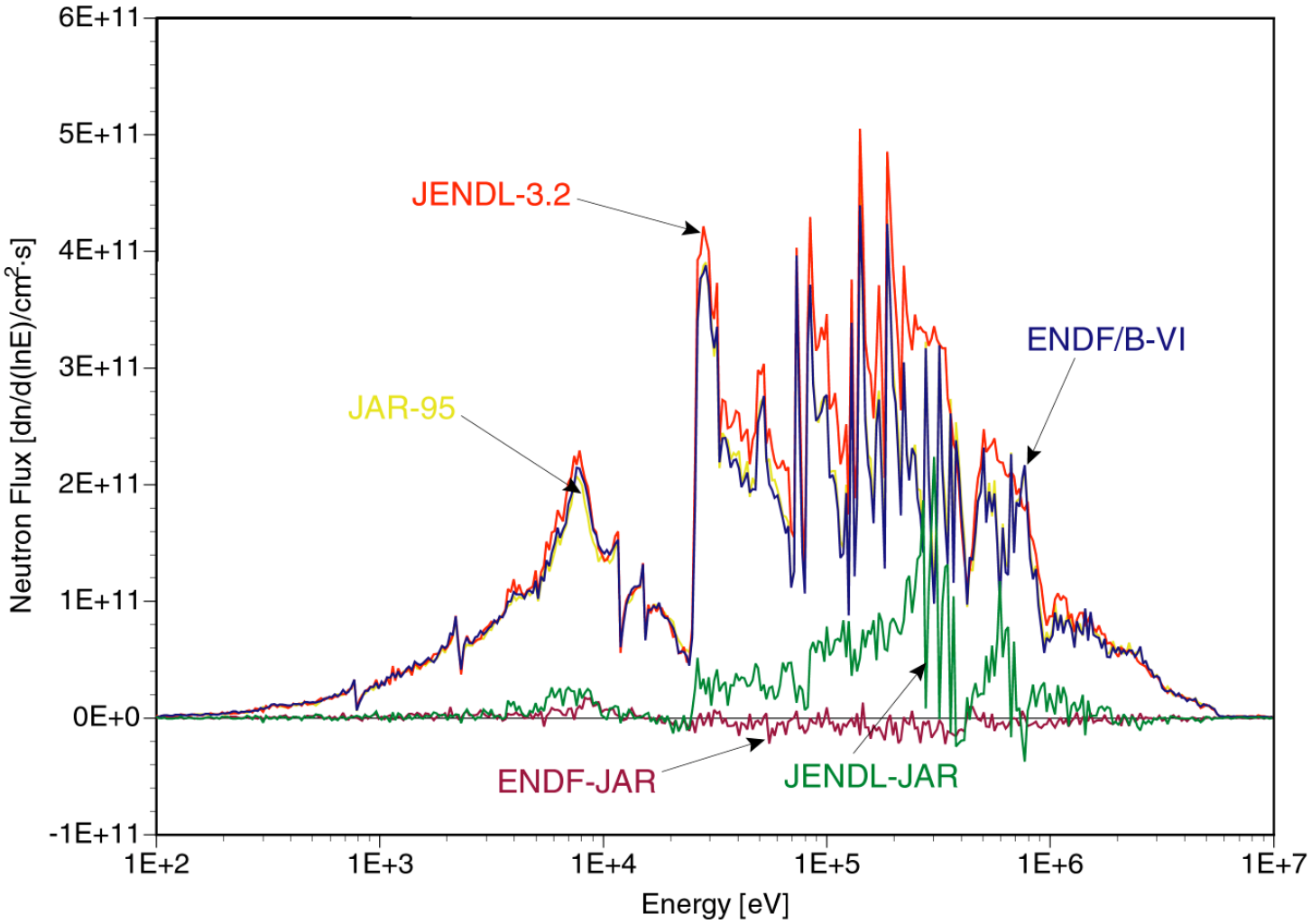
Spectrum Effect, Coolant



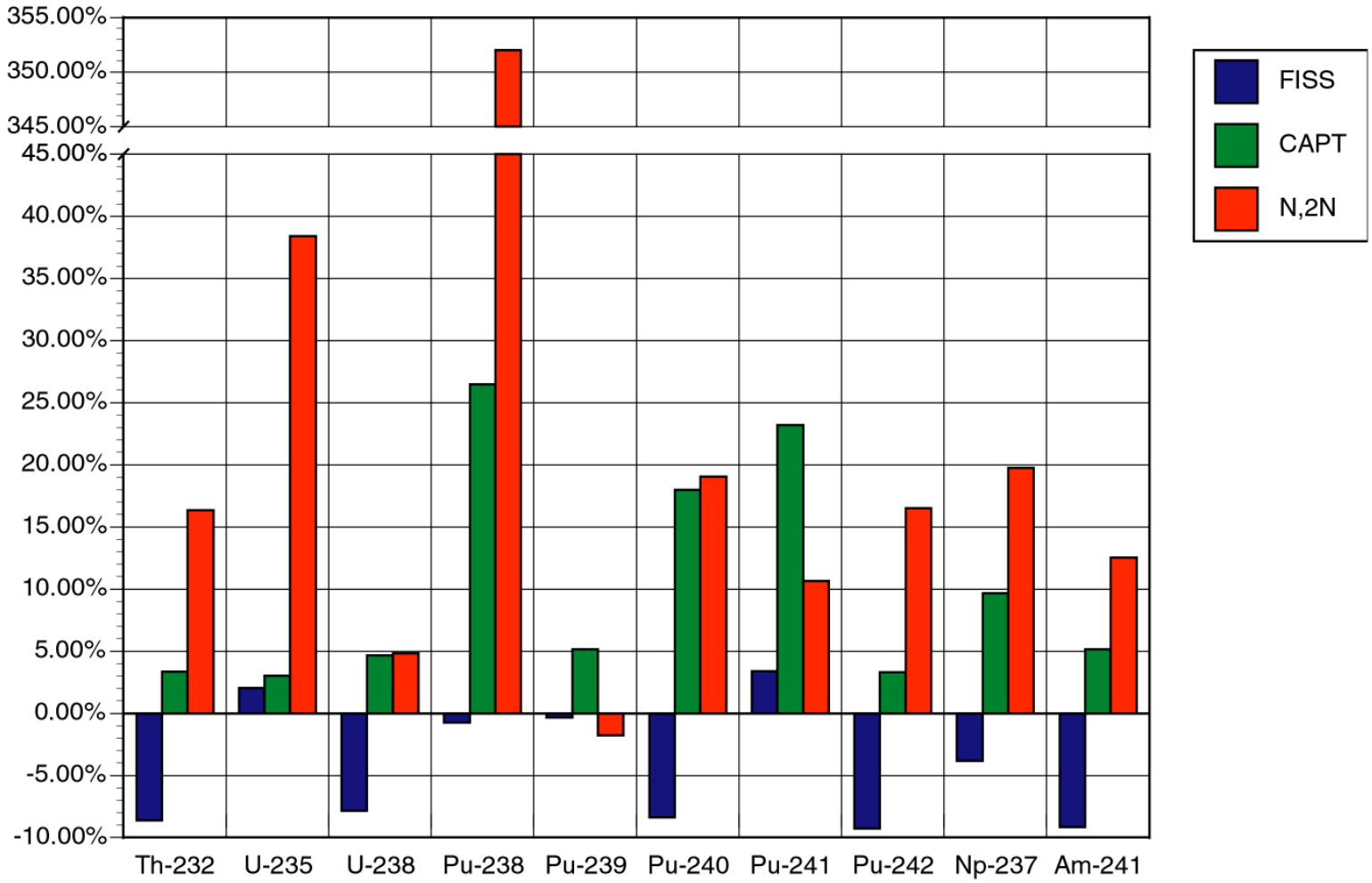
Spectrum Effect, Fuel



Spectrum Effect, Cladding



Comparison of 1-group XS



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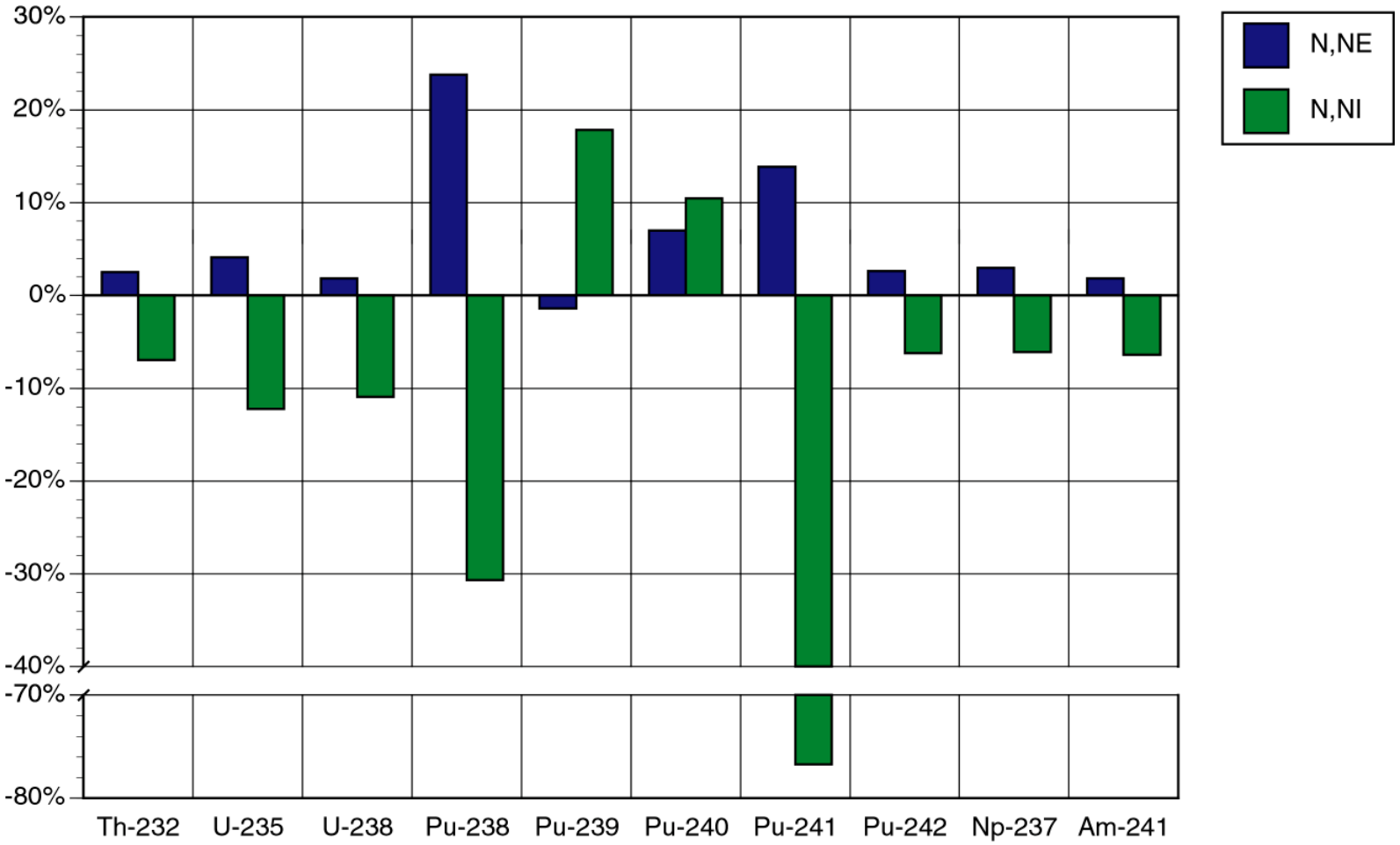

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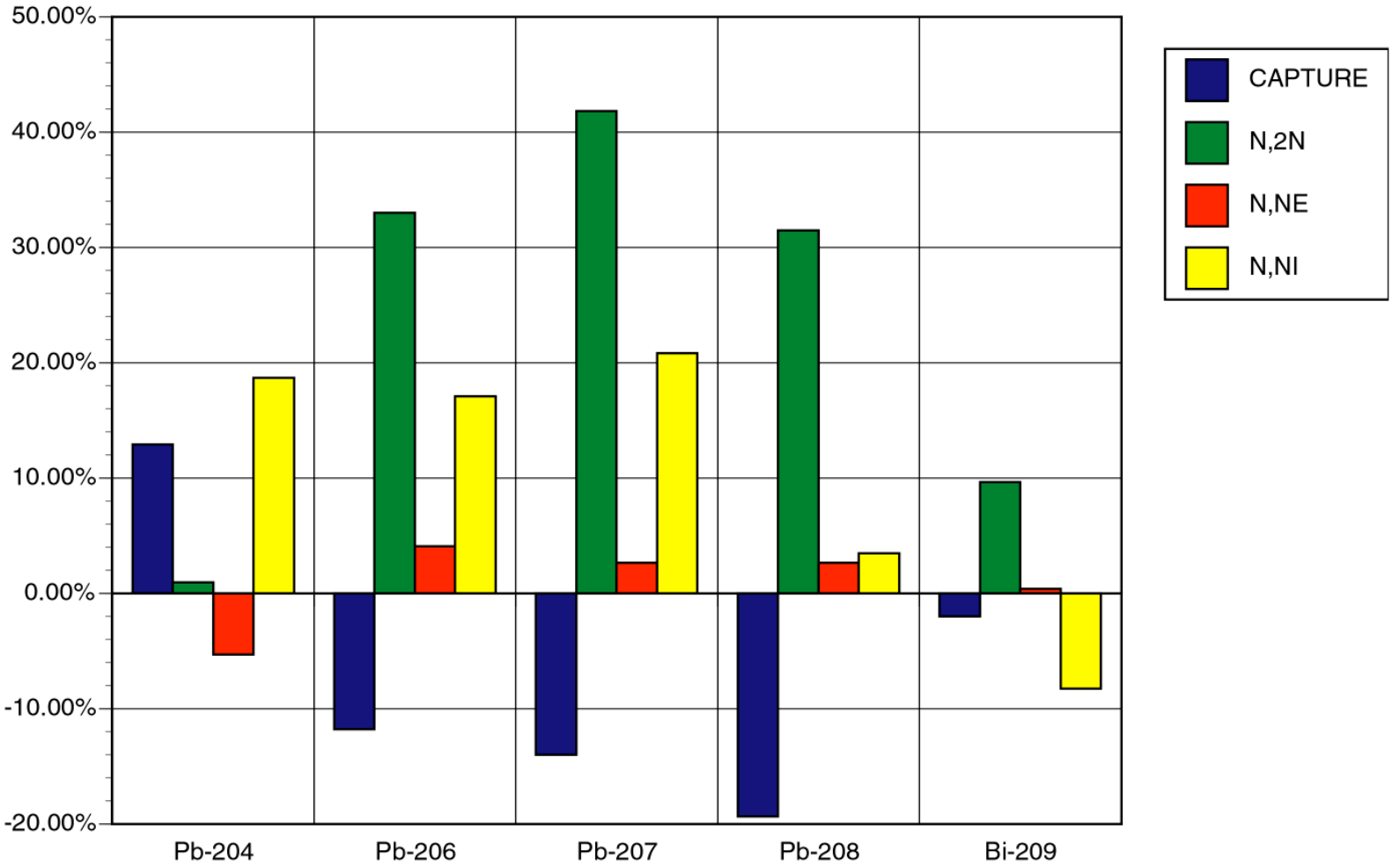
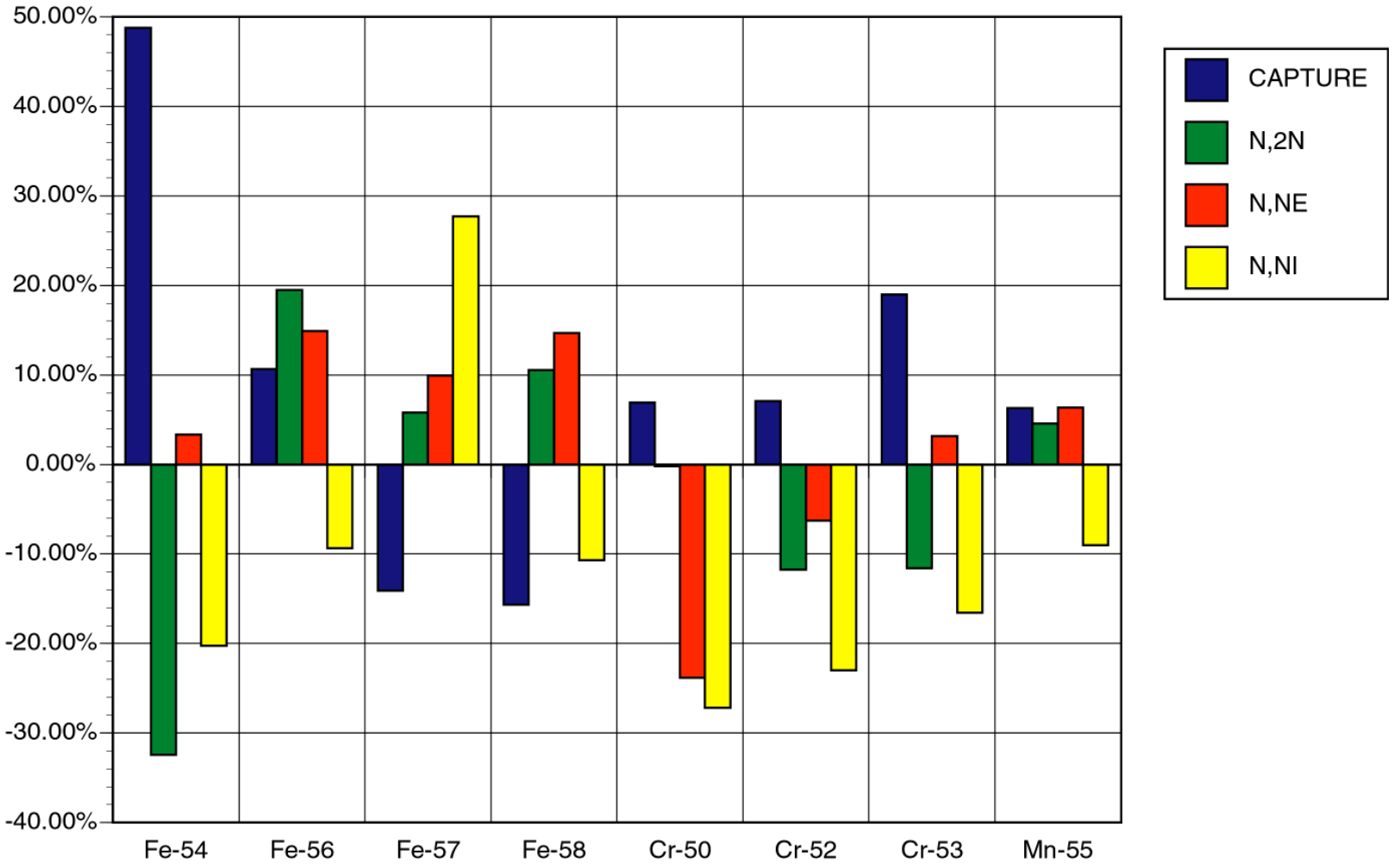


Comparison of 1-group XS



XS Data Effect on Transmutation Rates

Transmutation rates (kg/$TW_{th}h$) of plutonium and minor actinides and LLFPs

Nuclides	EADF (ThPuO2) ENDF/B-VI	EADF (UPuO2) ENDF/B-VI	EADF (UPuO2) JENDL-3.2	PWR (UO2)
^{233}U	+ 31.0			
Pu	– 42.8	– 7.39	– 5.55	+ 11.0
Np	+ 0.03	+ 0.25	+ 0.24	+ 0.57
Am	+ 0.24	+ 0.17	+ 0.14	+ 0.54
Cm	+ 0.007	+ 0.017	+ 0.020	+ 0.044
^{99}Tc prod	+ 0.99	+ 1.07	+1.22	+ 0.99
^{99}Tc trans	– 3.77	– 3.77		
^{129}I prod	+ 0.30	+ 0.31		+ 0.17
^{129}I trans	– 3.01	– 3.01		

Recommendations

- Discrepancies of 2000 pcm in k_{src} for different nuclear data libraries
- Spectrum effects were seen for JENDL
- In the fuel materials, improved XS determination needed for
  - fission in ^{232}Th, ^{238}U, ^{240}Pu and ^{242}Pu
  - capture in ^{238}Pu, ^{240}Pu and ^{241}Pu
  - (n,xn) in most nuclides (even ^{235}U)
  - elastic scattering in ^{238}Pu and ^{241}Pu
  - inelastic scattering in ^{238}Pu, ^{239}Pu, ^{240}Pu and ^{241}Pu

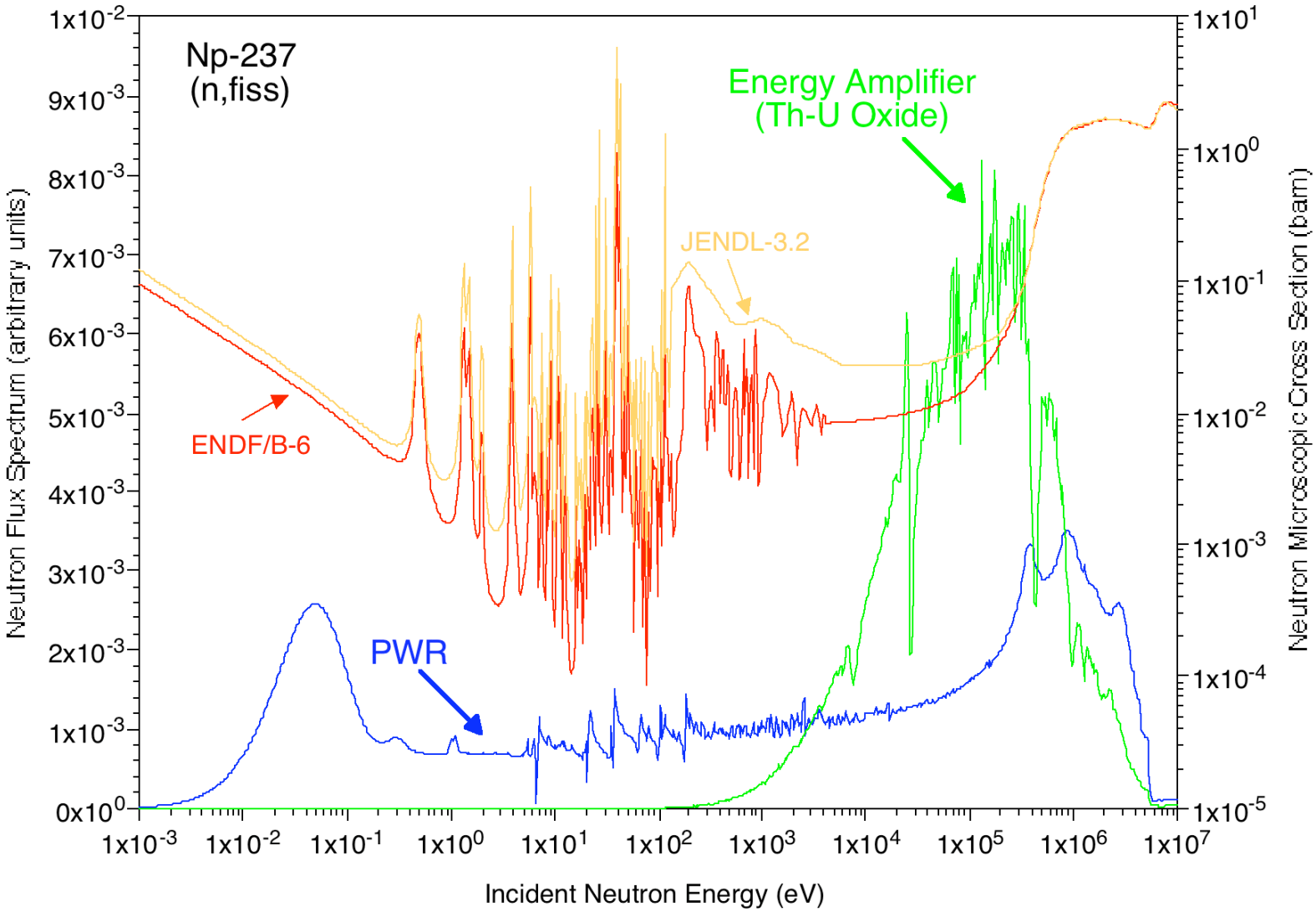
Recommendations

- In the coolant materials, improved XS determination needed for capture, (n,xn) and inelastic XS for the Pb isotopes

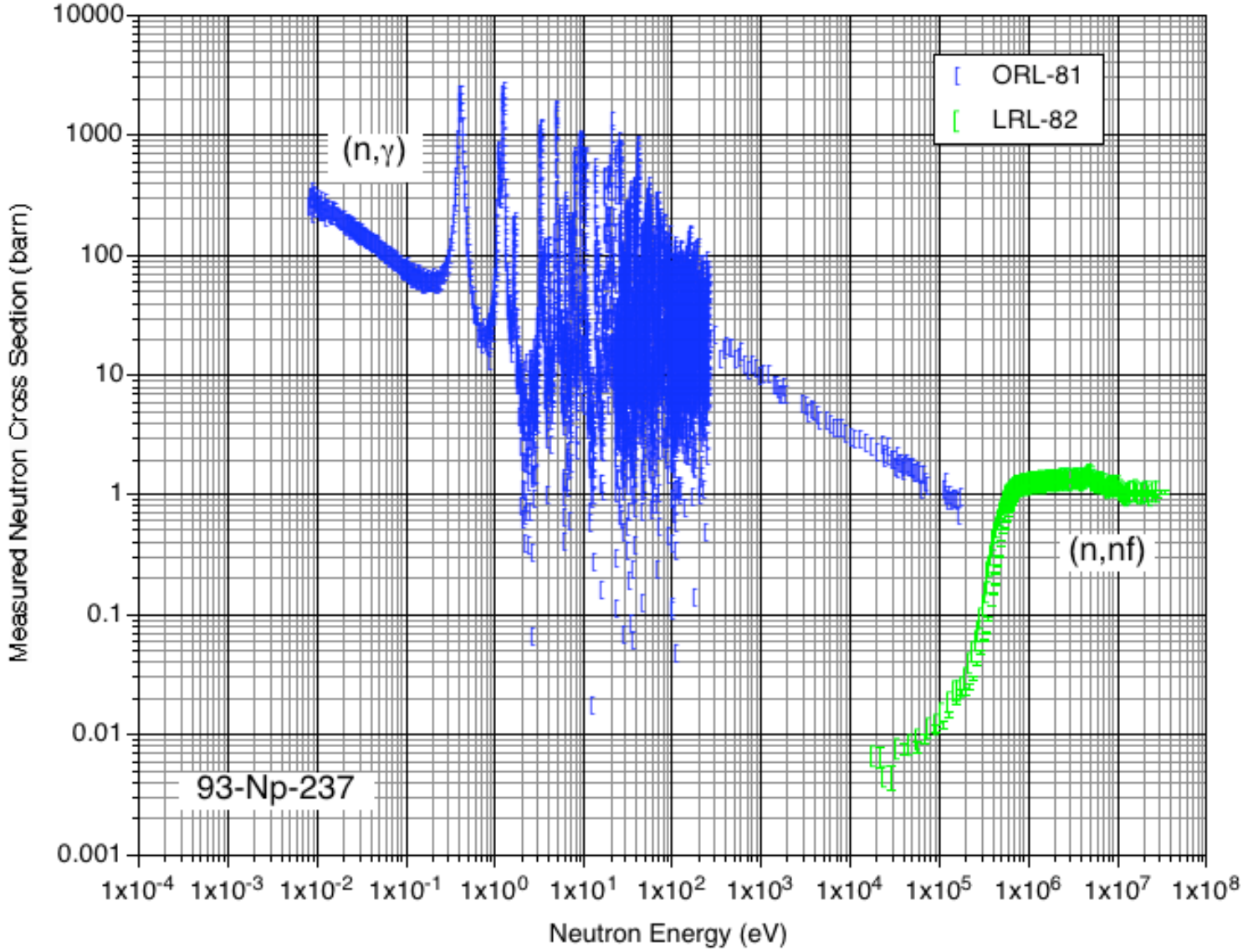
- In the cladding materials, improved XS determination needed for Fe isotopes, particularly ^{54}Fe (relative abundance 5.8%) has badly determined XS

- Analysis with a sensitivity-uncertainty code utilising XS data covariance files foreseen (deterministic code must be used)

Status of Nuclear Data: MA



Status of Nuclear Data: MA



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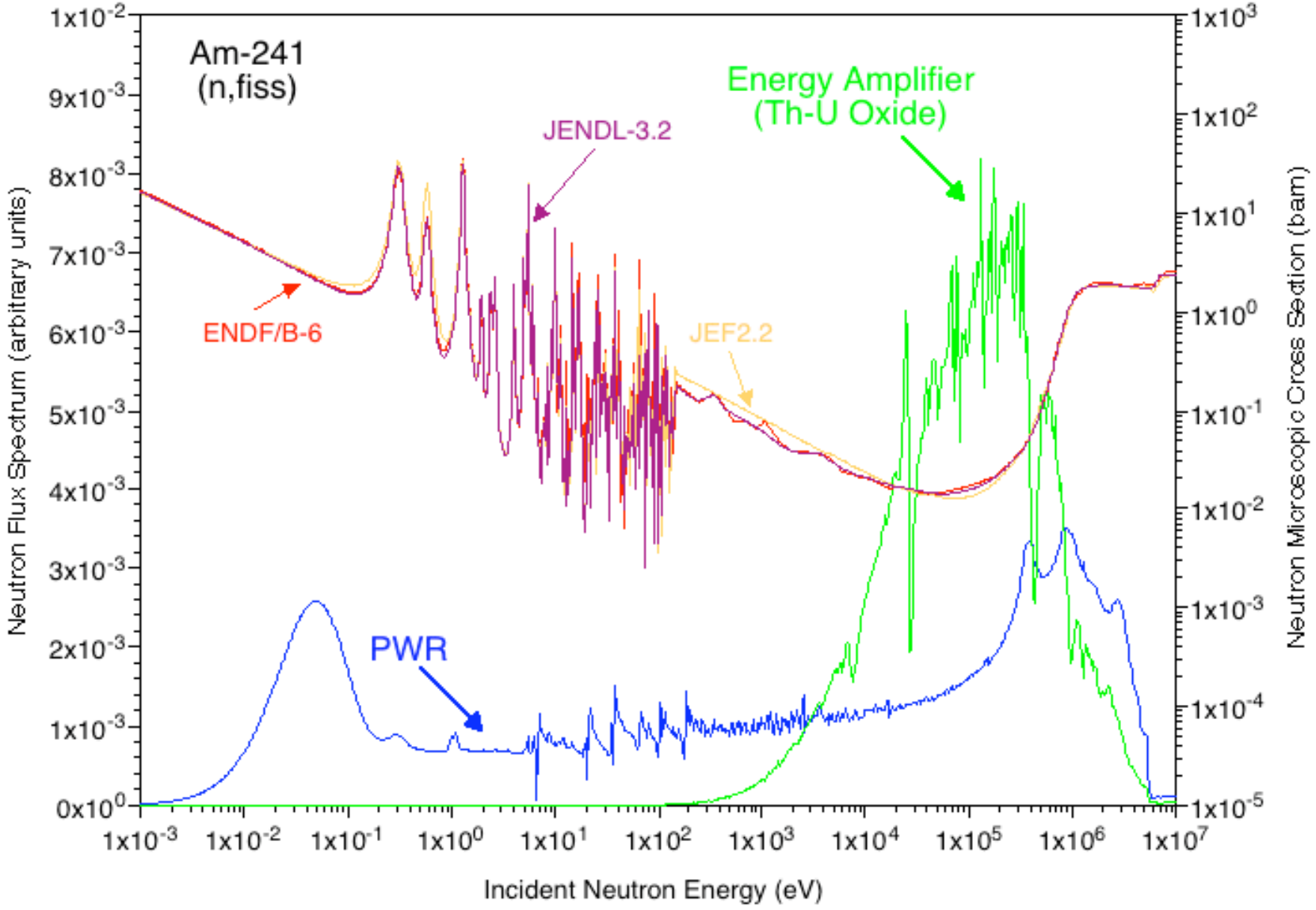

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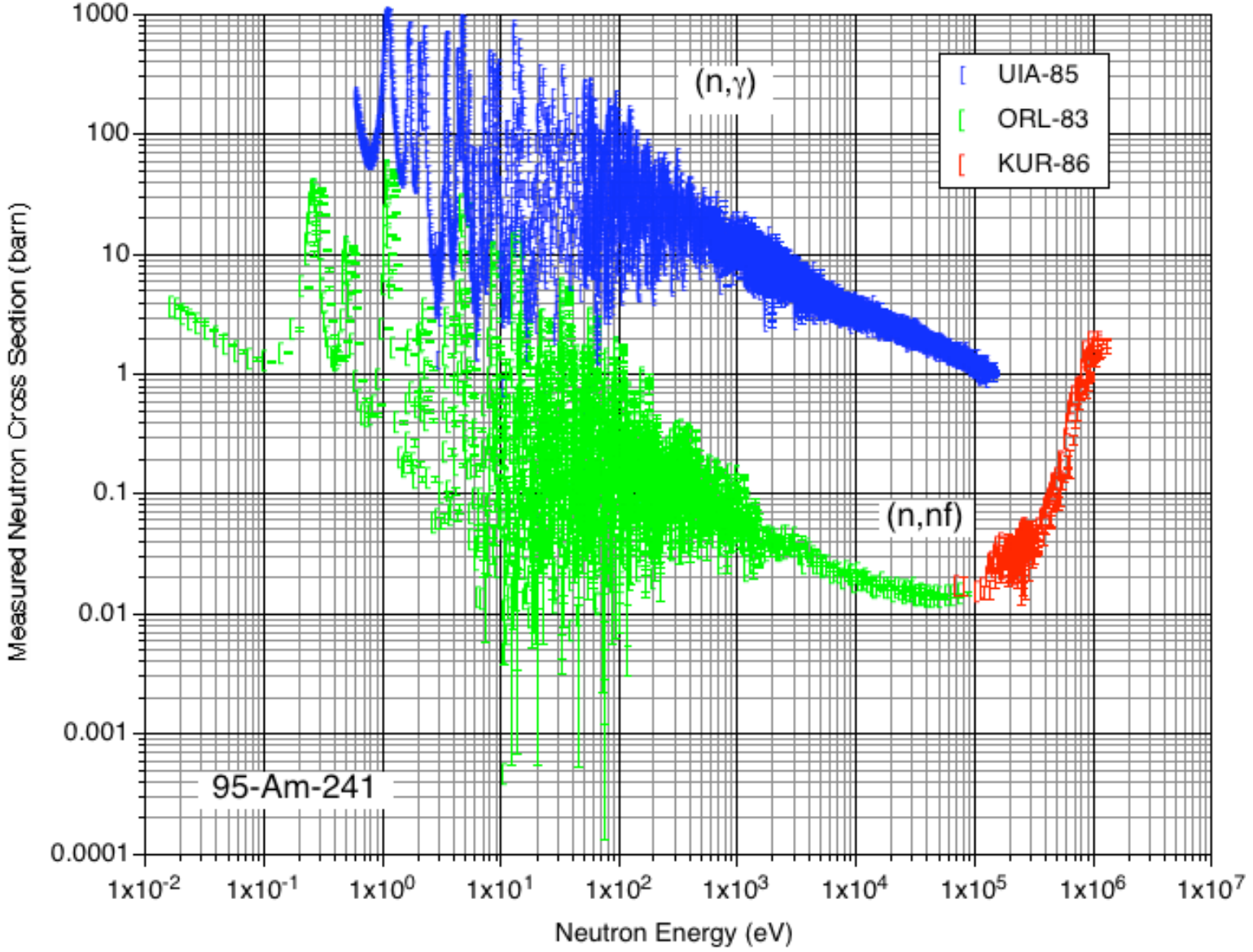

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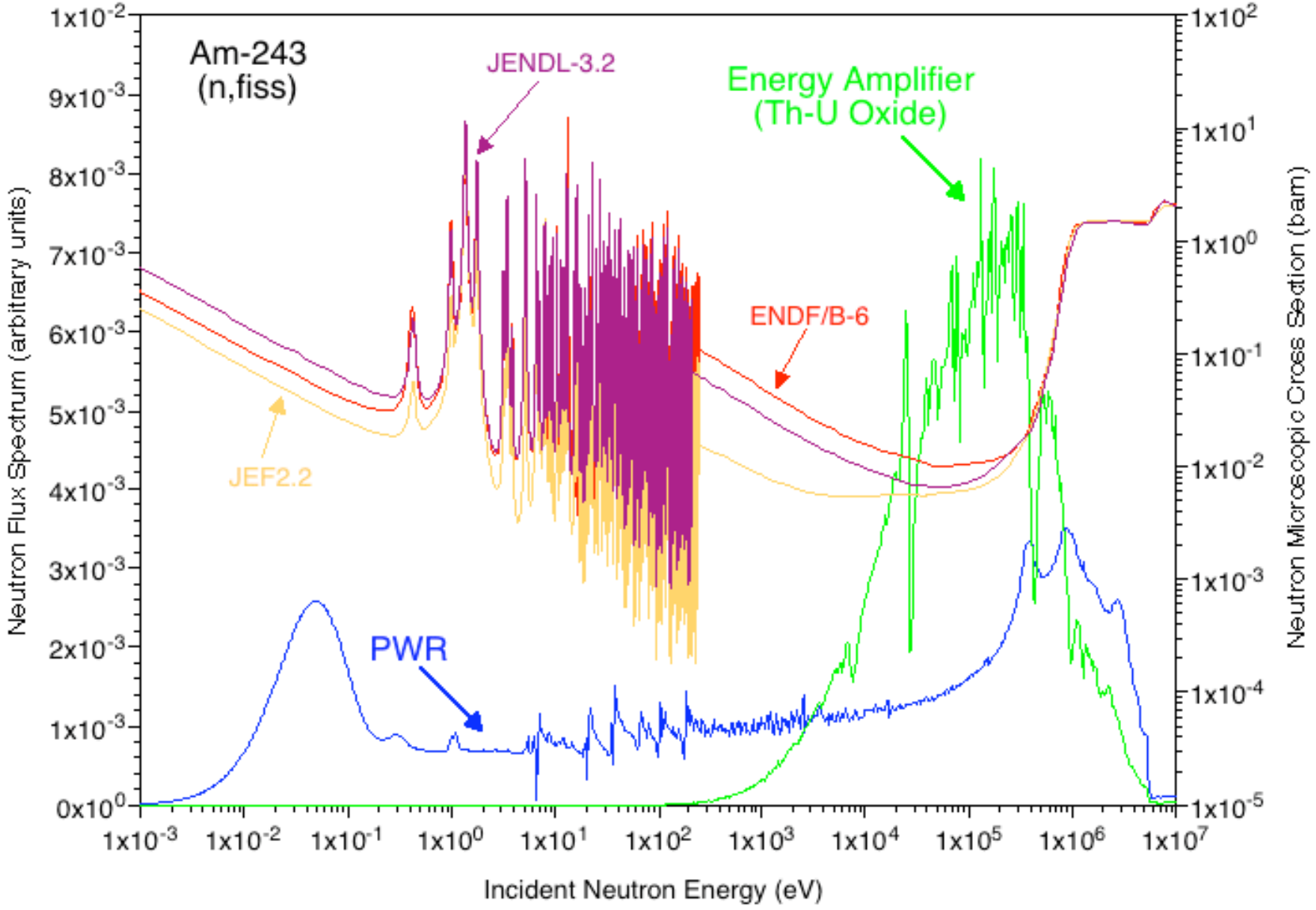

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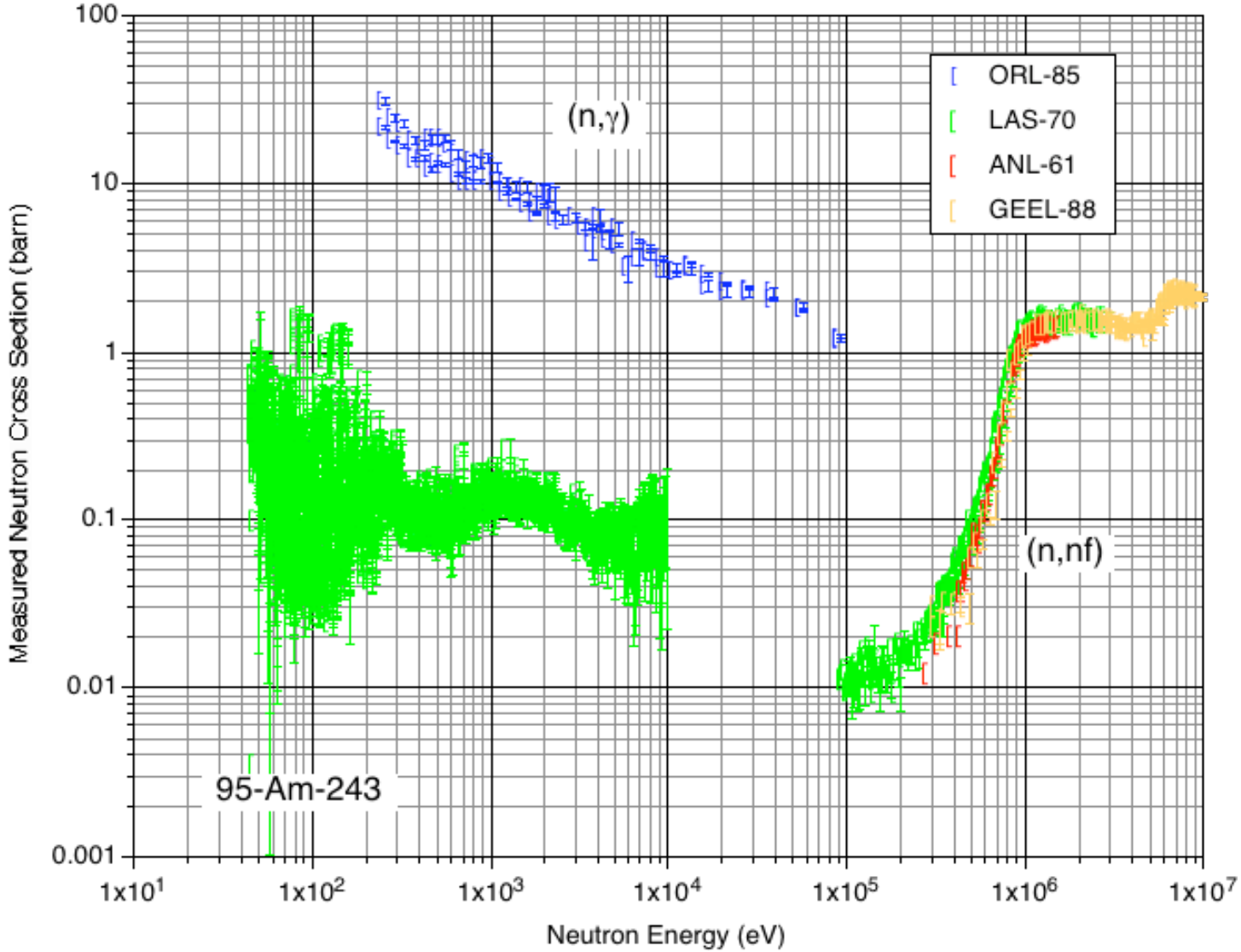

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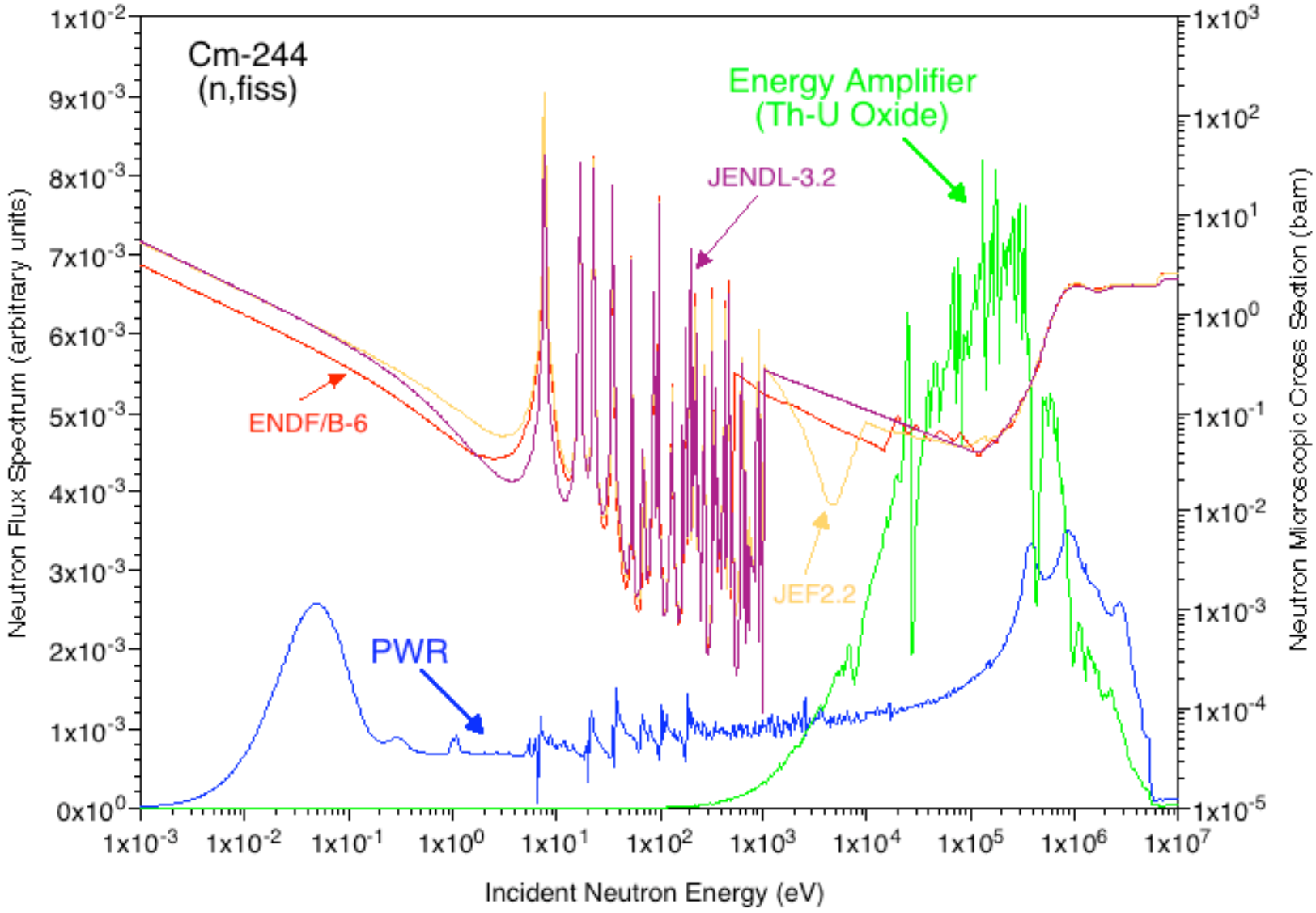

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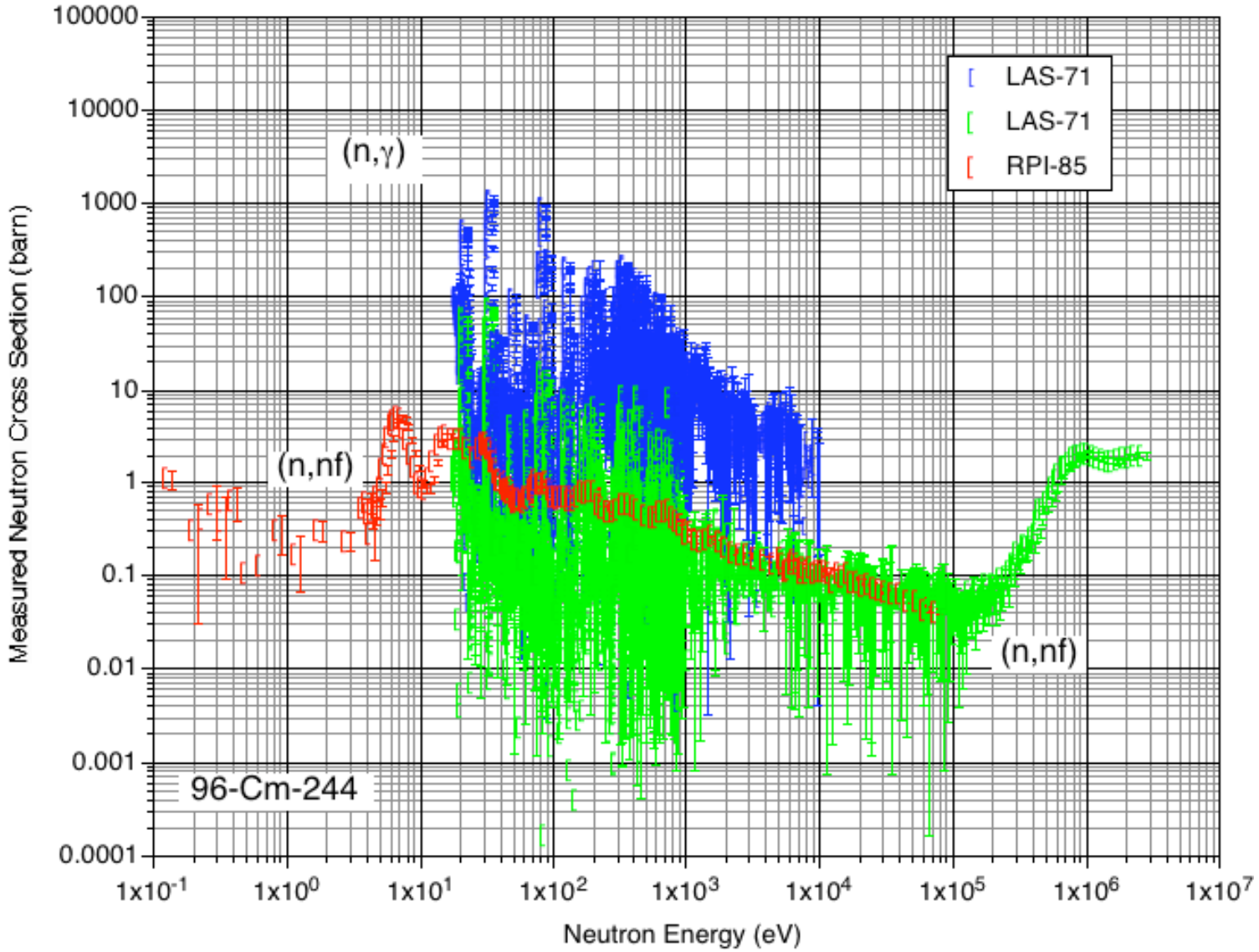

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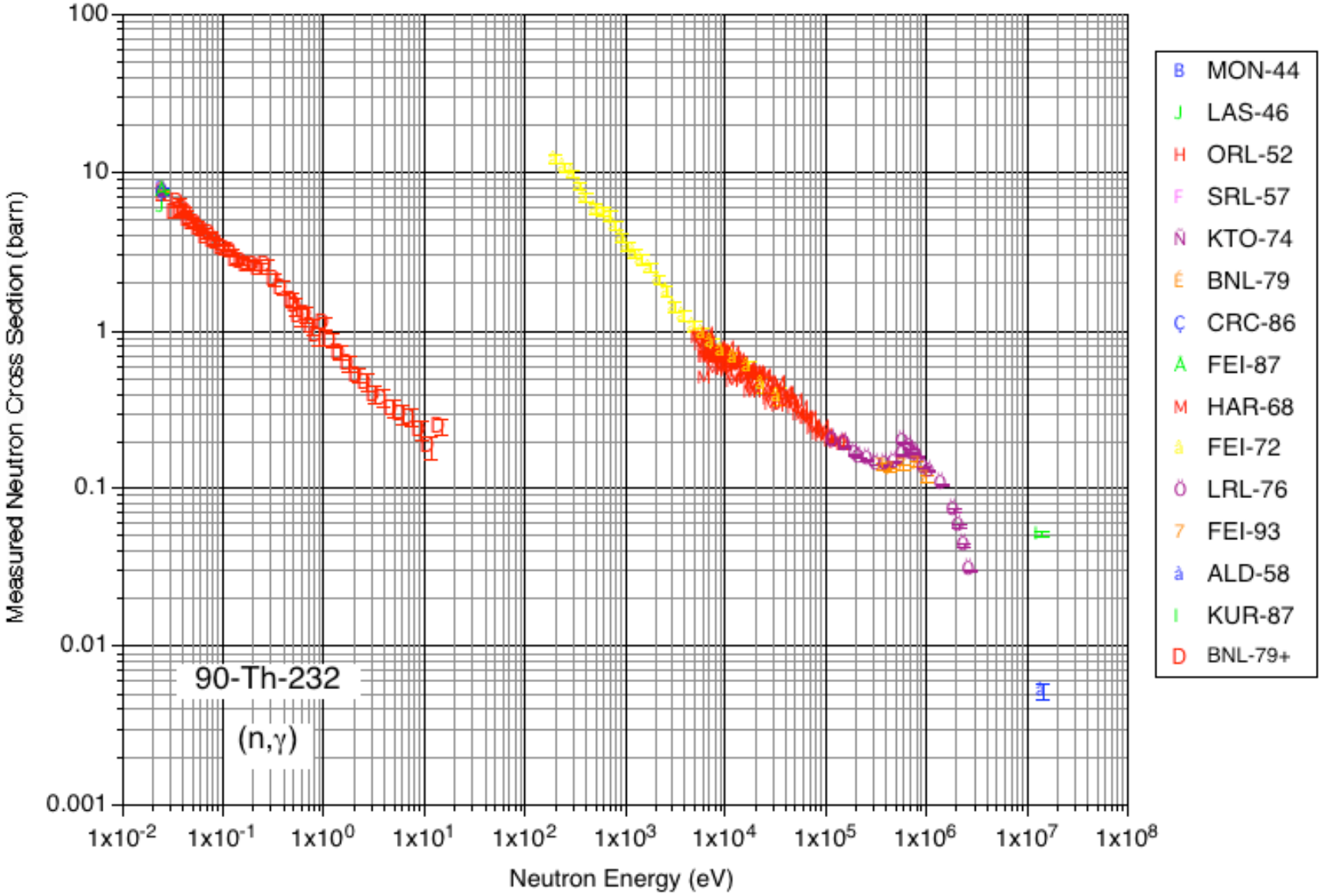

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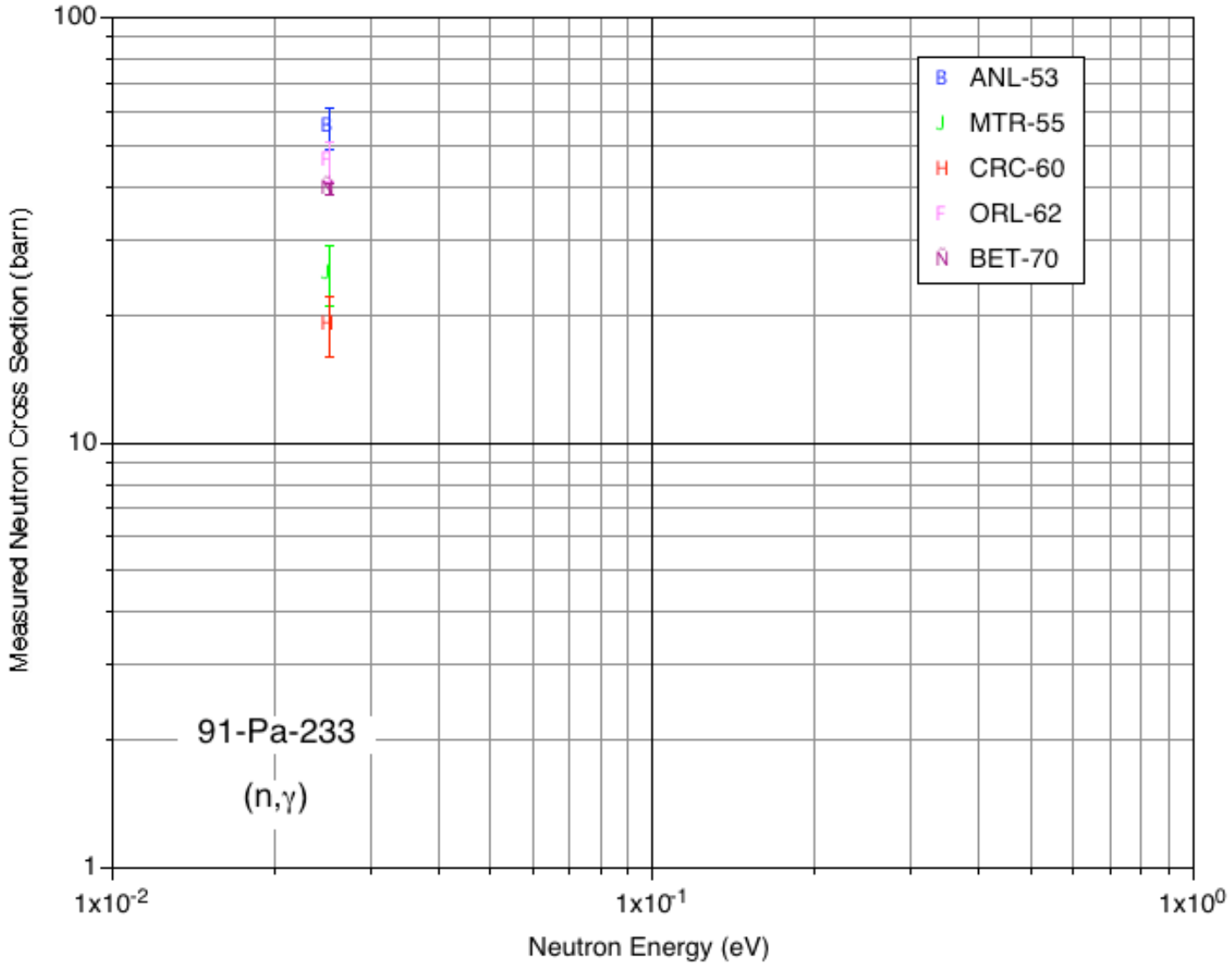
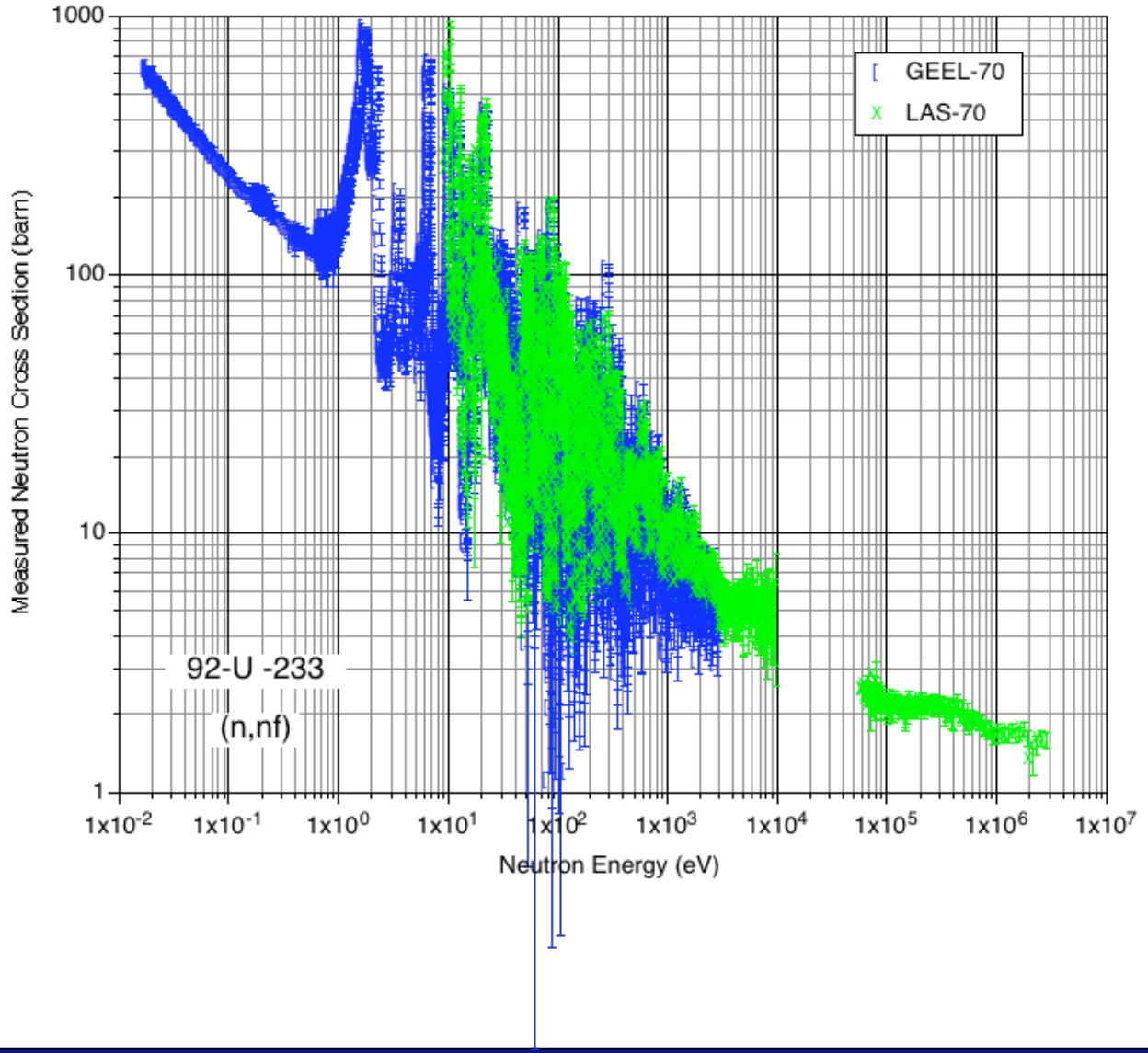
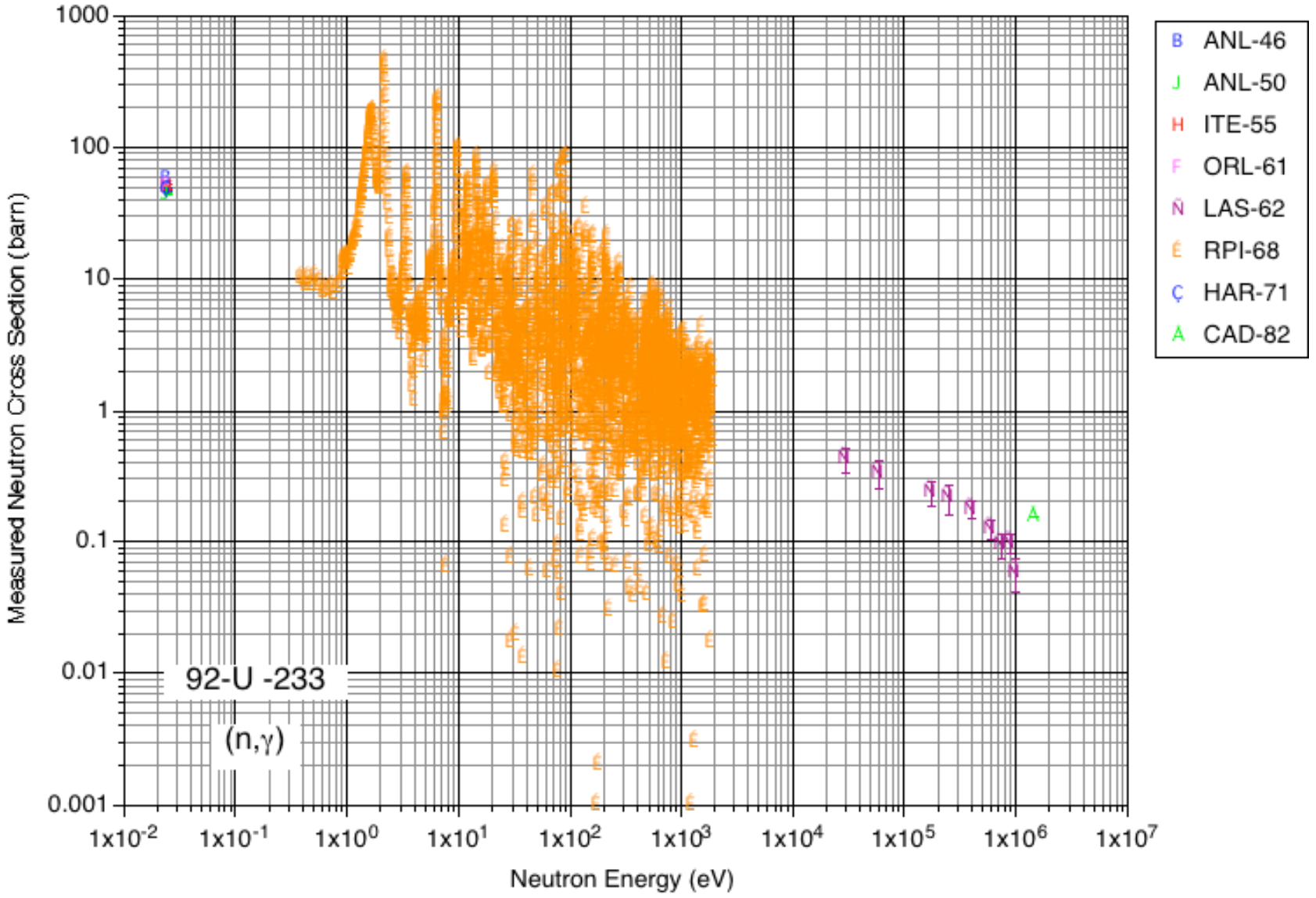


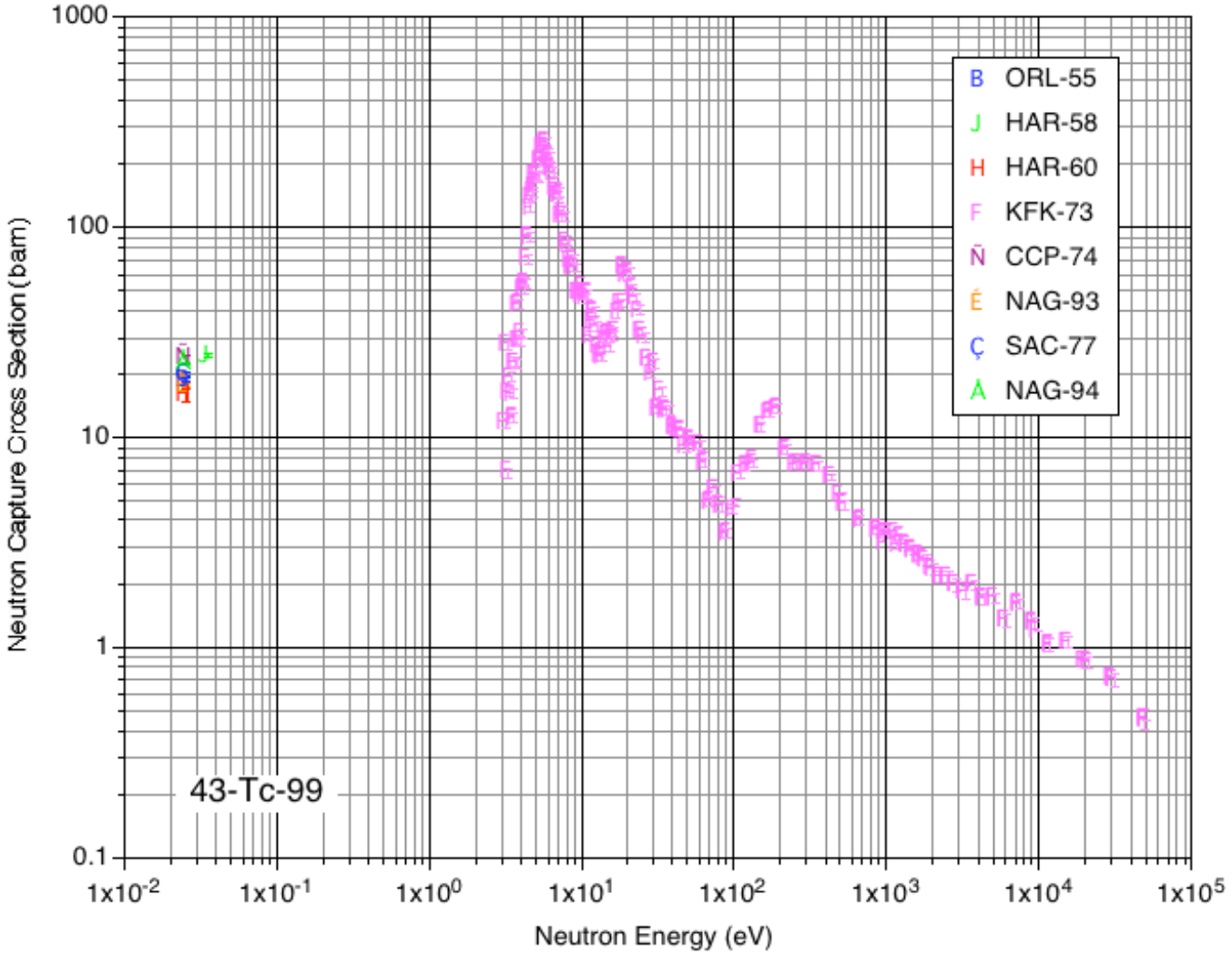
Status of Nuclear Data: Th-U Cycle



Status of Nuclear Data: Th-U Cycle



Status of Nuclear Data: LLFP



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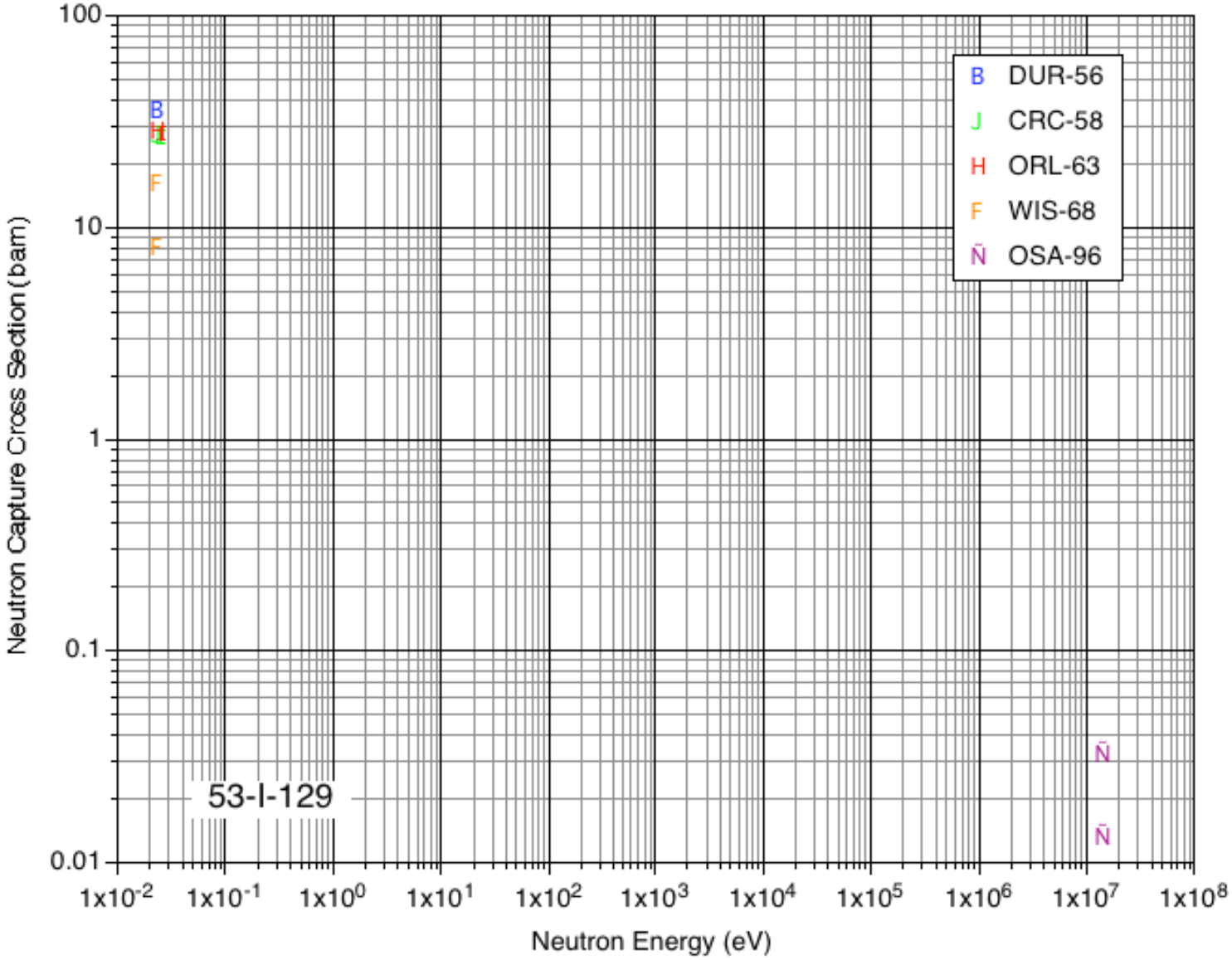

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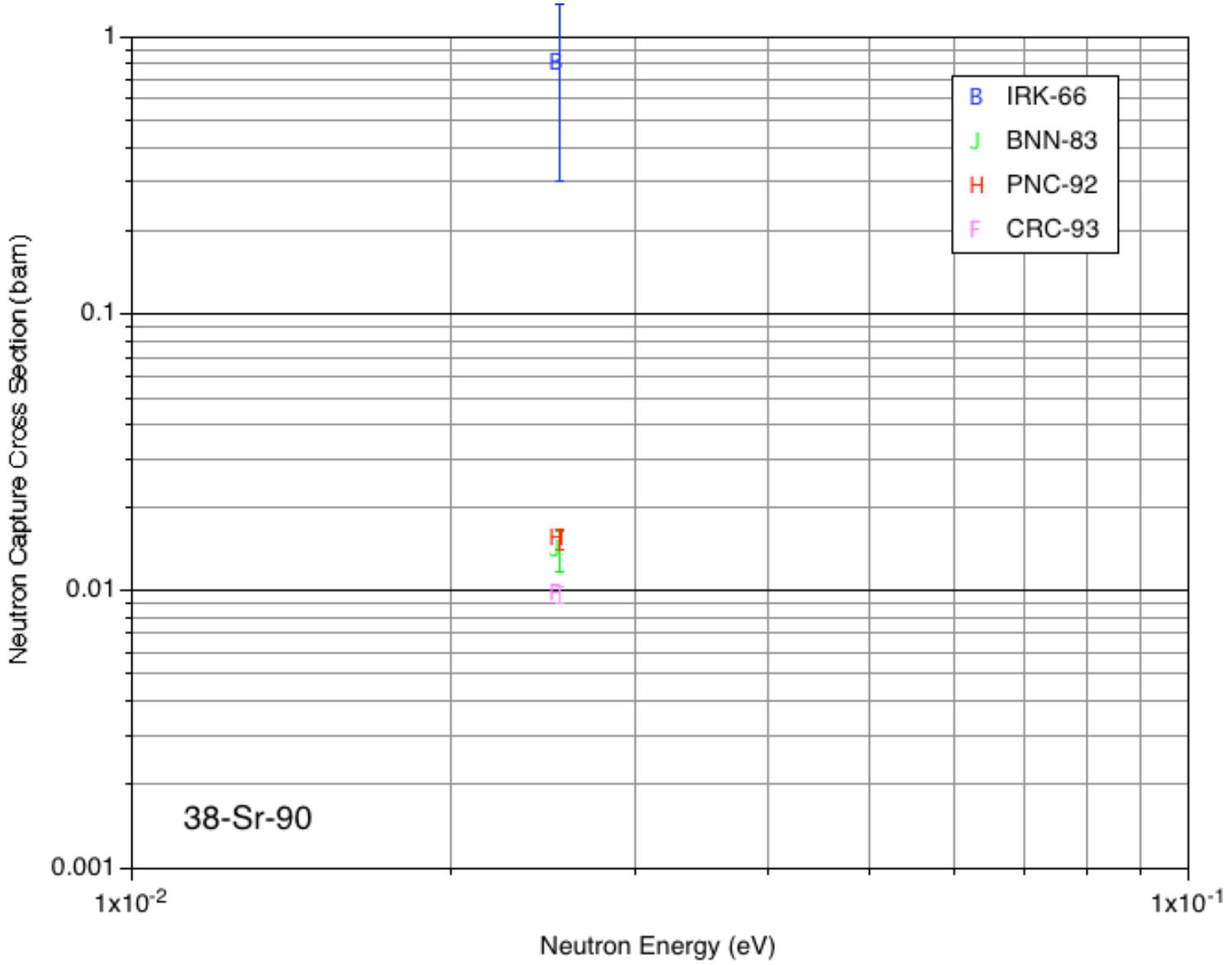

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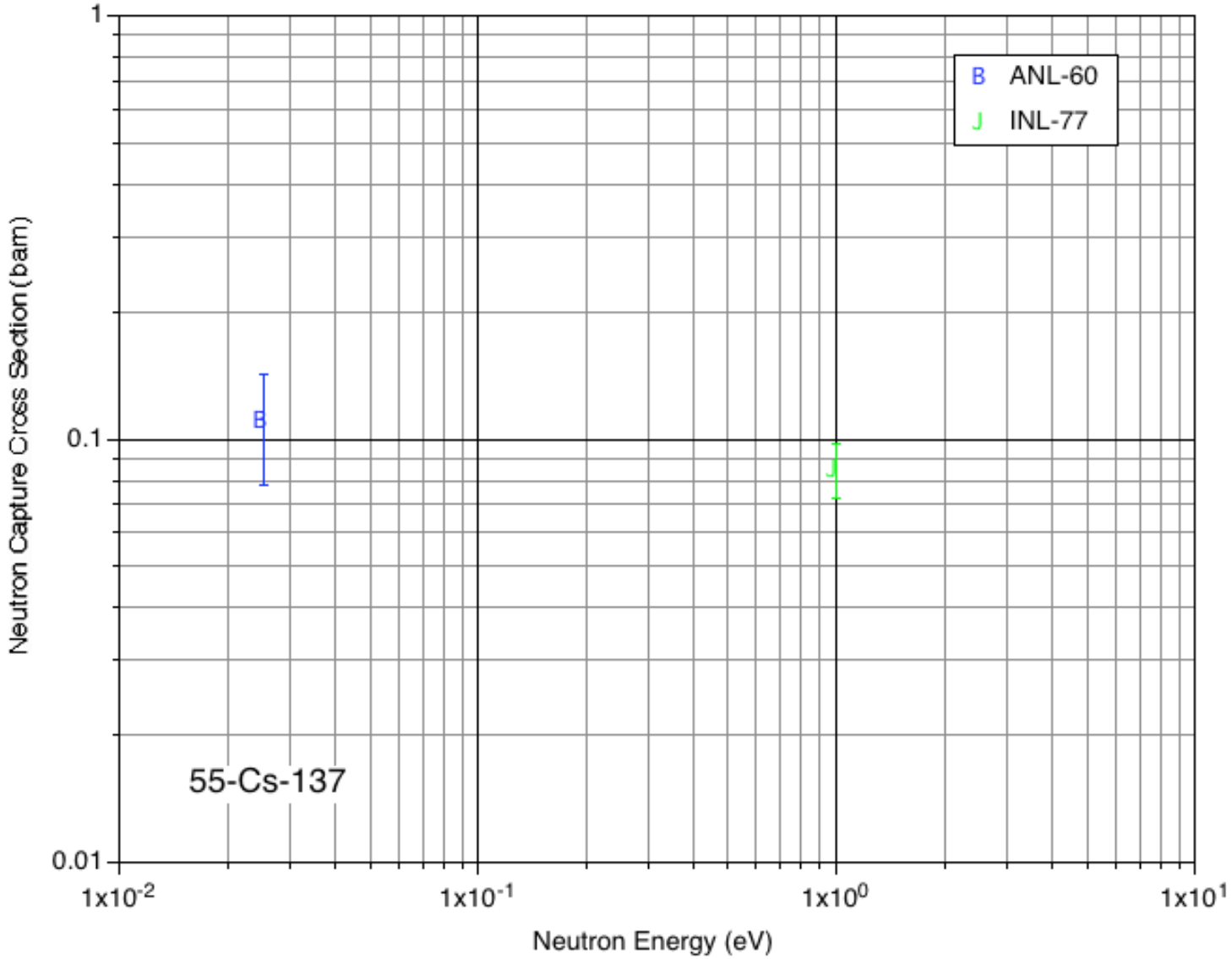

Conclusions

- The Designers would appreciate having a recommended XS-Library for:
  - ADS core design (fast core, driven by high energy spallation source); deterministic for engineering first approach calculation
  - ADS core Design for Monte-Carlo multi-group as well as continuous energy libraries below 150 MeV
  - ADS Shielding problems also Multi-group (deterministic and MC) and continuous energy ones (MC)
  - Burn-up treatment recommendations
  - Fuel Cycle analysis Nuclear data & codes

LECTURES OUTLINE

- ✓ LECTURE 1: Physics of Spallation and Sub-critical Cores, Fundamentals
  (Monday 17/10/05, 16:00 – 17:30)
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Nuclear Data & Methods for ADS Design II : EA-MC Code Package

Y. Kadi
CERN, Switzerland

18 October 2005, ICTP, Trieste, Italy

I – THE EA-MC MONTECARLO CODE PACKAGE

- Structure of the program
- Neutron transport & time evolution
- Limitations in the methodology
- Geometry Modelling
- 2D vs 3D
- Parallelisation

The EA-MC Code Package

- The EA-MC * code package is an innovative simulation tool developed at CERN by prof. C. Rubbia and his group.
- It describes the sequence of phenomena ranging from high-energy particle induced cascade in high-Z materials, producing neutrons that subsequently interact until they are absorbed or escape.
- It allows the study of complex systems such as:
  - Accelerator-Driven SubCritical Fission Devices for energy production and/or transmutation of nuclear waste
  - Accelerator-Driven Devices for the production of radioisotopes (medical applications, etc.)
  - Intense Spallation Neutron Sources (fundamental research)
  - Next generation of Nuclear Engines for space propulsion
  - Critical Fission Devices for nuclear power generation

* Energy Amplifier Monte Carlo

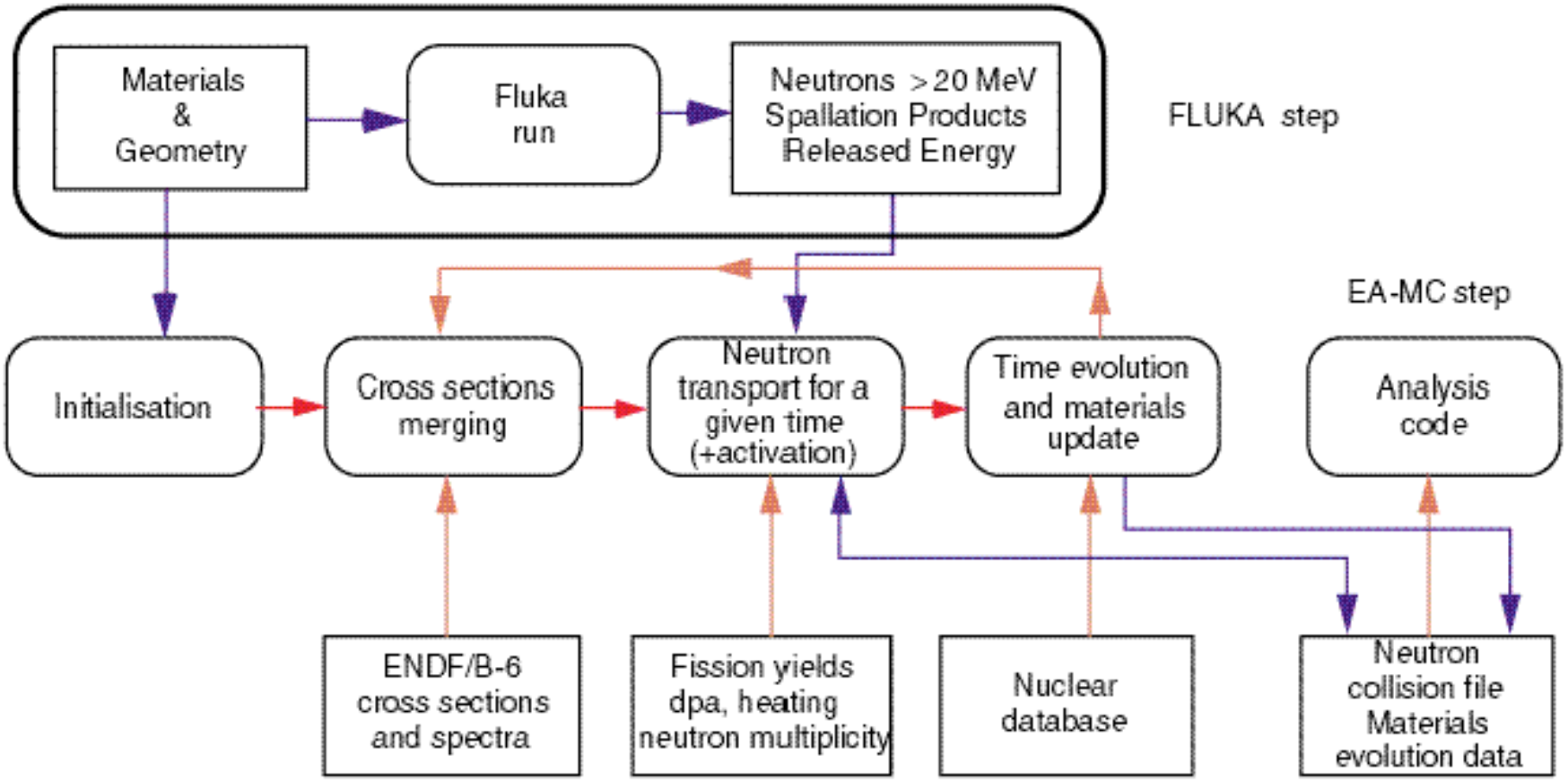
The EA-MC Code Package

The design of accelerator-driven fission devices (also called hybrid systems) requires powerful simulation tools for :

- ⇨ The modeling of the high-energy cascade and of the neutron production;
- ⇨ The transport of the low energy (E ≤ 20MeV) neutrons;
- ⇨ The description of the fuel evolution as a result of neutron interactions and nuclear decays;
- ⇨ The nuclear transmutation and activation of the structural materials and coolant due to the presence of a neutron fluence and of the proton beam induced high energy cascade.

Calculation Scheme

General architecture of the EA-MC Monte Carlo simulation of neutron transport and element evolution



Why a Monte Carlo code ?

- Fully analogous MonteCarlo simulations with point-like cross sections provide a host of information not easily available with analytic codes :
  - "Infinite" spatial resolution;
  - Full treatment of resonances;
  - "On-line" full 3D calculation of activation and spectrum-dependent transmutation effects;

- The fine interplay between resonances in a continuously time varying material composition can hardly be reproduced by a multi-group code (in a finite time) :
  - The self-consistent fluence field should be computed and then used to cen dense the cross sections at every burnup step… and so on;

Why a Monte Carlo code ? (2)

- The non-fission multiplicative processes can only be taken fully into account in a Monte Carlo code :
  - In fact they are ignored in many analytical codes, or taken into account by " modifying" the absorption cross section;
- The space-dependent time evolution of the fuel is difficult to describe in an analytical code, unless every region is evolved (with "0D" approximations ?) separately and with a self-consistent fluence :
  - But then all fluences have to be made to converge simultaneously, because the fluence in every region affects any other region and so on…;
- Compared to these problems the infamous $1/\sqrt{N}$ precision problem of the Monte Carlo is a small worry:

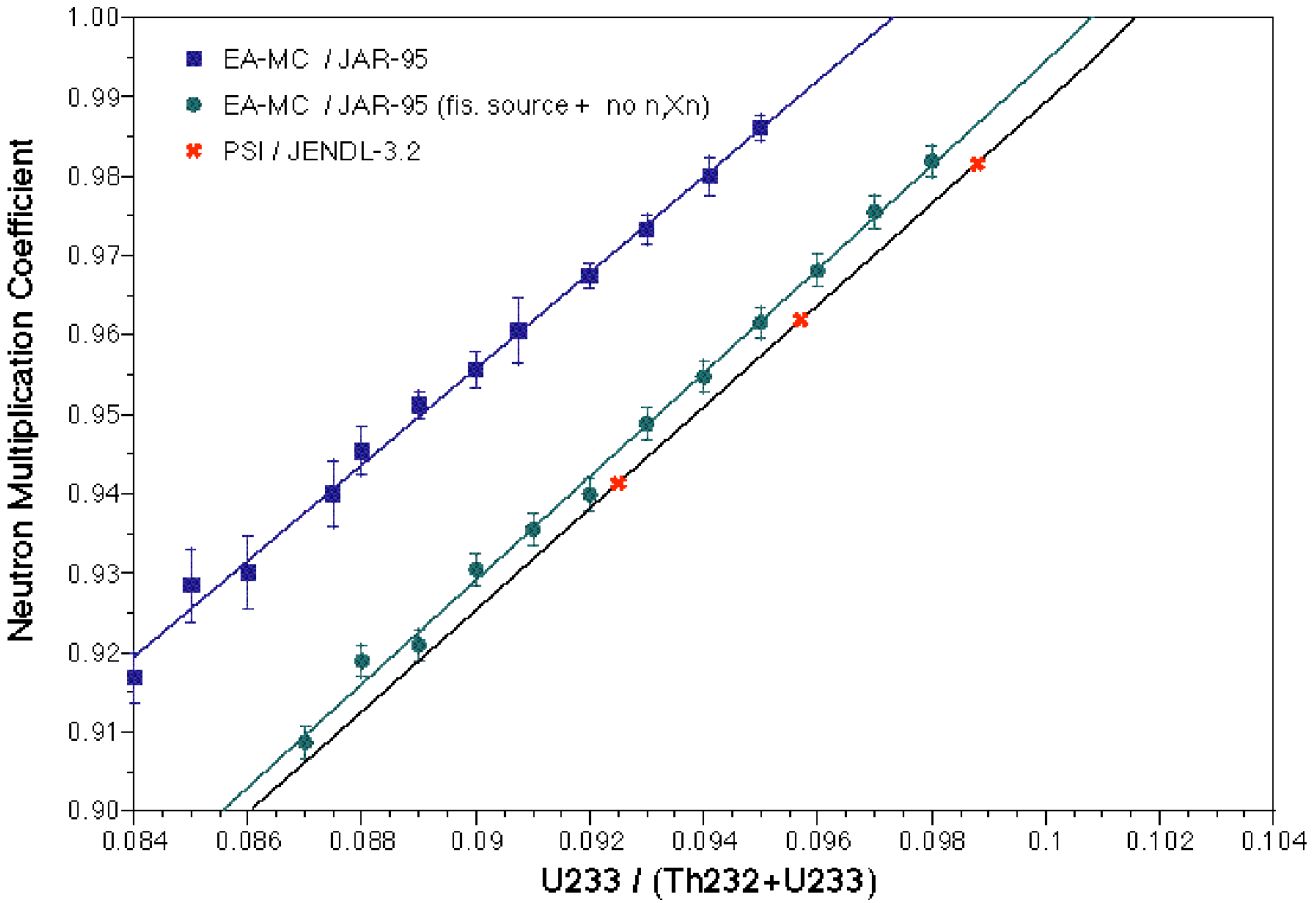
Why a Monte Carlo code ? (3)

- The approximations in an analytical code can be large :
  - Analytical codes are not suited to "explore" new problem domains where the effects of the approximations made in the treatment of cross sections is unknown;
  - The "convergence" of the differential equations gives the distance only to the mathematical solution, not to the physics reality;
  - Does it make sense at all to study the behaviour of a sub0critical system with the fundamental eigenfunction of the fluence, when we know that this is not its working mode ?
- Probably a correctly applied analytical model would not provide a time-to-solution shorter than a well implemented Monte Carlo
- The main limitations of the Monte Carlo method are :
  - The correctness of the cross sections, but this is common to all transport codes;
  - The physical model used, but for low energy neutron transport this is mainly expressed by the data;
  - The "statistics", and for this the Monte Carlo has to be written with "finesse" and then "brutally" handed over to the most power computer at hand.

Limitations in L-E Neutron Transport : Methodology (2)

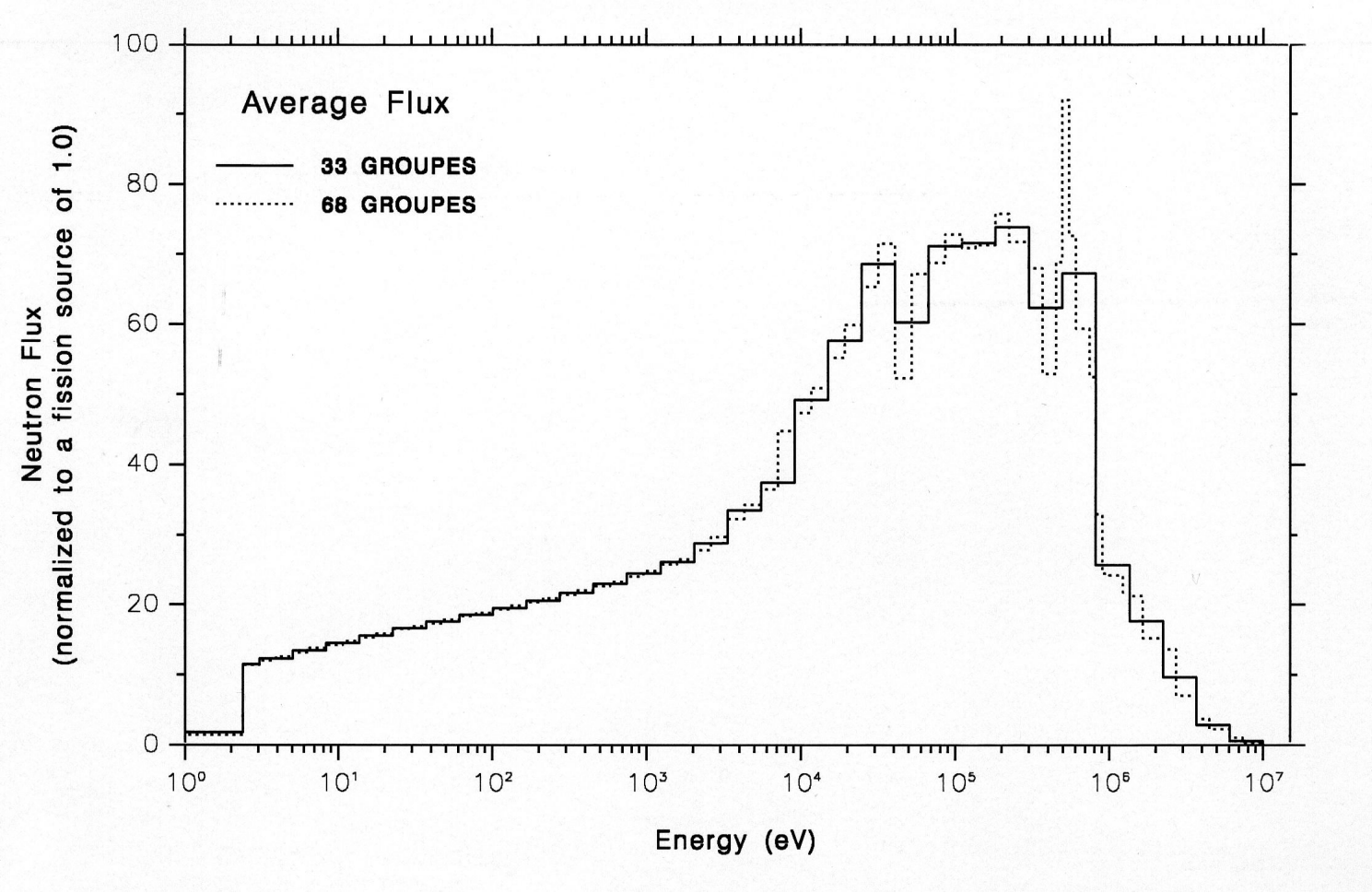
Comparison of the variation of k_{src} and k_{eff} as a function of the concentration of ^{233}U between EA Monte Carlo and PSI deterministic calculations

- ✓ Deterministic codes calculate k_{eff} via an eigenvalue search of the multi-group equation system.
- ✓ These codes often ignore in their scattering matrix non-fission multiplicative processes such as *(n, Xn)*, which are of great importance for lead cooled fast reactors.
- ✓ The large *(n, 2n)* cross section of thorium and lead increases the importance of this process for the EA, making the results obtained with deterministic codes even more unrealistic.
- ✓ Implementing in the EA Monte Carlo code the same assumptions used by standard deterministic codes enables us to reproduce their results.



Limitations in L-E Neutron Transport : Methodology (3)

Dependence of the neutron flux spectra on the number of energy groups used in calculations with TWODANT deterministic code



The EA-MC Code Package : *Other Codes*

- In spite of the fact that we have developed our own Monte Carlo code, we have installed and used some of the most important codes available :
  - Cross section treatment : NJOY-94 and PREPRO-2000;
  - Cell calculation code : TRANSX-2.9;
  - 2D analytical transport : TWODANT;
  - Monte Carlo calculations : MCNP-4A,B,C, FLUKA-2000 and HETC
  - Burnup calculations : ORIGEN and 2DB
  - Sensitivity studies : SUSD
- In particular we have made extensive comparisons between TWODANT and our code (EA-MC)

The Physics — EA-MC (1)

- The EA-MC Monte Carlo code follows all n eutrons generated in the cascade initiated by each "spallation neutrons" produced by the high-energy transport code FLUKA :
  - Neutron transport is done in time steps which vary adaptively according to the burnup phase;
  - Material evolution is performed between transport steps. The material composition is updated according to the neutron interactions simulated in every material zone;
  - High-energy spallation products coming from FLUKA are added to the material composition on a proton by proton basis;
  - The contribution of all fission, spallation, decay and activation products is considered explicitly during neutron transport;
  - Point cross sections for 35 reaction channels, provided by a rather complete and extensively checked library (combining data from the most authoritative available sources: ENDF/B-VI, JENDL-3.2, JEF-2.2, EAF-4.2 and BROND-2) are used.
- The cross sections are used directly as they come from the pre-processing codes, without any approximation : in some cases, [Th(ng)], the cross section for a single reaction channel can contain more than 60,000 points

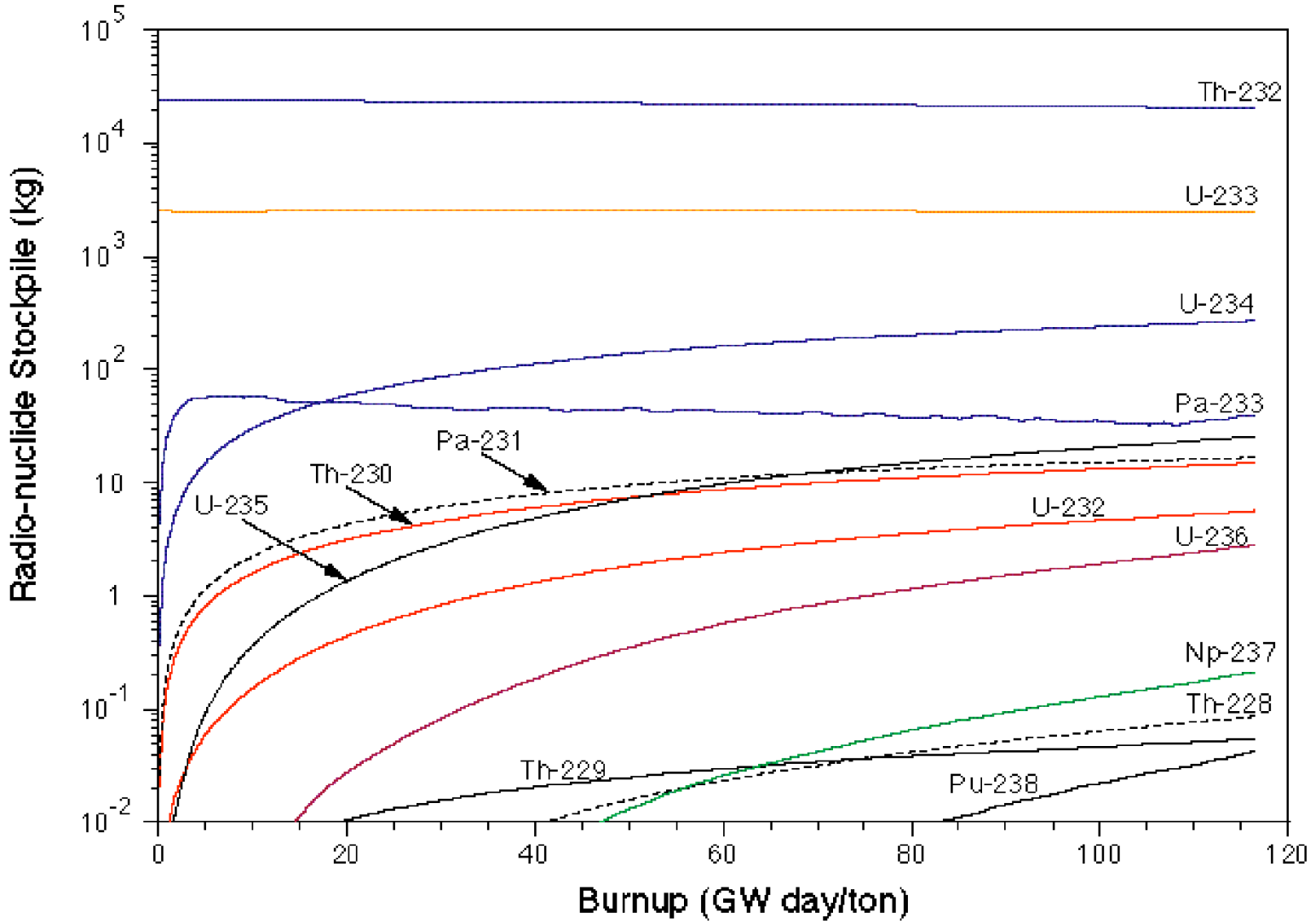
The Physics — EA-MC (2)

- The choice of the reactions has been highly optimised :
  - A clever algorithm allows a fast evaluation of the next interaction point, independently from the number of elements in the material;
  - Once the interaction point has been determined, a carefull dynamic allocation of the internal pointers allows an extremely fast sampling of the target nuclide and the reaction channel ≈ 10 μs/sampling;
  - All samplings of energy or angle of produced neutrons are done from tables, with one random number extraction;
  - The routine for elastic scattering has benn particularly well tuned, and it can perform a scattering with thermal motion of the target nucleus in few μs;
- At the end of every transport step all materials are evolved during a certain time step :
  - The underlying assumption is that the material composition changes very little during the time step;
  - As the gradient of change depends on the burnup phase, the time step changes during burnup;

Burnup capability

- To avoid all approximations in the concentration evolution, a complete solution to the Bateman equations involving thousands of elements is computed :
  - A combination of storage techniques and decay chain algorithms allows to evolve all materials in few seconds;
  - No time stepping is used, the solution is analytically correct within the assumptions made;
- D ifferent smoothing techniques have been developed in case of very short lived elements or strong concentration gradients :
  - The algorithm has been checked for stability against different time steps;

Burnup capability

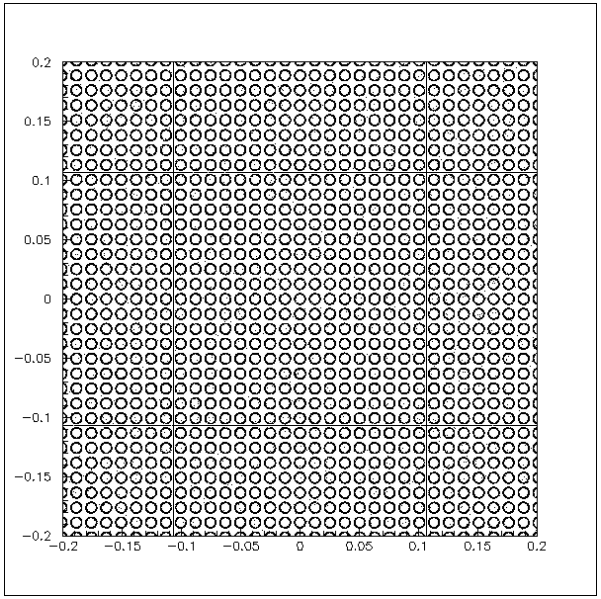


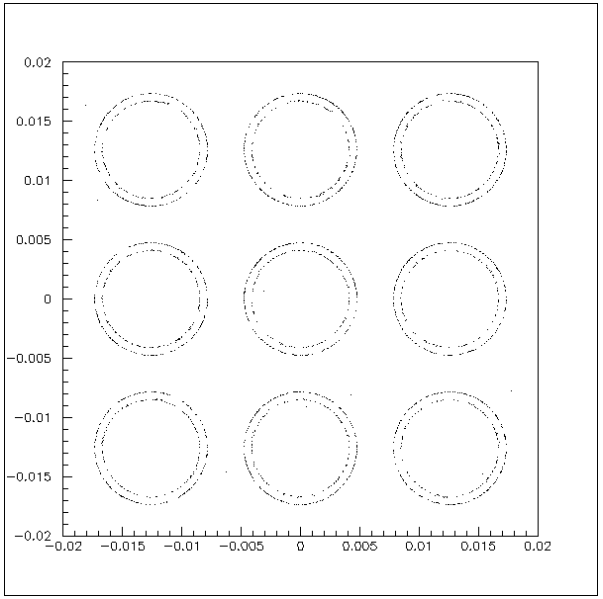
Geometry (1)

- No Monte Carlo is more precise than its geometry !
- The material regions in the system are described using simple geometry techniques which construct the material zones by the combination of simple geometric bodies :
  - The geometry allows for the separate specification of individual components of the geometry model (known as parts);
  - The parts can be included as a single item within other parts to form new parts;
  - the user can build an EA-MC geometry model as it is done in reality by assembling individual components to form larger components, which eventually form the completed system;
  - This allows a very accurate model of the system to be created;
- A lot of effort has been devoted to develop, test and optimise geometrical models for the EA :
  - Different libraries of geometry routines with a typical execution time of 5 – 10 us per call for the different configurations of the EA;
  - Specially optimised algorithms for square/ hexagonal lattice geometry;
  - Translation routines to CAD and ray tracing systems and to FLUKA geometry;

Geometry (2)

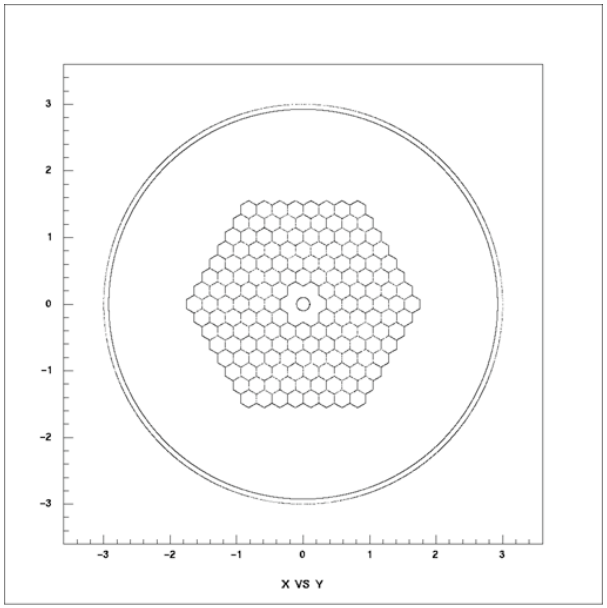
The following pictures are examples of boundary detection by the geometrical routines in the case of a PWR detailed representation (fuel sub-assemblies and fuel pins arranged in a square lattice).

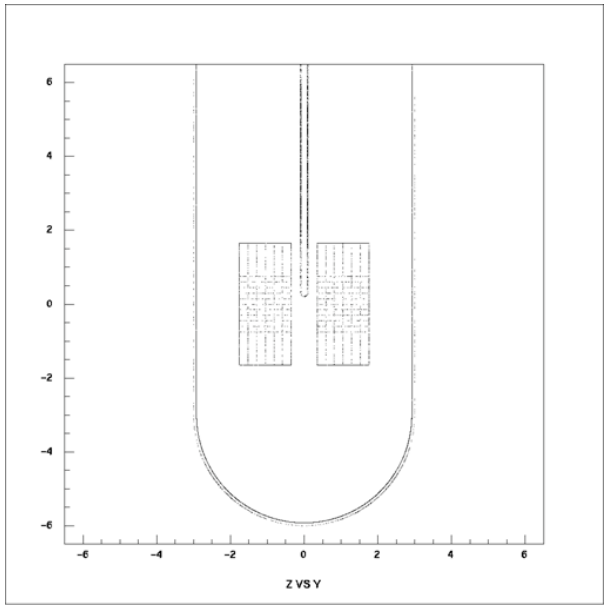




Geometry (3)

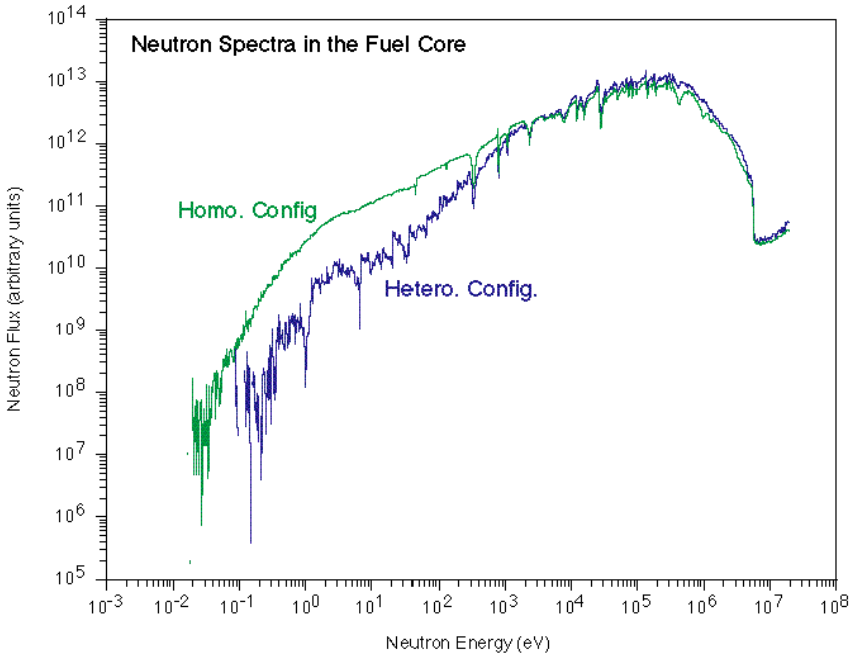
The following pictures are examples of boundary detection by the geometrical routines in the case of the Energy Amplifier (reactor vessel internal boundaries and hexagonal sub-assemblies arranged in an hexagonal lattice).

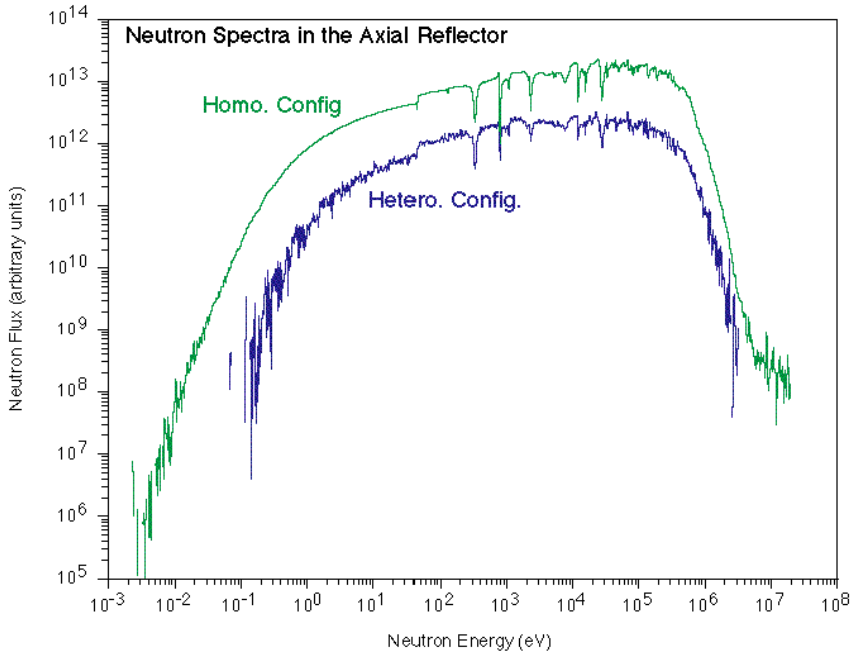




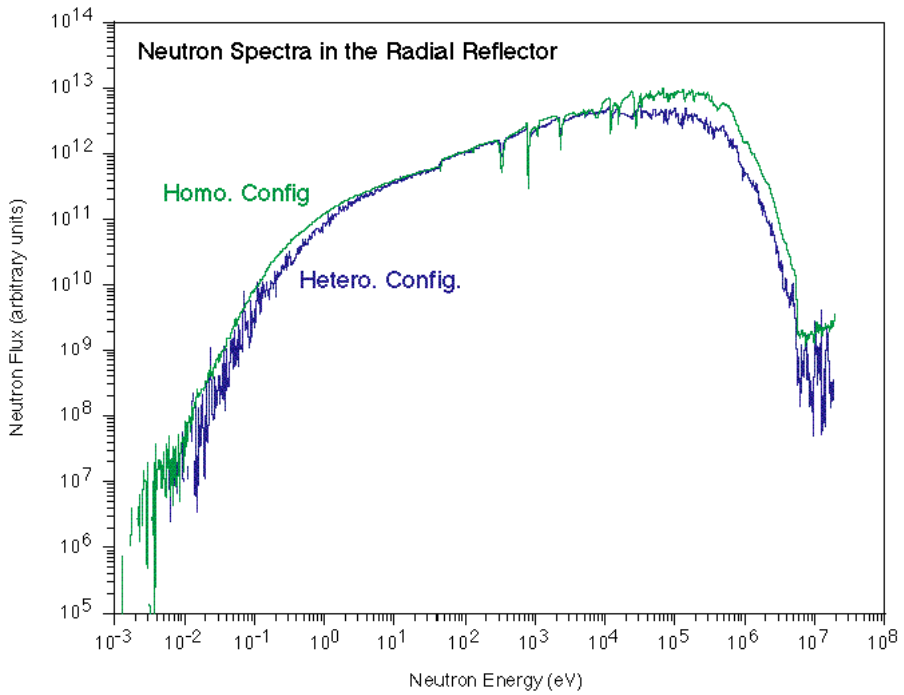
Limitations in L-E Neutron Transport : 2D vs 3D (1)

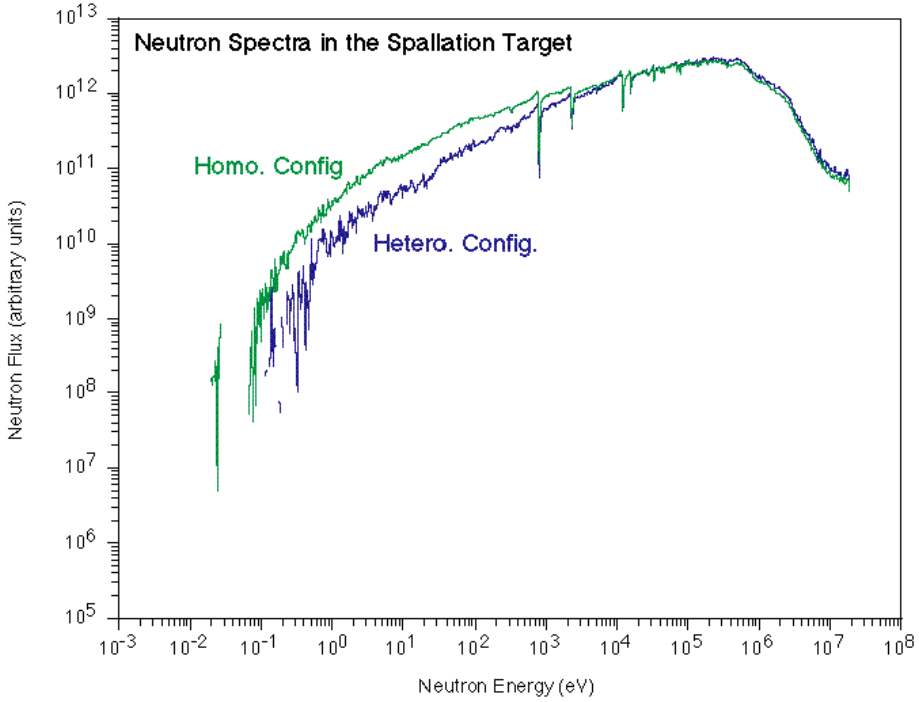
✓ the spatial resolution is limited, as space is digitized by a grid. Most of these codes are bi-dimensional, while the few available three-dimensional codes usually require a large amount of computing resources, leading to large computation times.





Limitations in L-E Neutron Transport : 2D vs 3D (2)





Limitations in L-E Neutron Transport : 2D vs 3D (3)

EAP80 reference configuration: Effect of core homogenisation

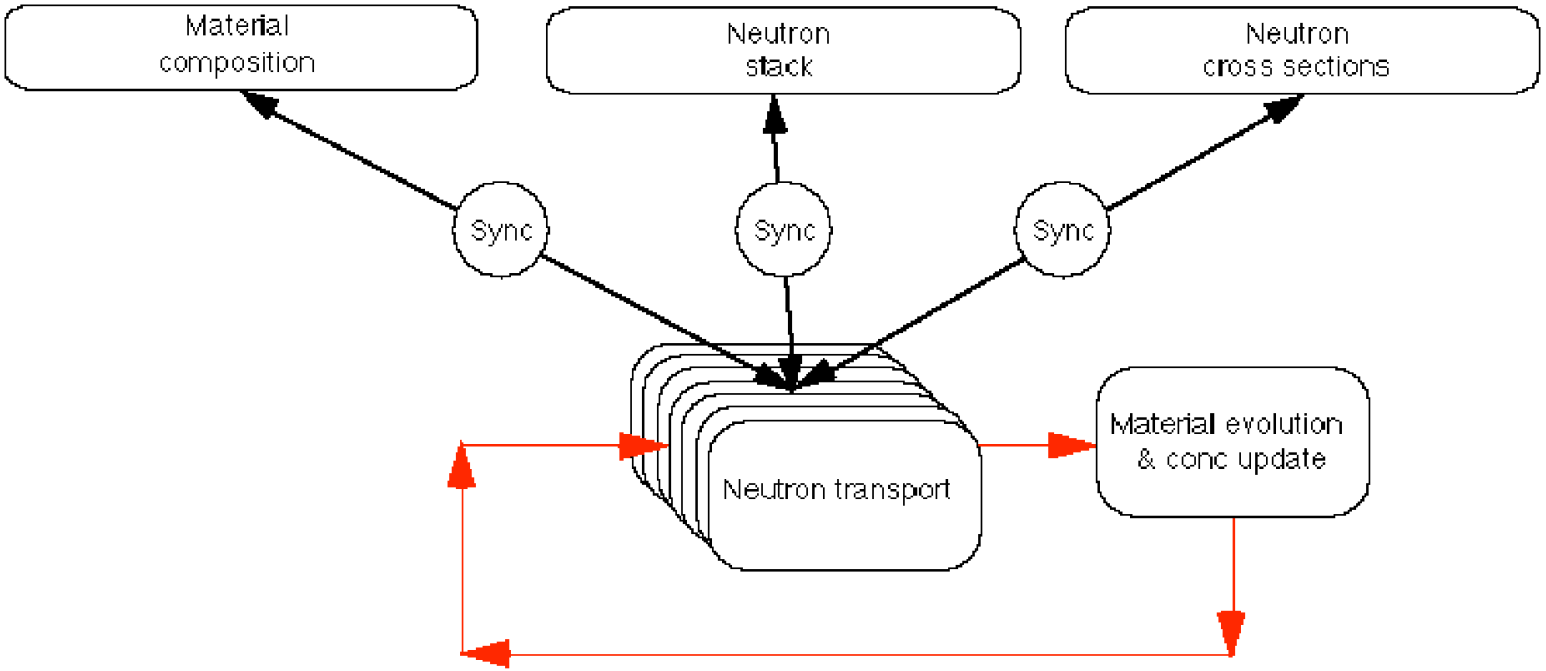
lobalParameters	Hetero.Config.	Homo. Config.	Units
Initial fuelmixture	(U-Pu)O_2	(U-Pu)O_2	
Initial fuelmass	3.804	3.804	ton
Initial Pu concentration	18.1	18.1	wt.%
Initial Fissileenrichment	18.6	18.6	wt.%
ThermalPower Output	80	80	MWatt
ProtonBeamEnergy	600	600	MeV
SpallationNeutron Yield	13.5 ± 0.1	13.6 ± 0.1	
Neutron multiplication	17.49 ± 0.48	20.67 ± 0.61	
MultiplicationCoefficient	0.9428 ± 0.00	0.9516 ± 0.0014	
EnergeticGain	24.7 ± 0.7	29.5 ± 0.9	
Gain coefficient	1.4	1.4	
AcceleratorCurrent	5.63 ± 0.17	4.69 ± 0.14	

==> $\Delta k/k \approx + 0.94\%$

Parallel Computing (1)

- One of the main problems of Monte Carlo codes is the control of the statistical fluctuations intrinsic to the sampling method
- The usual method is to run several Monte Carlo and to evaluate the dispersion and the average of the results
- In the EA-MC code several copies of the program are run in parallel and each one writes its own summary file
- A separate program (also parallel) can be run to merge all the files and estimate the associated statistical error
- Two parallel versions of the code were developed based on :
  - "Shared Memory" approach;
  - "Distributed Memory" approach;

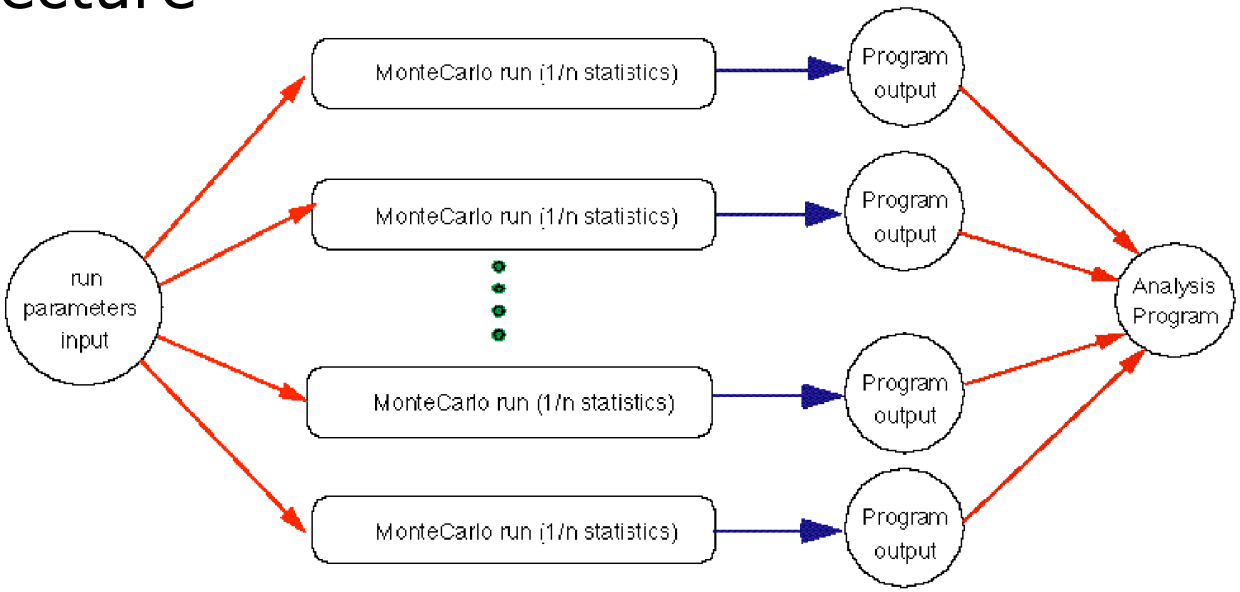
Shared memory parallel Monte Carlo architecture of the EA-MC code.



- Several processors share part of the storage and the access to the shared resources is synchronised
- This version showed a substantial performance improvement, but its performance did not behave linearly with the number of processors, hindering the full exploitation of the power of our machine

Parallel Computing (3)

Distributed memory in the parallel EA Monte Carlo architecture



- As there are no synchronisation points apart from the initial broadcast of the starting conditions, the performance is not degraded by the number of processors used
- We have run with a CERN system of 1 up to 64 processors in parallel where we observed a linear increase of the performance with the number of processors
- The implementation is portable and we have successfully installed and tested the program on several parallel platforms

Analysis Programs

- The decoupling of the production from the analysis allows the use of different offline routines for :
  - Fuel Reprocessing and Cool-Down;
  - Activity and Toxicity calculations;
  - Evolution of the global neutronic characteristics with burnup : neutron multiplication factor, acceler ator current, thermal power, neutron flux, reaction rates , material composition and stockpiles, etc…
  - Calculation of neutron flux spectra and derived one group cross sections;
  - Online monitoring of the main parameters;
  - Online modifications of the conditions of the run;

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Exercises OUTLINE

Exercise I: Generation of Neutron Induced Cross Sections from Standard Evaluated Nuclear Data Libraries using the PREPRO-2000 processing Code (Incl.: Description of process utility).

Exercise II: Simulation and Analyses of the Spallation Process using the FLUKA-2005 Particle Transport Code (Incl.:

- Standard FLUKA input file: Al_01.
- FLUKA geometry view file: Al_01.geo.
- Quick guide for processing FLUKA output files: how to fluka exercise).