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PCA benchmark analysis using the ADVANTG3.0.1/MCNP6.1.1b codes

Mario Matijević
University of Zagreb, Faculty of Electrical Engineering and Computing, Department of Applied Physics
Unska 3, 10000 Zagreb, Croatia

mario.matijevic@fer.hr

Contents:

1. PCA benchmark definition

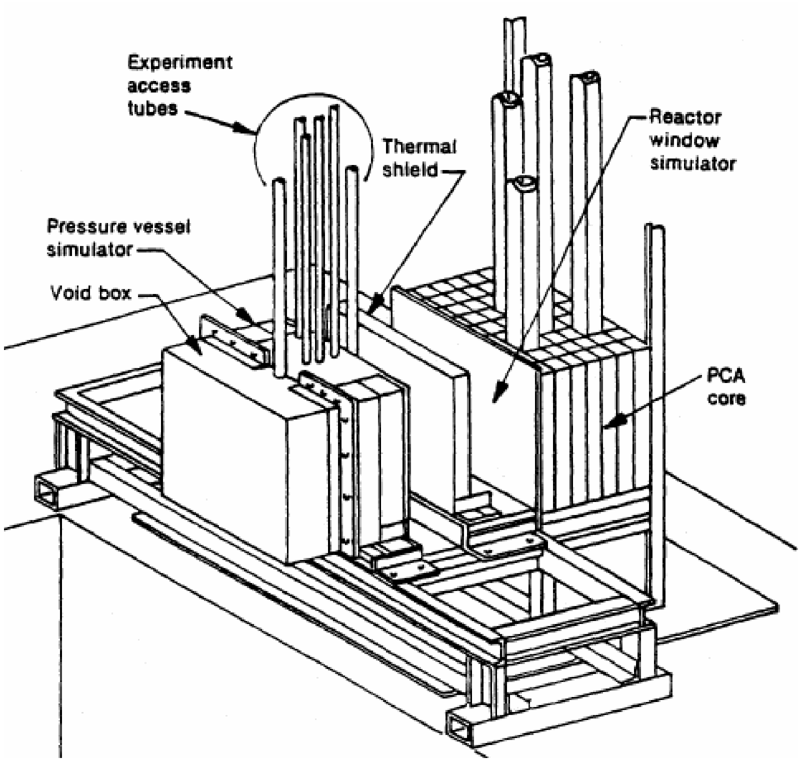
- **Pool Critical Assembly Pressure Vessel (PCA) benchmark**
  - A well known benchmark from the SINBAD database
  - Based on the PCA facility experiments at the ORNL
  - A small pool-type highly enriched experimental reactor
  - Measured and calculated (DORT) equivalent fission fluxes
  - Validation of transport theory codes and XS libraries
  - Prediction of the in-vessel neutron flux gradients

- **Scope of the PCA benchmark**
  - Validation of the methodology to predict the reaction rates in ex-core region
  - Qualification of the pressure vessel fluence calculation methodology
  - Simulation of the neutron flux gradient inside carbon steel (RPV)
  - RPV surveillance programs of existing USA NPPs (RPV damage)
  - Measured RR inside RPV (A4, A5, A6) and water gap in-front (A3, A2)
  - Well defined neutron source, materials, and simple geometry
  - DORT libraries in the PCA benchmark: BUGLE-93, SAILOR-95, BUGLE-96
  - Computational requirements by the U.S. NRC Regulatory Guide 1.190

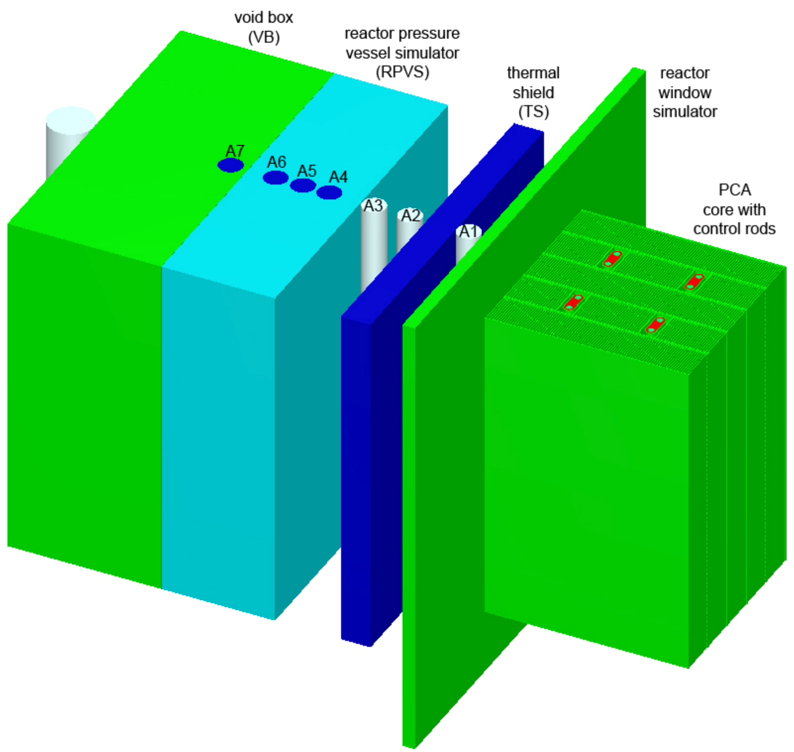
2. PCA benchmark description

❑ PCA benchmark "12/13" configuration

- PCA core with components mock up the core-to-cavity region in PWRs
- Al plate, Thermal shield (TS), pressure vessel simulator (PVS), void box (VB)
- Water gap between Al plate and TS: 12 cm
- Water gap between TS and RPVS: 13 cm
- PCA facility is immersed in a large pool of water (coolant and moderator)
- PCA core has 25 material test reactor (MTR) plate-type elements (e=93%)



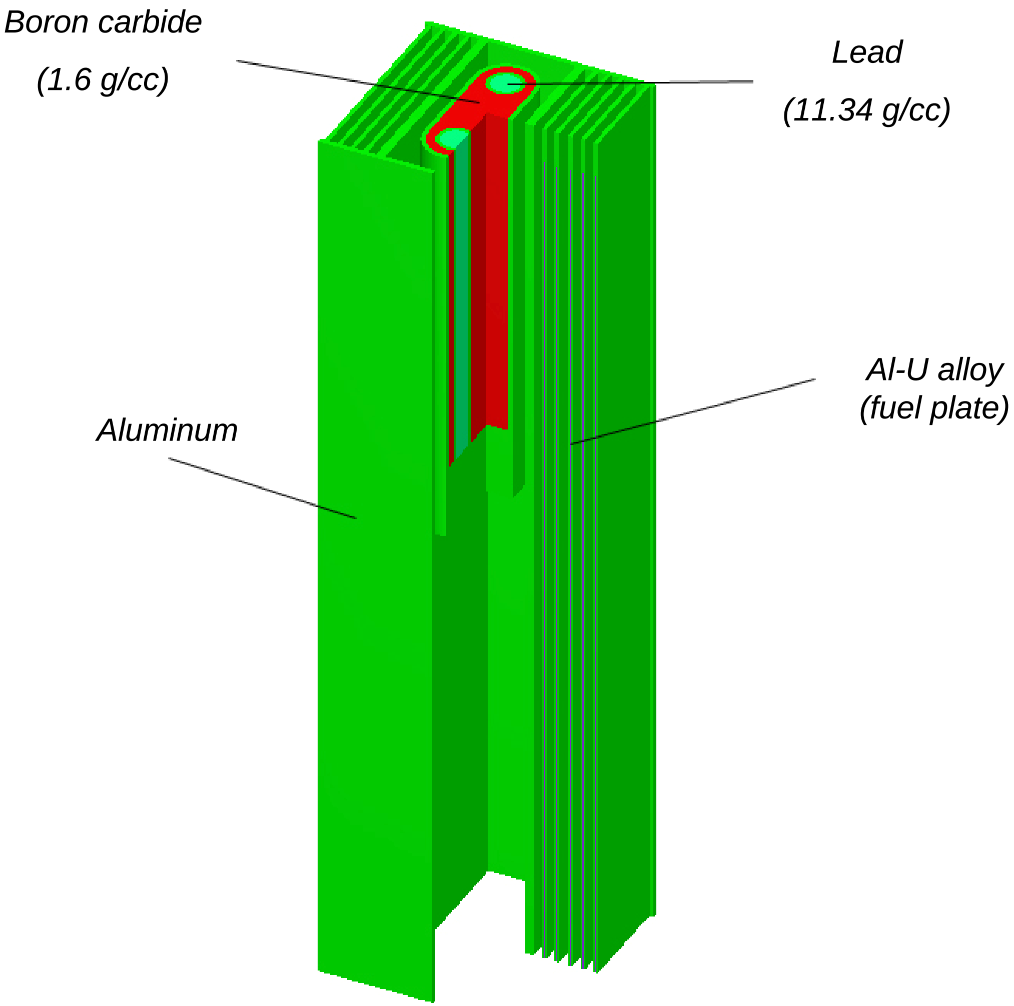
PCA pressure vessel wall benchmark facility



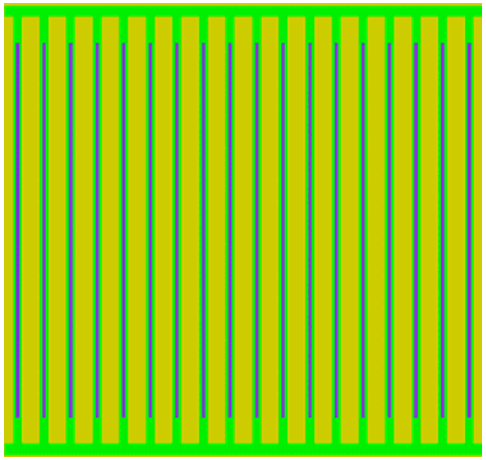
MC model of PCA benchmark facility (water removed)

2. PCA benchmark description

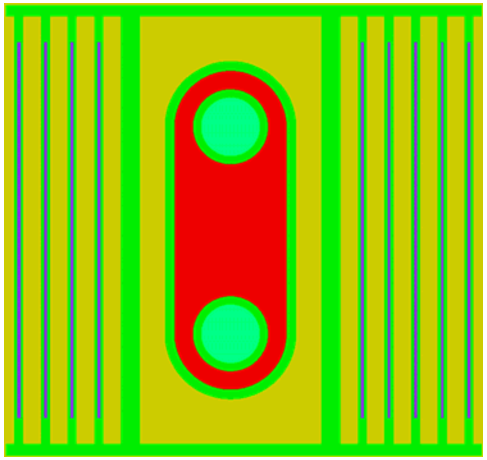
❑ PCA benchmark “12/13” configuration



Cross sectional view through the control element



PCA standard MTR fuel element (water included)



PCA control rod (water included)

2. PCA benchmark description

❑ PCA benchmark "12/13" configuration

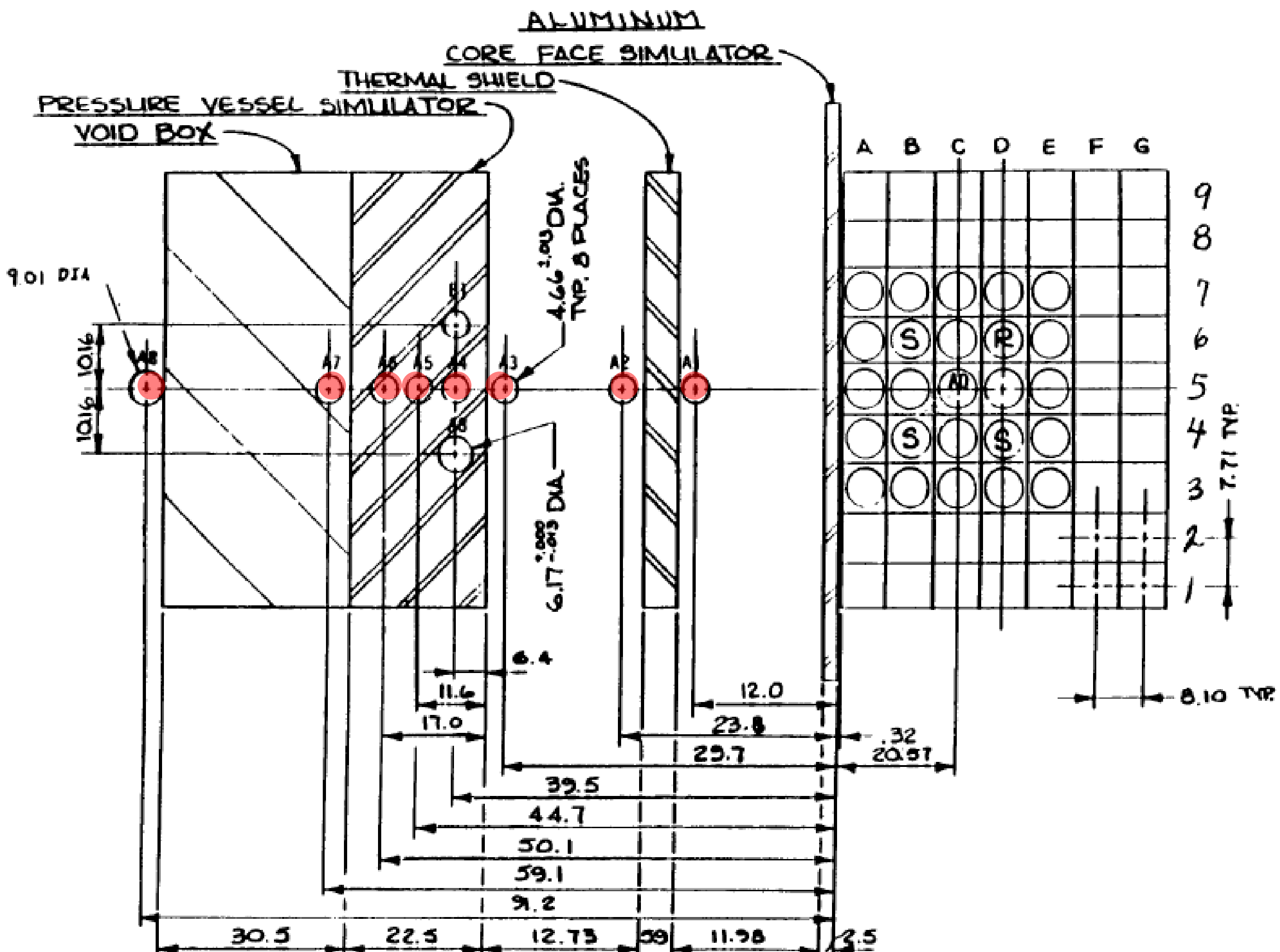


Fig. 1.2 Horizontal cross section of the PCA pressure vessel benchmark facility 12/13 configuration
(dimensions are in cm)

2. PCA benchmark description

❑ PCA benchmark "12/13" configuration

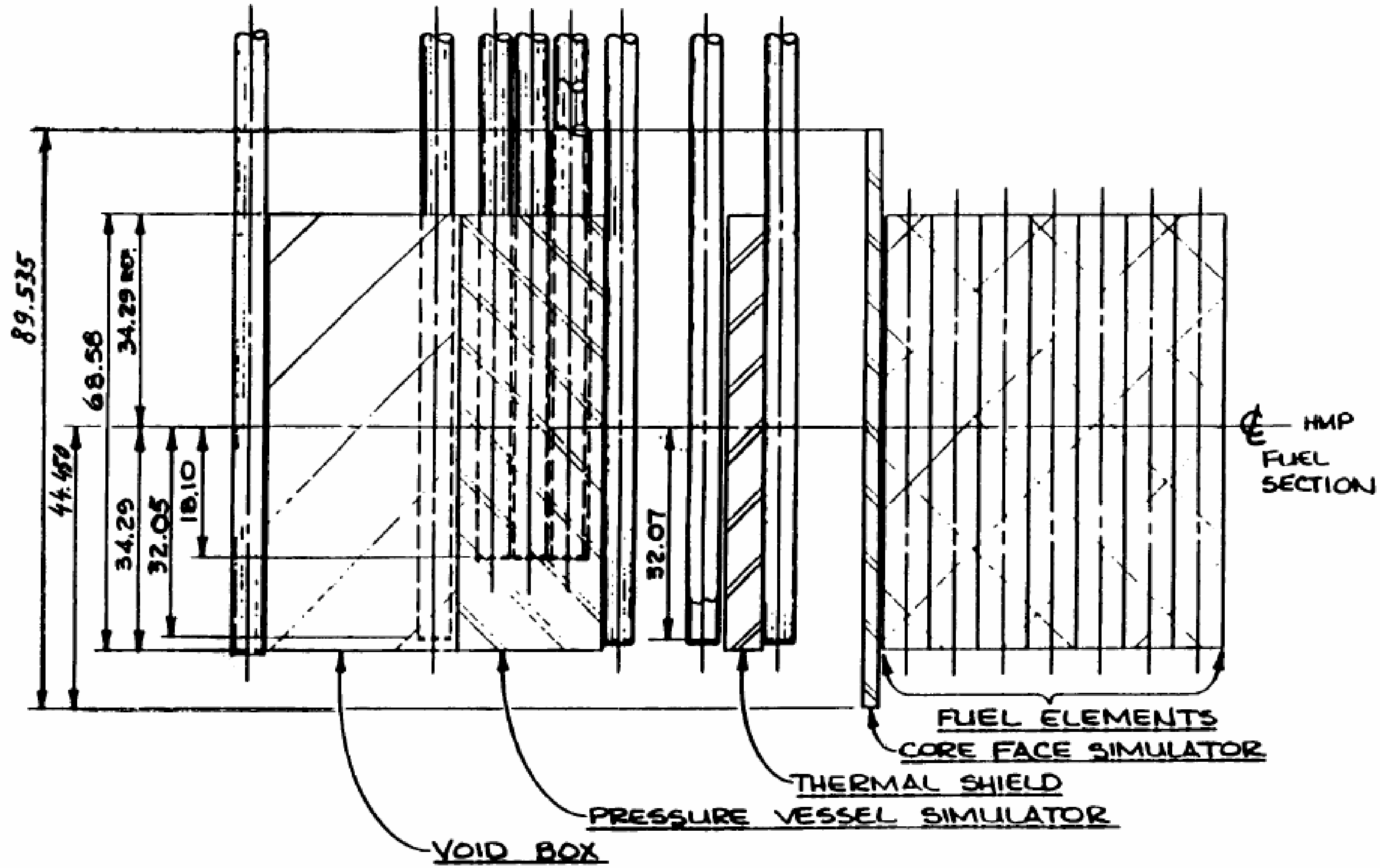


Fig. 1.3 Vertical cross section of the PCA pressure vessel benchmark facility (dimensions are in cm)

2. PCA benchmark description

❑ Experimental measurements: A1 – A7

Table 1.6 Experimental results for fission chamber and radiometric measurements of equivalent fission fluxes

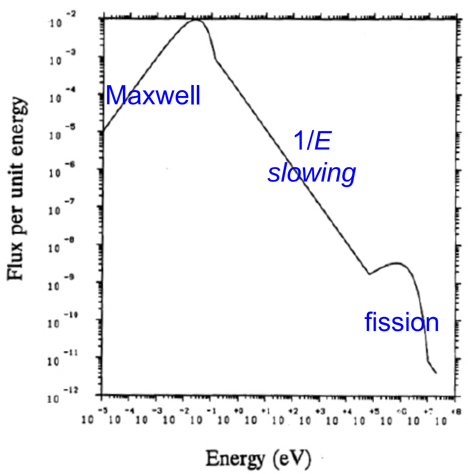
Location	Distance* (cm)	Equivalent fission fluxes** [per 1 PCA core fission neutron per second (cm⁻²)] ^{237}Np	^{238}U	^{103}Rh	^{115}In	^{58}Ni	^{27}Al
A1	12.0	6.64 E-6 ± 6.2%	-	5.54 E-6 ± 1.0%	5.61 E-6 ± 1.0%	5.83 E-6 ± 1.4%	7.87 E-6 ± 1.0%
A2	23.8	-	-	-	6.06 E-7 ± 2.0%	6.18 E-7 ± 2.0%	1.02 E-6 ± 2.0%
A3	29.7	2.27 E-7 ± 6.3%	-	-	1.99 E-7 ± 1.0%	2.31 E-7 ± 1.4%	4.48 E-7 ± 1.0%
A4	39.5	9.27 E-8 ± 5.5%	6.11 E-8 ± 6.9%	7.74 E-8 ± 1.5%	5.87 E-8 ± 0.7%	5.30 E-8 ± 1.0%	1.02 E-7 ± 2.0%
A5	44.7	5.18 E-8 ± 5.7%	2.74 E-8 ± 6.8%	4.35 E-8 ± 5.0%	2.76 E-8 ± 1.5%	2.09 E-8 ± 1.8%	4.10 E-8 ± 2.2%
A6	50.1	2.70 E-8 ± 5.8%	1.12 E-8 ± 7.1%	2.19 E-8 ± 5.0%	1.17 E-8 ± 3.0%	7.43 E-9 ± 2.2%	1.54 E-8 ± 2.2%
A7	59.1	7.25 E-9 ± 9.2%	-	-	-	-	-
Reaction cross sections, averaged over ^{235}U fission spectrum *** (mb)							
		1312 ± 50	305 ± 9	733 ± 38	189 ± 8	109 ± 6	0.705 ± 0.040

* Distance to core face of the aluminum window.

Equivalent fission fluxes at detector locations:

$$\phi_{eq} = \frac{\text{reaction rates}}{\bar{\sigma}_i}$$

$$\phi_{eq} = \frac{\int_E \sigma_i(E)\phi(E)dE}{\frac{\int_E \sigma_i(E)\varphi(E)dE}{\int_E \varphi(E)dE}}$$



2. PCA benchmark description

- **Reactions of interest (*shielding calculations*)**
  - $^{237}Np(n,f)^{137}Cs$, $^{238}U(n,f)^{137}Cs$, $^{103}Rh(n,n')^{130m}Rh$, $^{115}In(n,n')^{115m}In$, $^{58}Ni(n,p)^{58}Co$, $^{27}Al(n,\alpha)^{24}Na$
  - Results are given per unit PCA core neutron source (normalized)
  - Calculated-to-measured (C/M) ratios of equivalent ^{235}U fission fluxes
  - Measurements in core midplane (z=0 and y=0) at locations A1 to A7
  - Experimental access tubes: steel in PV and Plexiglas in water locations
  - Minimization of the perturbations of the neutron field
  - DORT reaction rates (/atom/s) are given for dosimeters A1-A8

- **Critical configuration (*eigenvalue calculations*)**
  - Fully inserted control rod reaches bottom of the fuel
  - Withdrawn length is measured from the bottom of the fuel
  - Safety rods (S1, S2 and S3) critical positions: 48.26 cm
  - Regulating rod (RR) position: 38.43 cm
  - Total critical mass of ^{235}U: 3336.01 g

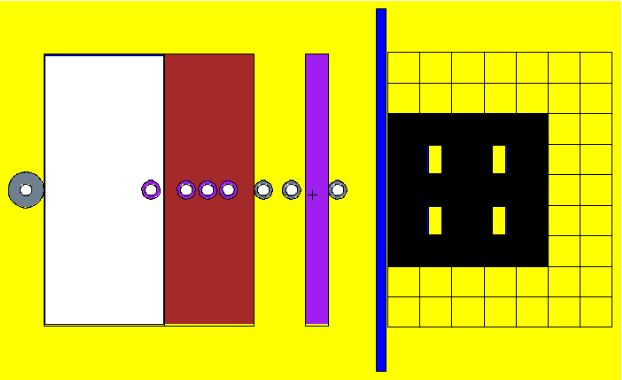
3. ADVANTG3.0.1 / MCNP6.1.1B codes

❑ ADVANTG3.0.1 code (ORNL)

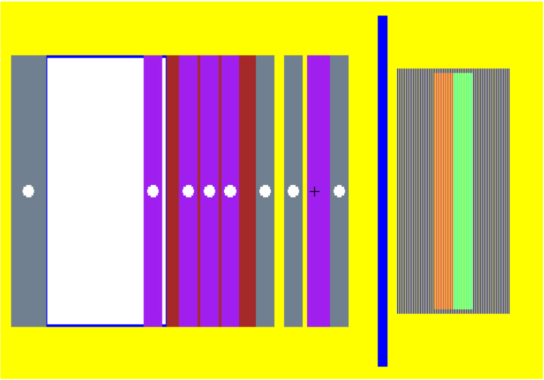
- Automated mesh-based tool for generating VR parameters for MCNP code
- Approximate 3-D multigroup SN forward/adjoint transport solutions
- Denovo SN solver developed at ORNL with CADIS/FW-CADIS formalism
- VR parameters: space-energy weight-windows (WW) and biased source distributions (SB) cards for the MCNP input

❑ MCNP6.1.1b code (LLNL)

- general-purpose Monte Carlo N-Particle code with arbitrary 3D geometry
- neutron, photon, electron, or coupled n/p/e transport
- XS libraries: continuous, discrete, multigroup, S(a,b) law, dosimetry,…
- powerful general source, rich collection of VR techniques, flexible tallies
- Pointwise XS data with MAKXSF for XS libraries with Doppler broadening

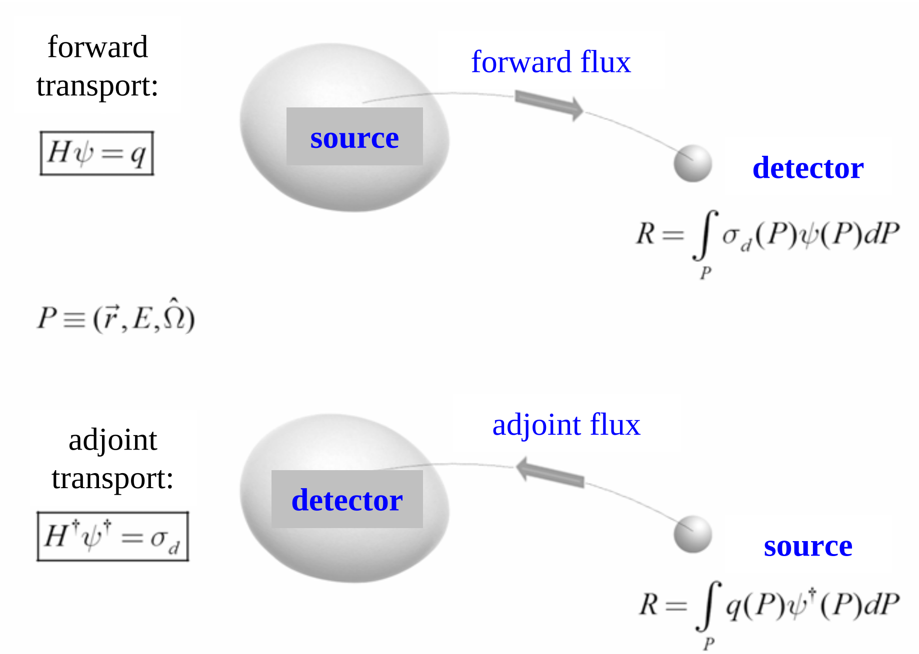


PCA model with MCNP in z=0 cm plane



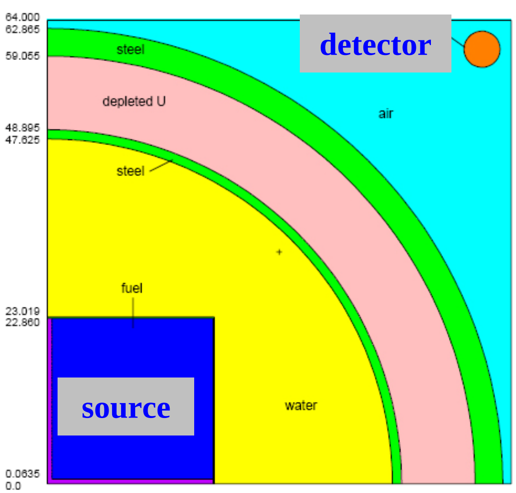
PCA model with MCNP in y=30.84 cm plane

3. ADVANTG3.0.1 / MCNP6.1.1B codes

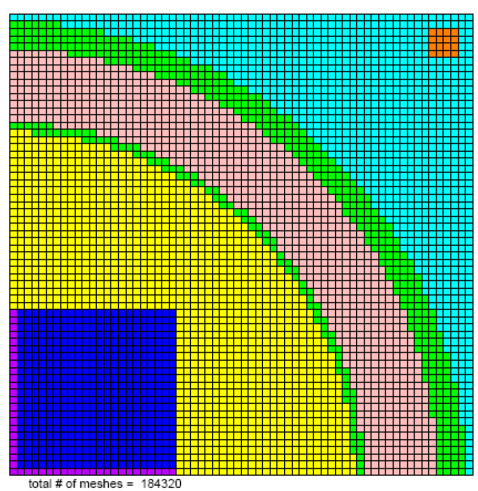


Hybrid shielding

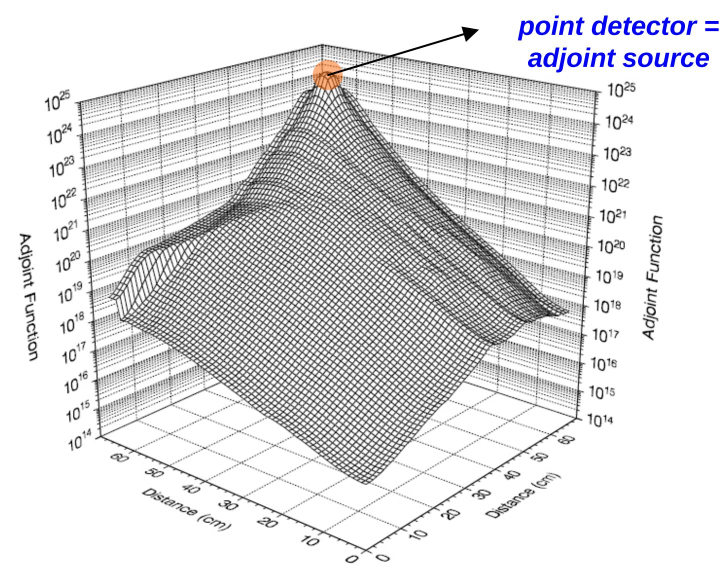
$q^\dagger(\vec{r},E) = \sigma_d(\vec{r},E)$	Adjoint source	CADIS
$\hat{q}(\vec{r},E) = \frac{1}{R} q(\vec{r},E)\phi^\dagger(\vec{r},E)$	Biased source	
$\overline{w}(\vec{r},E) = \frac{R}{\phi^\dagger(\vec{r},E)}$	Target weight	
$w_0(\vec{r},E) = \frac{q(\vec{r},E)}{\hat{q}(\vec{r},E)} = \frac{R}{\phi^\dagger(\vec{r},E)}$	Initial weight	
$q^\dagger(\vec{r},E) = \frac{\sigma_d(\vec{r},E)}{\int \sigma_d(\vec{r},E)\phi(\vec{r},E)}$	Weighted adjoint source	FW-CADIS



MCNP model of the ¼ cask



ADVANTG SN mesh for VR parameters



Adjoint function (1.8-2.4) MeV

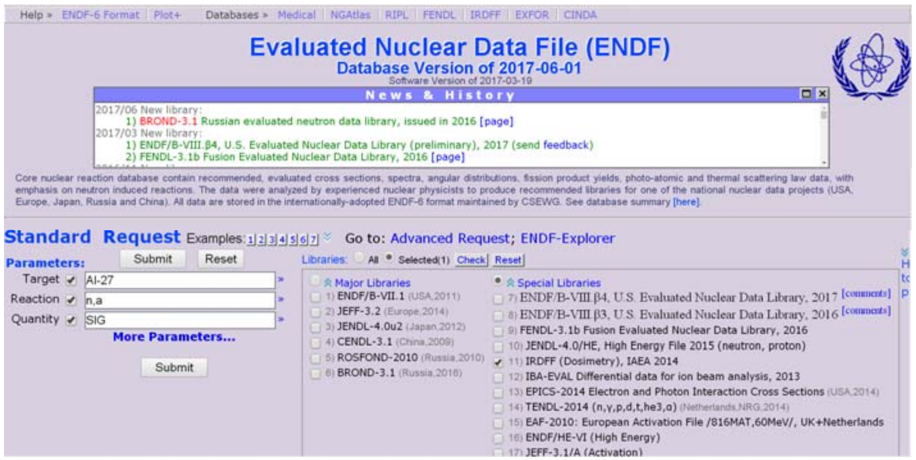
4. PCA response functions

❑ Cross sections from the IAEA NDS service

– **ENDF/B retrieval service (www-nds.iaea.org)**

– **IRDF-2002 and IRDFF-2014 dosimetry libraries**

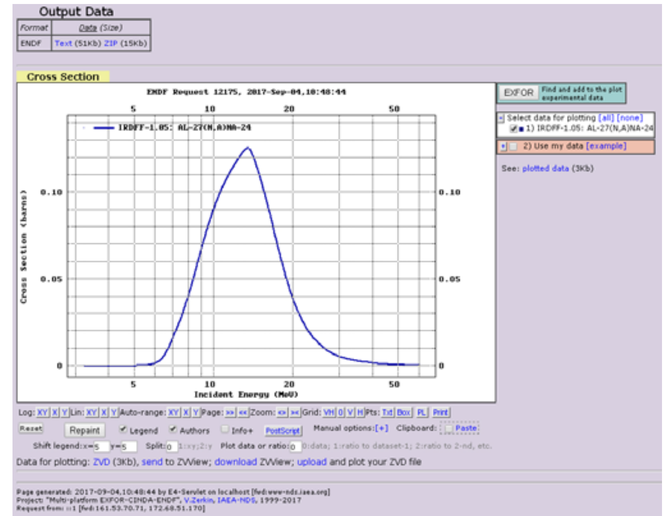
Cross sections with reconstructed resonances and applied Doppler broadening at the temperature 293 K



Selection of XS library and reaction type

IRDFF-1.05 library

Al-27(n,a)Na-24



XS reaction plotting and extracting for MCNP

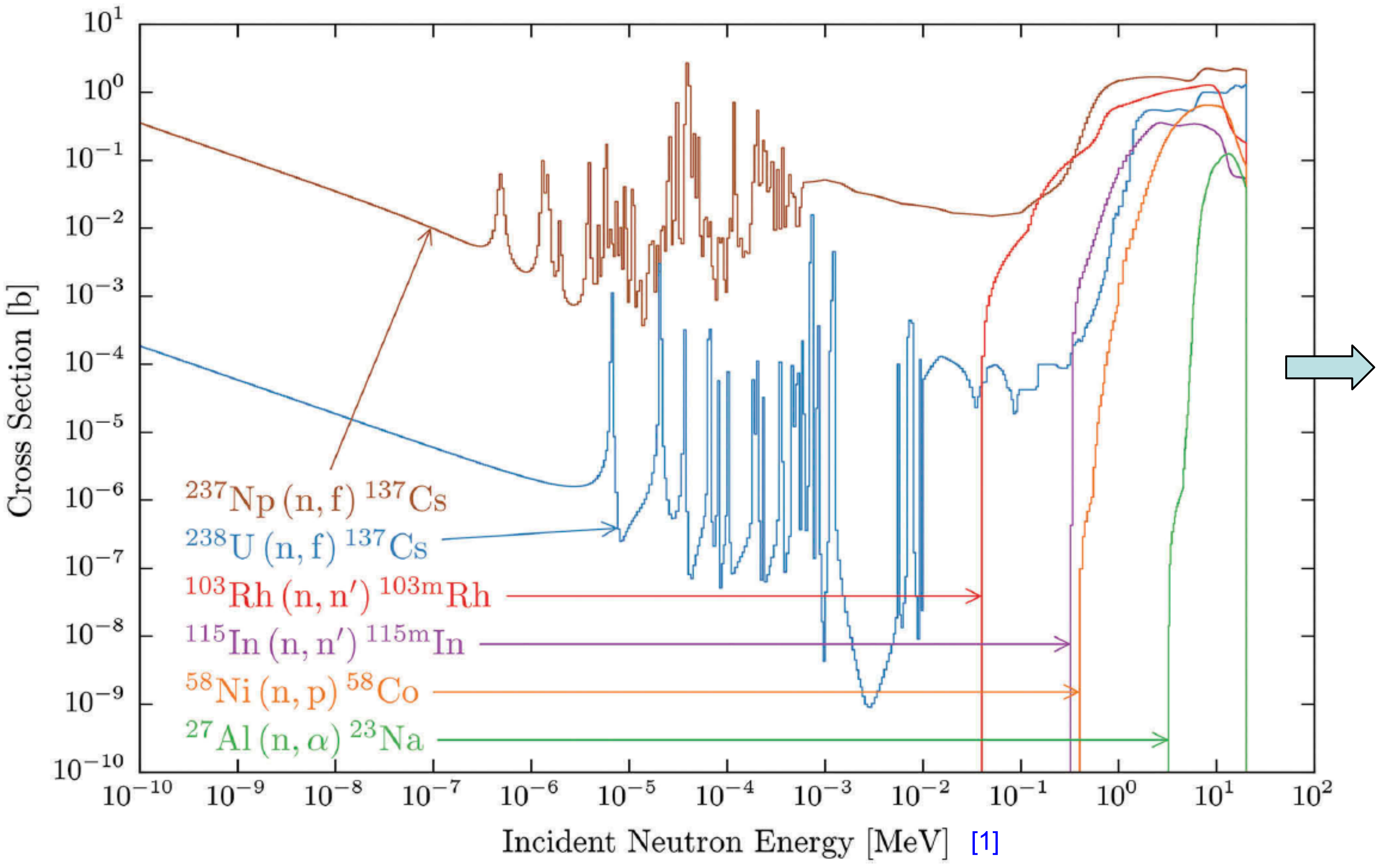
XS reaction explorer

```
 1.302700+4 2.674980+1          0          0          0          01325 3107    1
-3.132140+0-3.132140+6          0          0          1       2651325 3107    2
        265          2                                         1325 3107    3
 3.249265+6 0.000000+0 4.250000+6 5.30733-13 4.500000+6 2.800000-81325 3107    4
 4.638899+6 1.439246-6 4.642116+6 1.491115-6 4.644190+6 1.525042-61325 3107    5
 4.750000+6 3.734485-6 4.816437+6 5.720716-6 5.000000+6 1.338863-51325 3107    6
 5.162467+6 5.232525-5 5.203279+6 6.509141-5 5.250000+6 8.108130-51325 3107    7
 5.500000+6 2.250280-4 5.600000+6 3.732320-4 5.700000+6 5.656270-41325 3107    8
 5.800001+6 8.110670-4 5.900001+6 1.121560-3 6.000000+6 1.513930-31325 3107    9
 6.100000+6 2.012190-3 6.200001+6 2.650500-3 6.300001+6 3.475370-31325 3107   10
 6.400001+6 4.544200-3 6.500000+6 5.914000-3 6.600000+6 7.615680-31325 3107   11
 6.700001+6 9.621631-3 6.800001+6 1.183530-2 6.900001+6 1.412760-21325 3107   12
 7.000000+6 1.639810-2 7.100001+6 1.860930-2 7.200001+6 2.077670-21325 3107   13
 7.210001+6 2.099240-2 7.220001+6 2.120820-2 7.230000+6 2.142400-21325 3107   14
 7.240001+6 2.163990-2 7.250000+6 2.185600-2 7.260001+6 2.207220-21325 3107   15
 7.270000+6 2.228860-2 7.280001+6 2.250520-2 7.290000+6 2.272220-21325 3107   16
 7.300001+6 2.293950-2 7.310000+6 2.315720-2 7.320001+6 2.337520-21325 3107   17
 7.330001+6 2.359370-2 7.340001+6 2.381270-2 7.350001+6 2.403220-21325 3107   18
 7.360001+6 2.425220-2 7.370001+6 2.447280-2 7.380001+6 2.469400-21325 3107   19
 7.390001+6 2.491580-2 7.400001+6 2.513830-2 7.410001+6 2.536140-21325 3107   20
 7.420001+6 2.558530-2 7.430011+6 2.580980-2 7.440011+6 2.603510-21325 3107   21
 7.450011+6 2.626120-2 7.460011+6 2.648810-2 7.470011+6 2.671580-21325 3107   22
```

XS reaction data in the ENDF-6 format

4. PCA response functions

- **Cross sections from the IAEA NDS service**
  - **IRDFF-2014 and IRDF-2002 dosimetry library**
  - **Neutron excitation (n,n') of the first isomeric state Rh (56.12 min) and In (4.486 h)**
  - **Metastable isomers ^{103m}Rh and ^{115m}In with reactions MF/MT = 3/51**



[1]

DE/DF cards define the response spectrum for point detector tallies

[1] Joel A. Kulesza & Roger L. Martz (2017) Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry Using MCNP6, Nuclear Technology, 197:3, 284-295, DOI: 10.1080/00295450.2016.1273711

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

- MCNP6.1.1b eigenvalue results:

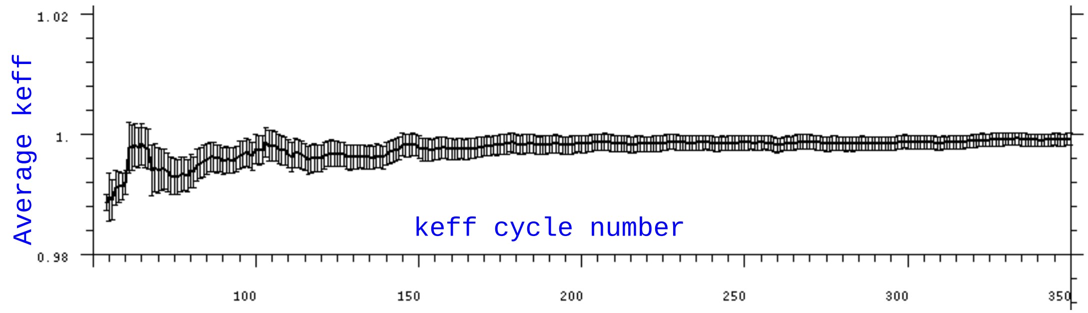
keff = (0.99924 ± 0.00100)

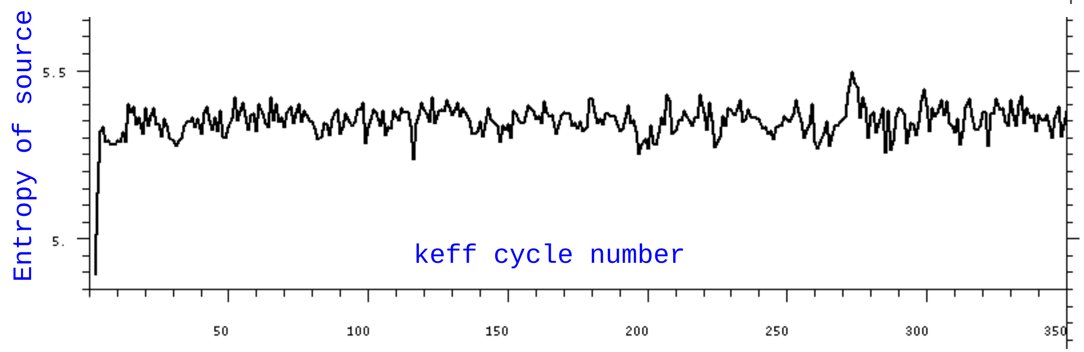
c --------- criticality source -----------

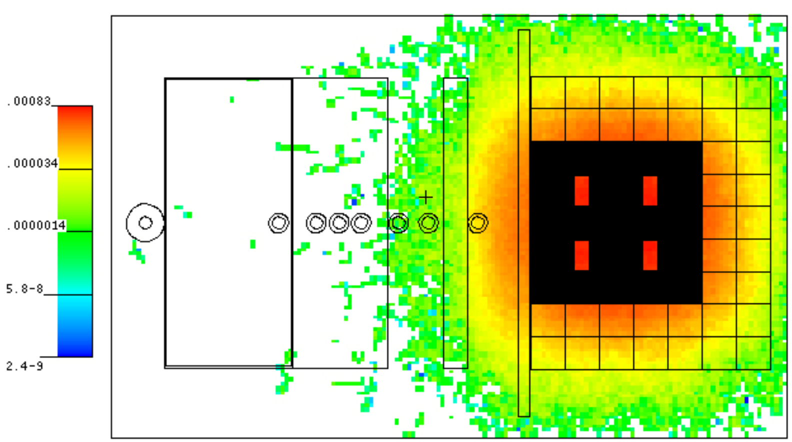
kcode 2000 1.0 50 350 1e4

ksrc 20.22 31.46 0 $ starting point

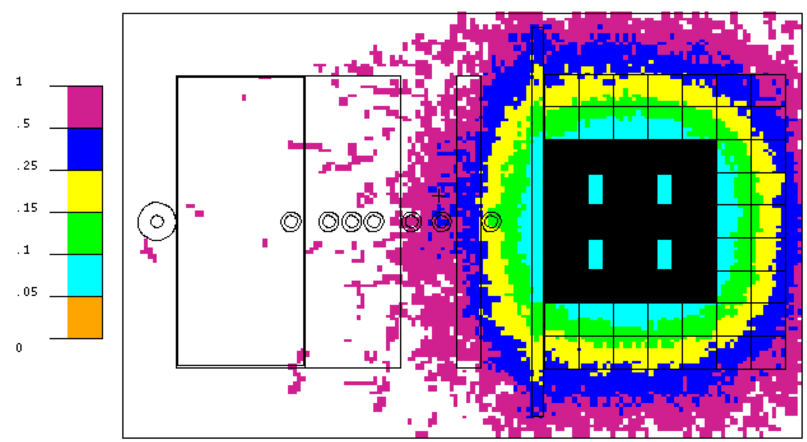
c ---







keff neutron flux in z=0 cm plane



keff neutron flux RE in z=0 cm plane

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

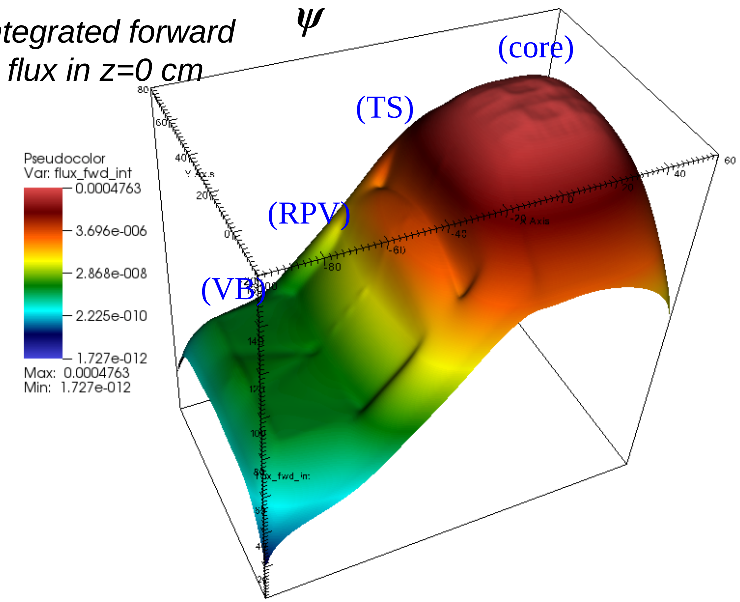
- **ADVANTG3.0.1 parameters:**
  - FW-CADIS method for one reaction on all detectors (A1-A8)
  - S4/P1, SC spatial differencing, eps=1e-3, 1.6e6 mesh cells
  - ANISN-format coupled n-g multigroup library BPLUS (updated BUGLE-96)
  - BUGLE-96 library: LWR shielding, PV dosimetry, VITAMIN-B6 collapsing
  - 5 weighting spectra of 1-D model of a reactor cavity and bioshield
  - BPLUS library: 47n/20g, 393 isotopes, ENDF/B-VII.0 evaluation
  - Mixed 11 pure materials into 26857 macro materials
  - Memory requirements (GB): 6-9 FW Denovo, 10-14 ADJ Denovo

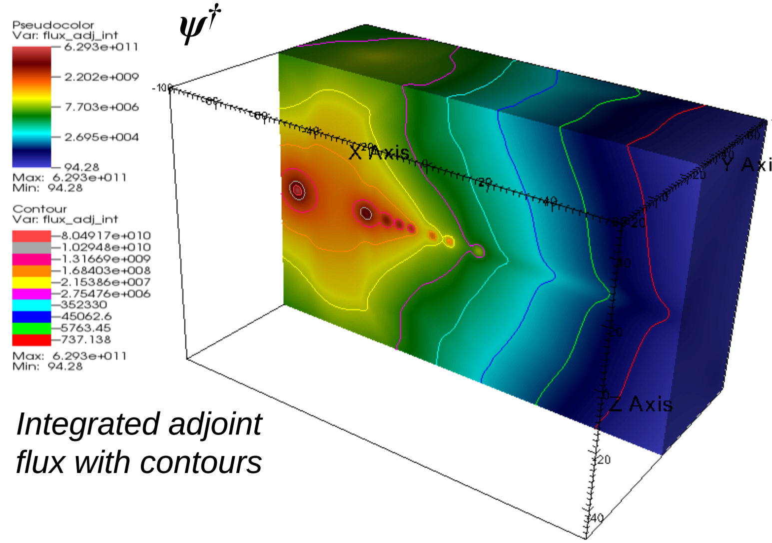
- **MCNP6.1.1b parameters:**
  - Continuous XS for neutron transport with Doppler correction and S(a,b) law
  - MCNP6.1.1b with distributed (PVM) calculation on Quad Core CPU
  - Using point detectors inside small void spheres at centers of A1-A8
  - Mesh tally for capturing the global MC neutron transport
  - card “ctme 720” $ cumulative time in min
  - About 2e6 neutron histories per MC simulation
  - Point detectors have *RE* on average 1-2 %

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

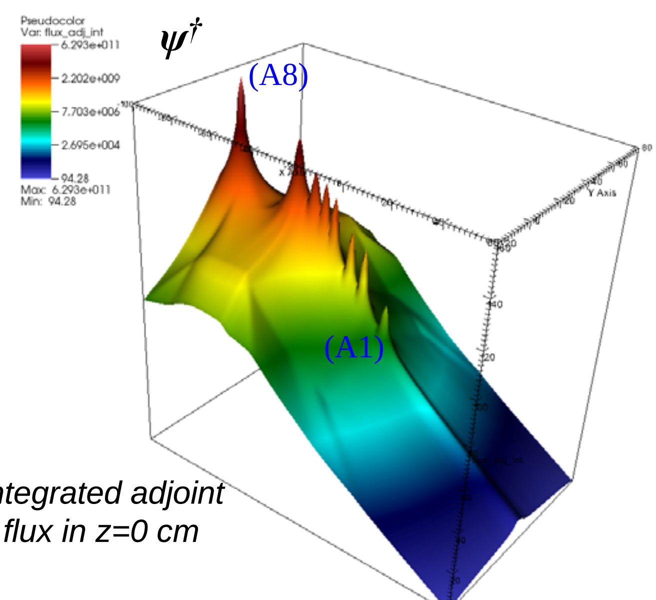
❑ADVANTG3.0.1 FW-CADIS results for $^{27}Al(n,a)^{24}Ni$

Integrated forward flux in z=0 cm



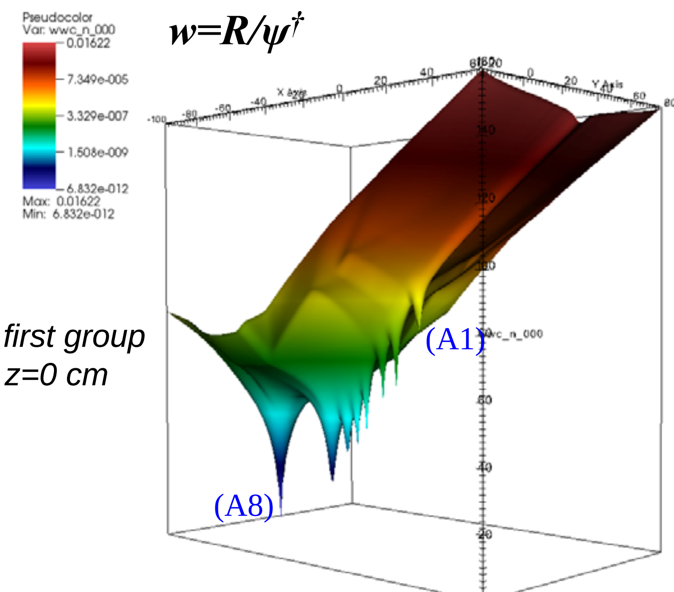


Integrated adjoint flux with contours



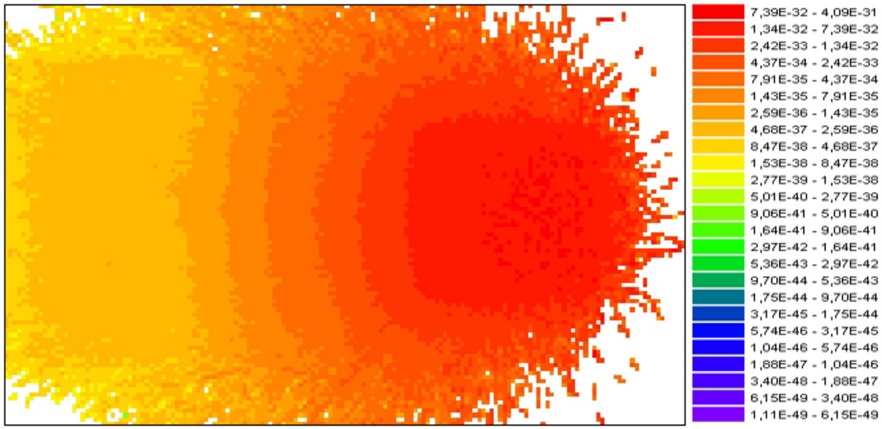
Integrated adjoint flux in z=0 cm

WW first group in z=0 cm

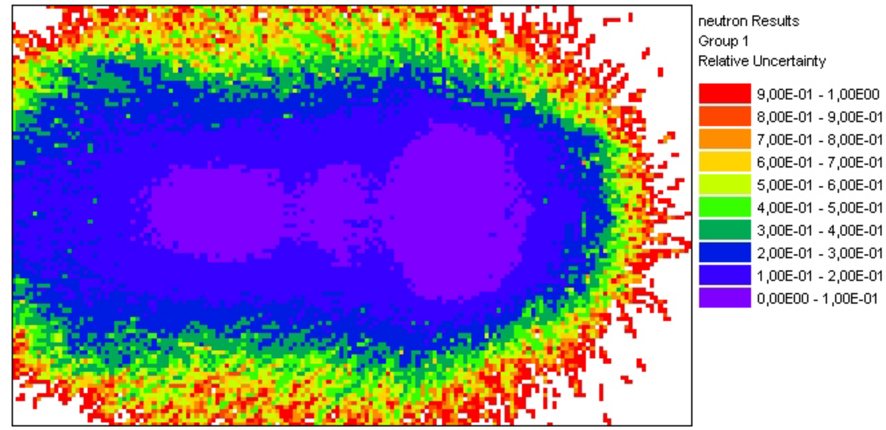


5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

❑ MCNP6.1.1b results for all reactions



MC neutron flux solution for Al-27(n,a)Ni-24 in z=0 cm plane



MC neutron flux RE on 1 sigma level for Al-27(n,a)Ni-24 in z=0 cm plane

Equivalent fission fluxes C/M ratios

("-" experimental result not provided in the PCA benchmark)

	Location	^{237}Np(n,f)	^{238}U(n,f)	^{27}Al(n,a)	^{58}Ni(n,p)	^{115}In(n,n')	^{103}Rh(n,n')	MCNP Avg ± sig	DORT Avg ± sig
	A1	0.862	-	0.801	0.887	0.902	0.945	0.88 ± 0.02	0.91 ± 0.02
	A2	-	-	0.852	0.938	0.986	-	0.93 ± 0.04	0.92 ± 0.01
	A3	0.908	-	0.765	0.835	0.877	-	0.85 ± 0.03	0.96 ± 0.02
RPV	**A4**	0.869	0.882	0.874	0.898	0.935	0.905	0.90 ± 0.01	0.94 ± 0.03
RPV	**A5**	0.914	0.880	0.929	0.919	0.935	0.877	0.91 ± 0.01	0.92 ± 0.03
RPV	**A6**	0.878	0.884	0.968	0.957	0.969	0.881	0.92 ± 0.02	0.91 ± 0.04
	A7	0.939	-	-	-	-	-	0.94 ± 0.00	0.89 ± 0.00
	A8	-	-	-	-	-	-	-	-

[Lower quality results since ADVANTG was used with default eps=1e-3]

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

❑ Isotopes of Fe and self-shielding

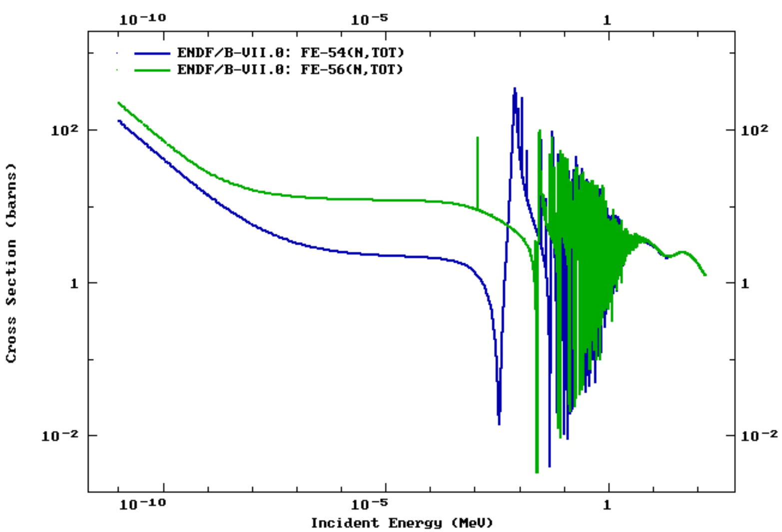
- Neutron spectrum “softening” inside the RPV simulator
- Neutrons > 1 MeV are shifted to resonance region of Fe => self-shielding!
- Important reaction becomes inelastic neutron scattering (n,n’)

$$\sigma_{t,l}(E) = \frac{N\pi\bar{\lambda}^2 g\Gamma_n}{(E-E_0)^2 + 1/4\Gamma^2}\left(\Gamma - 2\Gamma\sin^2\delta_l + 2(E-E_0)\sin 2\delta_l\right) + 4N\pi\bar{\lambda}^2(2l+1)\sin^2\delta_l$$

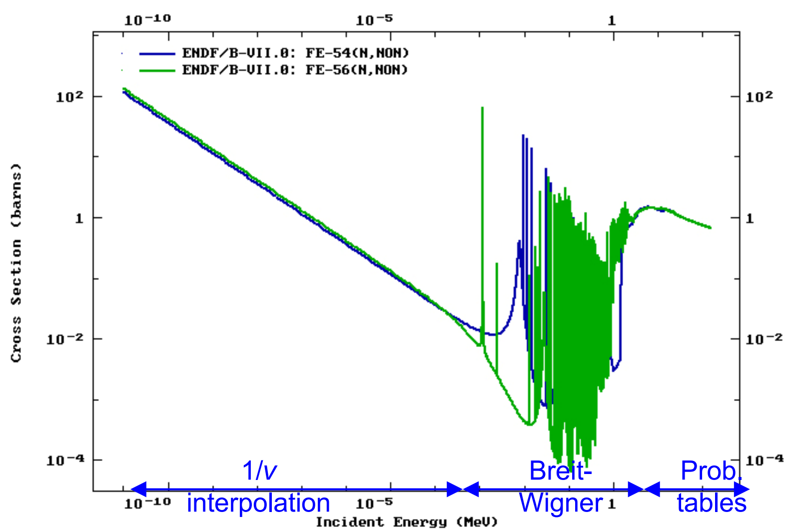
Hard-sphere nuclear model ⇨ $\tan\delta_l = \frac{J_l(R/\bar{\lambda})}{N_l(R/\bar{\lambda})}$

- l=0 (s-wave) neutrons $\delta_0 = R/\bar{\lambda}$ (LWR)
- l=1 (p-wave) neutrons $\delta_1 = \delta_0 - \tan^{-1}(R/\bar{\lambda})$ (FBR)

$$\sigma_{t,0}(E) = \sigma_0\sqrt{\frac{E_0}{E}}\frac{\Gamma^2}{4(E-E_0)^2+\Gamma^2}\left[1 + \frac{4(E-E_0)}{\Gamma}\frac{R}{\bar{\lambda}}\right] + \sigma_{pot}$$



Total cross section (MT=1) of iron isotopes

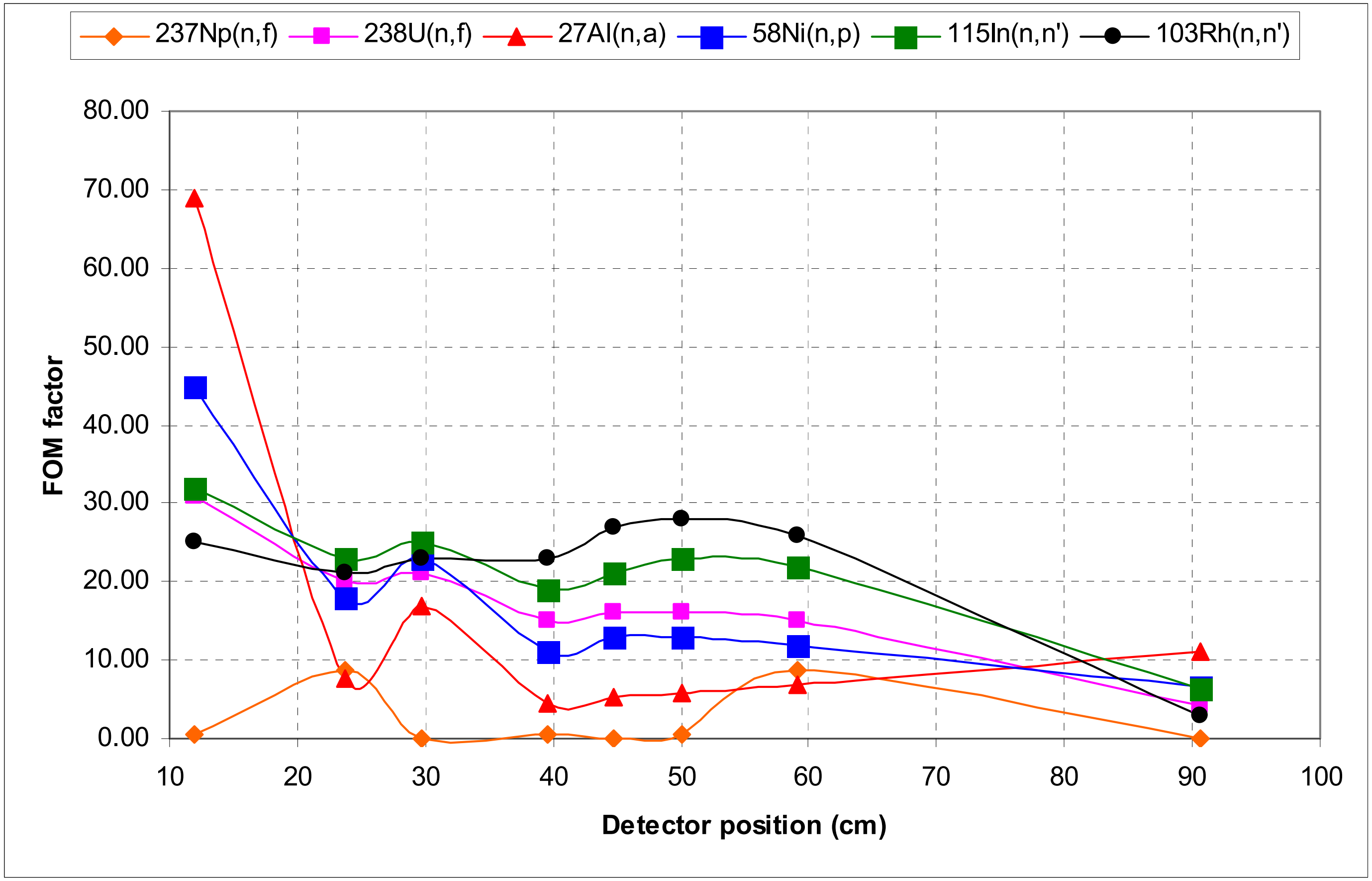


Inelastic scattering (MT=3) of iron isotopes

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

❑ MCNP FOM factors for all reactions

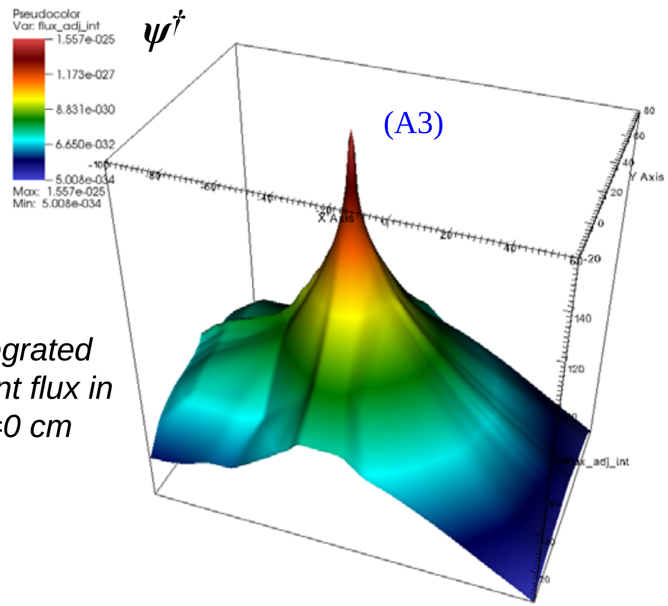
- ❑ Computational model metric addressing memory and CPU time
- ❑ Figure-of-merit (FOM) factor: CPU time necessary to reach a given level *RE*
- ❑ FOM = $1/(RE^2 x T)$, where *RE* is MC rel.error and *T* is CPU time in min



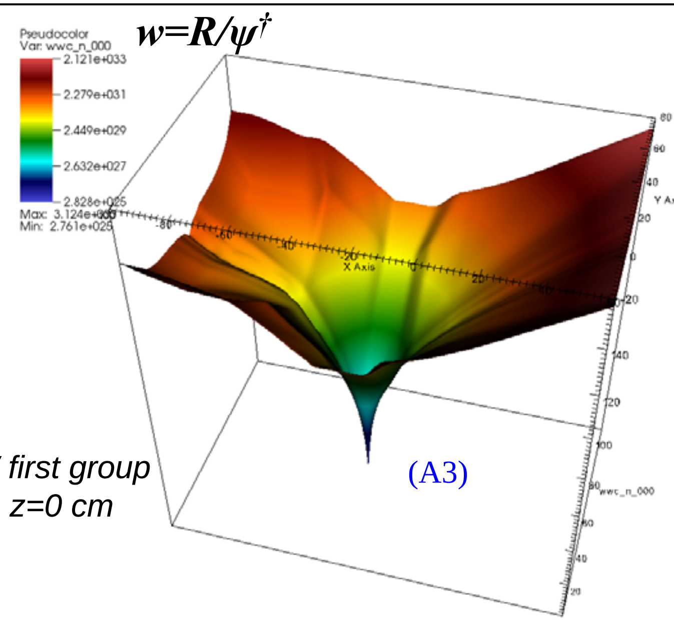
FOM factors for different detector locations

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

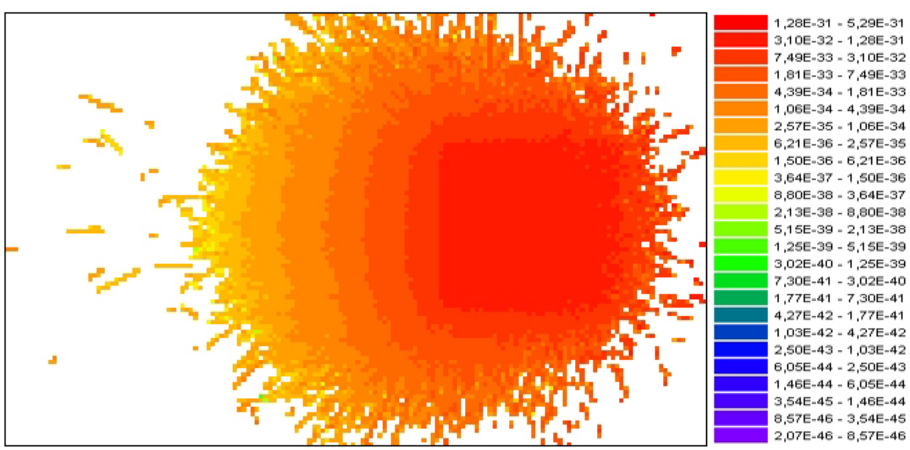
❑ ADVANTG3.0.1 CADIS optimization of A3 detector



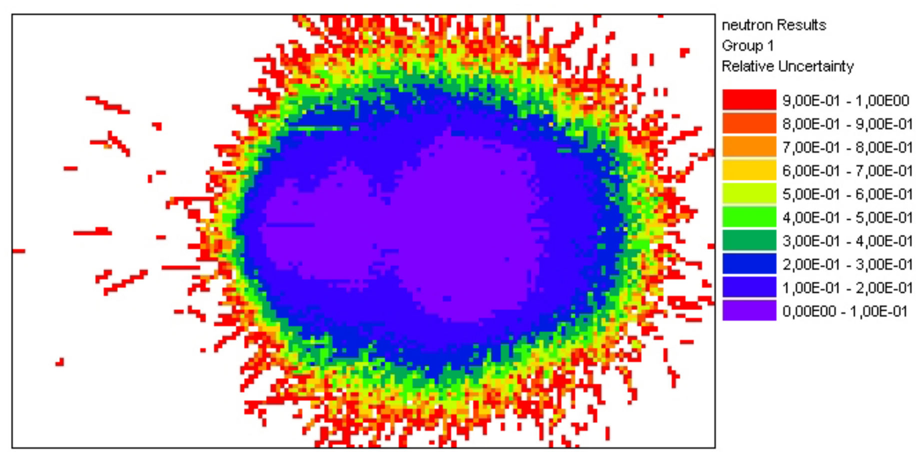
Integrated adjoint flux in z=0 cm



WW first group in z=0 cm



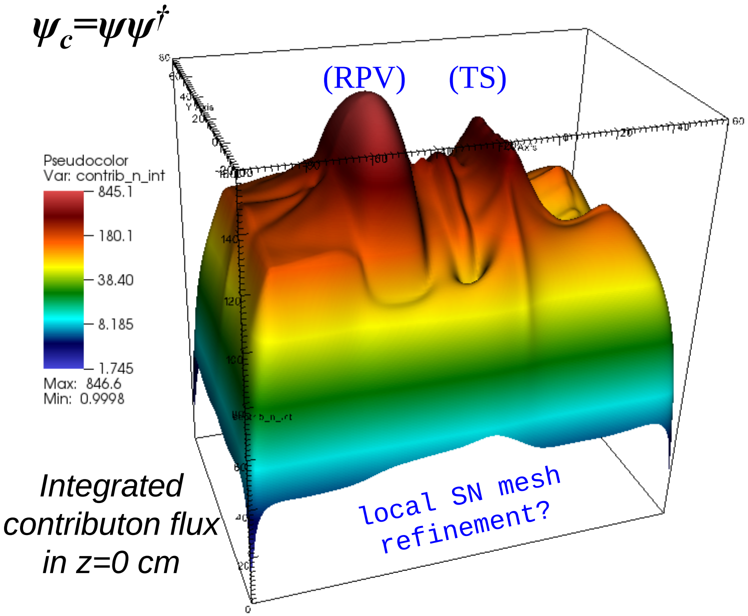
MC neutron flux solution for Al-27(n,a)Ni-24 in z=0 cm plane



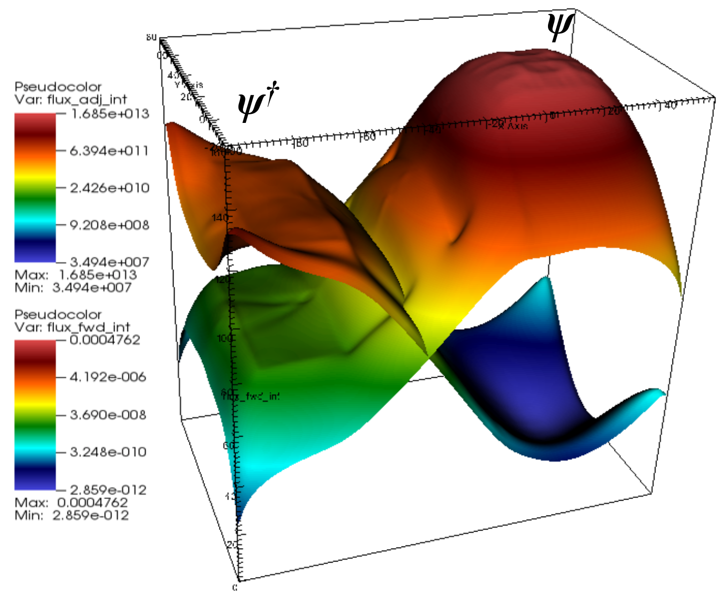
MC neutron flux RE on 1 sigma level for Al-27(n,a)Ni-24 in z=0 cm plane

5. PCA results using ADVANTG3.0.1 / MCNP6.1.1b

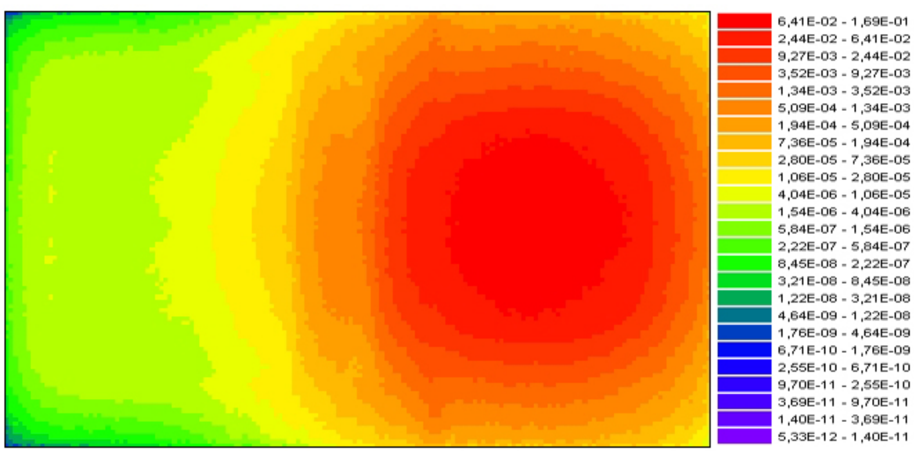
❑ ADVANTG3.0.1 FW-CADIS global flux solution



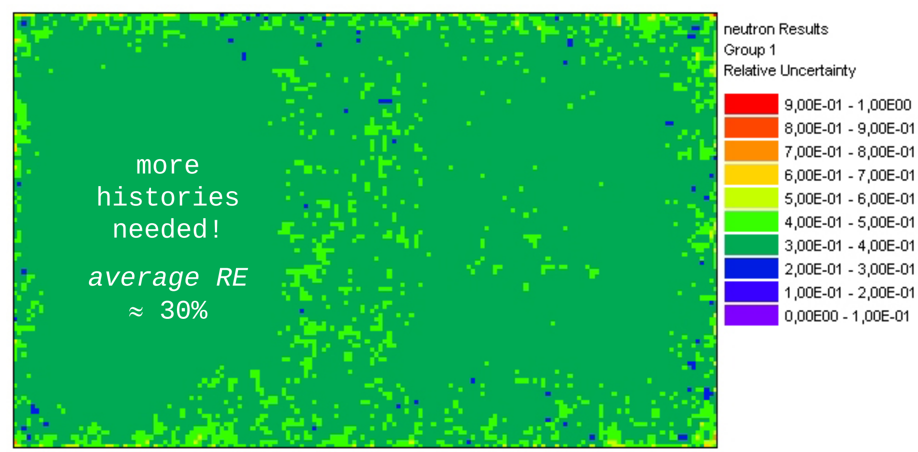
Integrated contributon flux in z=0 cm



Integrated forward and adjoint flux in z=0 cm



MC neutron flux global solution in z=0 cm plane



MC neutron flux RE in z=0 cm plane

6. Summary and conclusions

- **Hybrid shielding:**
  - FW-CADIS for distributed detectors and global flux solution
  - CADIS for local answers, would require 6 reactions x 8 locations = 48 runs!
  - SN based VR technique removes burden of manual VR preparation
  - Computational trade-off between SN and MC simulations
- **PCA benchmark:**
  - Good agreement between calculated (C) and measured (M) results
  - Obtained results in accordance with the Regulatory Guide 1.190
  - Sensitivity of BPLUS shielding library on the iron XS (self-shielding)
  - Differences due to XS libraries, weighting spectrum, core modeling,…
  - More neutron groups are preferred due to spectral effects
- **Commercial hybrid shielding codes today:**
  - SCALE6.2 (CADIS/FW-CADIS in MAVRIC)
  - ADVANTG3.0.1 + MCNP5v1.6 (or MCNP6.1.1b)
  - A[3]MCNP (TORT + MCNP5v1.6)
  - ATTILA + MCNP6.1.1B

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MCNP6

scale

Nuclear Systems Modeling & Simulation

ADVANTG—An Automated Variance Reduction Parameter Generator

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