A³MCNP

(Automated Adjoint Accelerated MCNP)

A. Haghighat

Overview - History

- A^3MCNP was developed by John Wagner* and Alireza Haghighat in 1997 (Wagner's PhD dissertation)
- Since then we have used the code system for various important problems successfully
- The A^3 Patch is marketed through the HSW Technologies; five copies have been sold thus far
- In 2003, we implemented a new volumetric source distribution (sponsored by Mitsubishi Heavy Industries – MHI)
- We are planning to combine the neutral and charge particle algorithms

Contents

CADIS – Consistent Adjoint Driven Importance Sampling

Description:

Uses a 3-D S_N importance function distribution for

source biasing

transport biasing

in a consistent manner, within the weight-window* (r, E) *technique* **.**

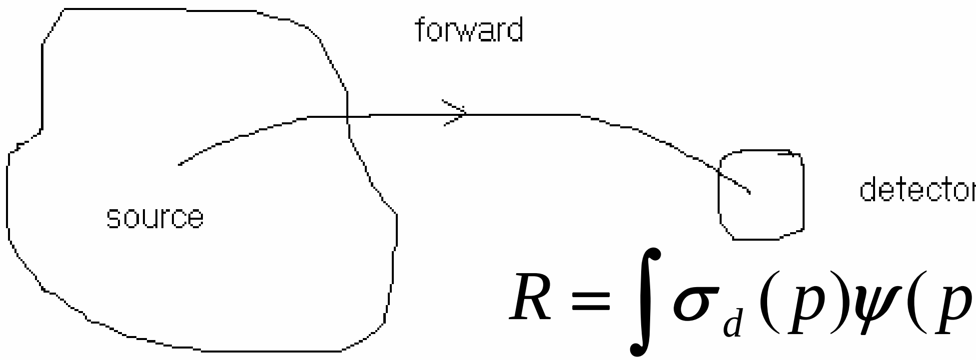
*their biasing formulations are derived based on importance sampling applied to the source integral and transport integral.

CADIS

Source biasing

Detector (σ_d) response formulation

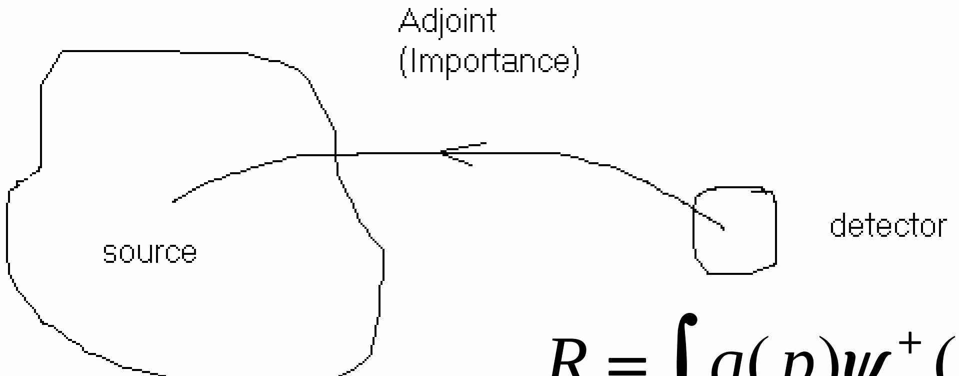
$$H\psi = s$$



$$R = \int_p \sigma_d(p)\psi(p)dp$$

where $p \equiv (\bar{r}, E, \hat{\Omega})$

$$H^+\psi^+ = \sigma_d$$



$$R = \int_p q(p)\psi^+(p)dp$$

CADIS

Source biasing

Biased source

$$\hat{q}(p) = \frac{\phi^{+}(p)q(p)}{\int_{p} \phi^{+}(p)q(p)dp} = \frac{\phi^{+}(p)q(p)}{R}$$

Particle weight

$$W(p) = \frac{R}{\phi^{+}(p)}$$

CADIS – Consistent Adjoint Driven Importance Sampling

Transport biasing

Transport equation

$$\phi(p) = \int_{p'} K(p' \to p)\phi(p')dp' + q(p)$$

Transport equation for the biased source

$$\hat{\phi}(p) = \int_{p'} \hat{K}(p' \to p)\hat{\phi}(p')dp' + \hat{q}(p)$$

where

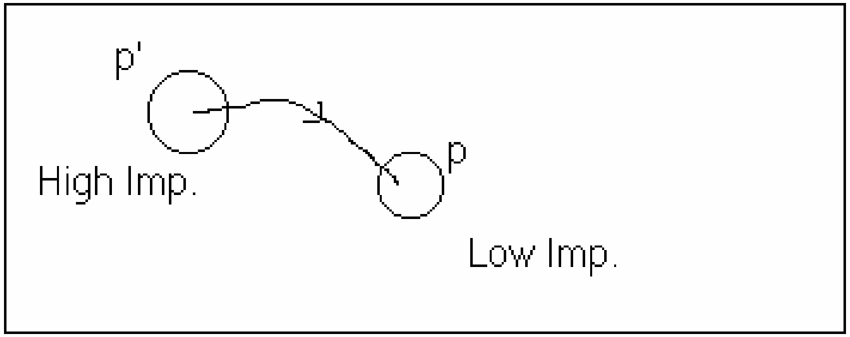
$$\hat{\psi}(p) = \frac{\psi^{+}(p)\psi(p)}{R} \qquad \hat{q}(p) = \frac{\psi^{+}(p)q(p)}{R}$$

$$\hat{K}(p' \to p) = K(p' \to p)\left[\frac{\phi^{+}(p)}{\phi^{+}(p')}\right]$$

CADIS

Transport biasing

$$\hat{K}(p' \to p) = K(p' \to p)\left[\frac{\phi^+(p)}{\phi^+(p')}\right]$$



•***If*** $\left(\frac{\psi^+(p)}{\psi^+(p')}\right)$ ***<1, particles are processed through the Russian roulette, Otherwise, particles are split***

•***Particle statistical weight***

$$w(p) = \left(\frac{\psi^+(p')}{\psi^+(p)}\right) w(p')$$

Note:

The word "consistent" in CADIS refers to the transport biasing formulation is derived consistently based on the biased source.

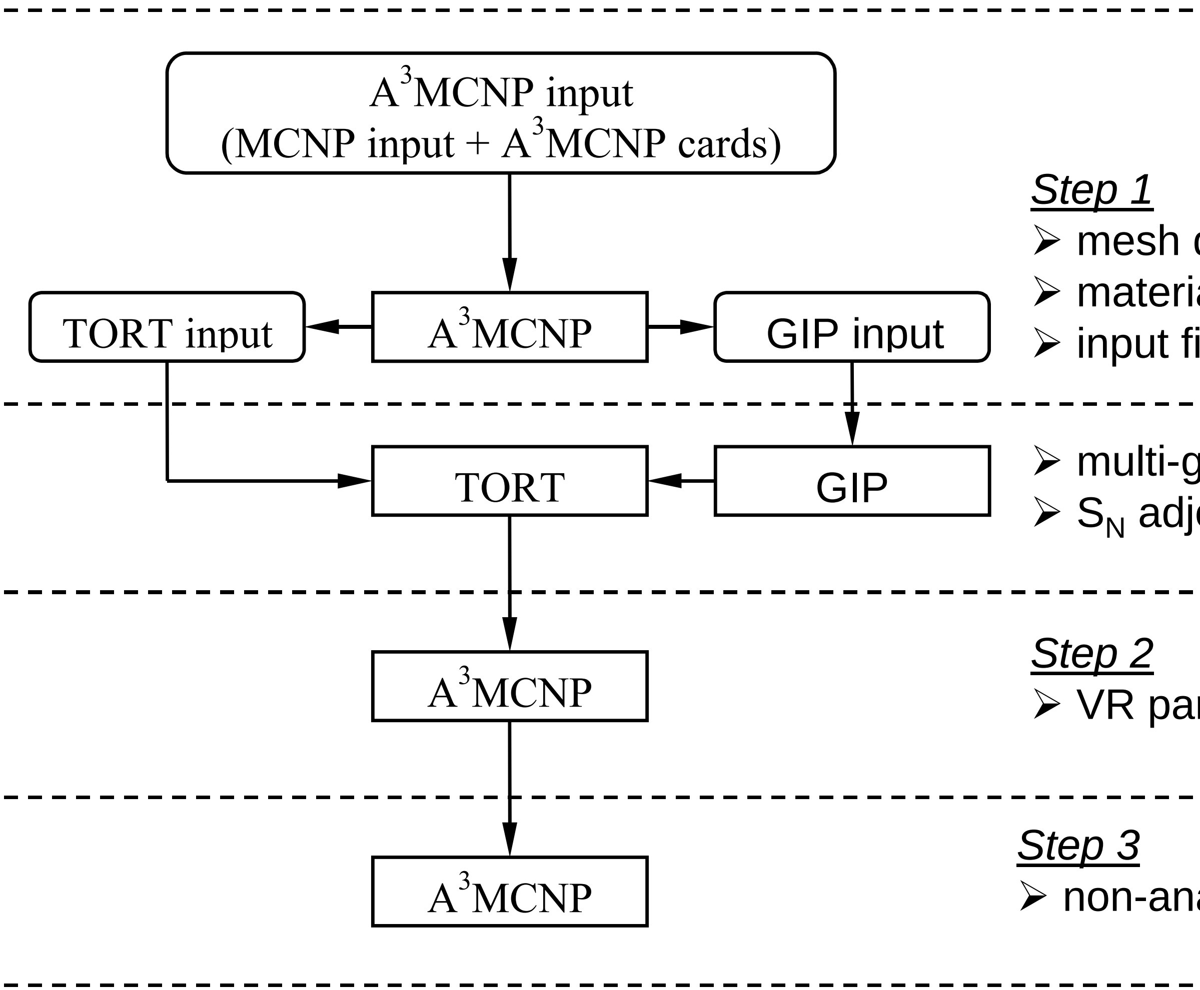
A^3MCNP – Automated Adjoint Accelerated MCNP

- CADIS methodology effective, but

- Automation tools are needed for determination of "importance" function

- Hence, we developed A^3MCNP

A^3MCNP Calculations



Step 1

- mesh distribution
- material composition
- input files

- multi-group cross sections
- S_N adjoint function

Step 2

- VR parameters

Step 3

- non-analog MC Calculation

Application of A^3MCNP

- PWR Cavity dosimetry

  For determination of neutron interaction rates with dosimetry materials placed at the reactor cavity, and estimation of fluence at the reactor pressure vessel

- BWR Core Shroud

  Determination of neutron and gamma fields at the reactor pressure vessel

- Storage cask

  Determination of neutron and gamma fields at the cask's outside surface

Application

PWR cavity dosimetry

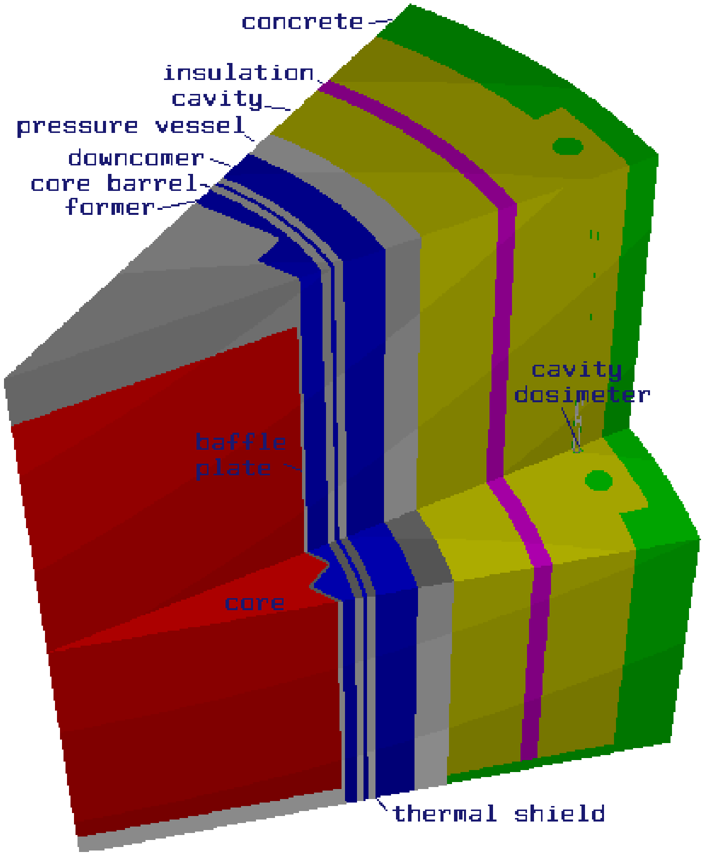
•Objective: Estimation of neutron reaction rates at the cavity dosimeter for benchmarking of the PV fluence.

•Problem size: R=350 cm, θ=45°, z= 400 cm

•Deep penetration

•Detector size (radius of ~2 cm , ~height of the model)

•R-θ, Sn DORT calculation: 8500 meshes, S8, 47-group/P3; CPU time = 15 min



Application

PWP cavity dosimetry (continued)

$$\frac{FOM(CADIS)}{FOM(MCNP)} \cong 50{,}000$$

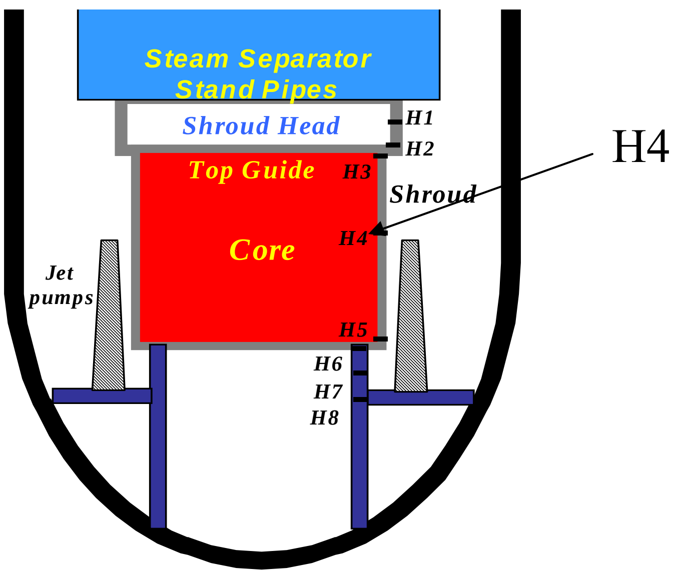
Relatively speaking, DORT CPU time is negligible, hence

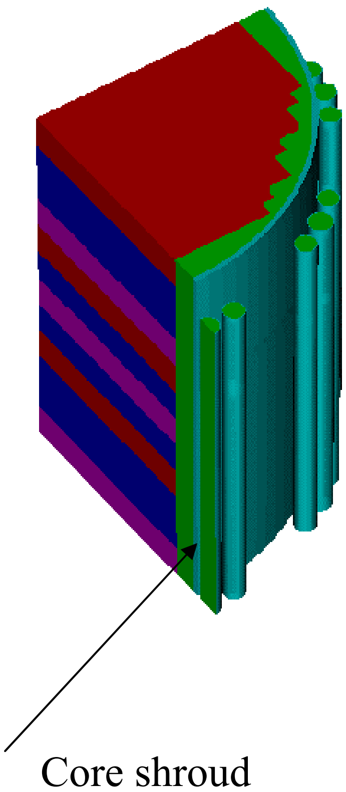
$$\frac{CPU(CADIS)}{CPU(MCNP)} \cong 50{,}000$$

Application

BWR Core Shroud

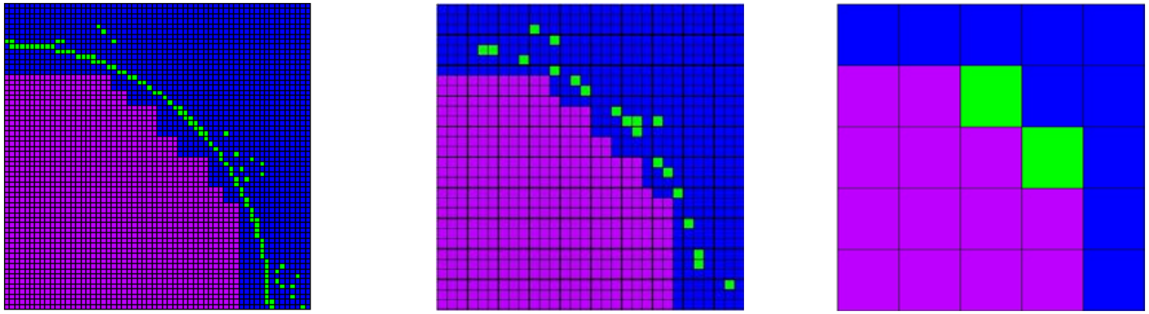
Determination of neutron and gamma DPA at the core shroud





Application

Different A^3MCNP meshing for the core shroud problem was developed to examine the performance of the code, e.g.



Case	Total # of meshes (# axial meshes)	Mesh size (x, y, z) (cm)
1	86400 (24)	5,5,15.875
2	43200 (12)	5, 5, 31.75
3	38400 (24)	7.5,7.5,15.875
4	10800 (12)	10, 10, 31.75
5	2700 (12)	20, 20, 31.75
6	1200 (12)	30, 30, 31.75
7	300 (12)	60, 60, 31.75

Table 2 - *Different back-thinned cases.*

Case	No. of Meshes (axial mesh)		Max. mesh size (cm) in Fuel, moderator, steel
	Ref.	Back-thinned	
8	86400(24)	65067(24)	5.0, 10.0, 5.0
9	43200(12)	32557(12)	5.0,10.0,5.0
10	38400(24)	18525(24)	15.0,15.0,7.5

Application

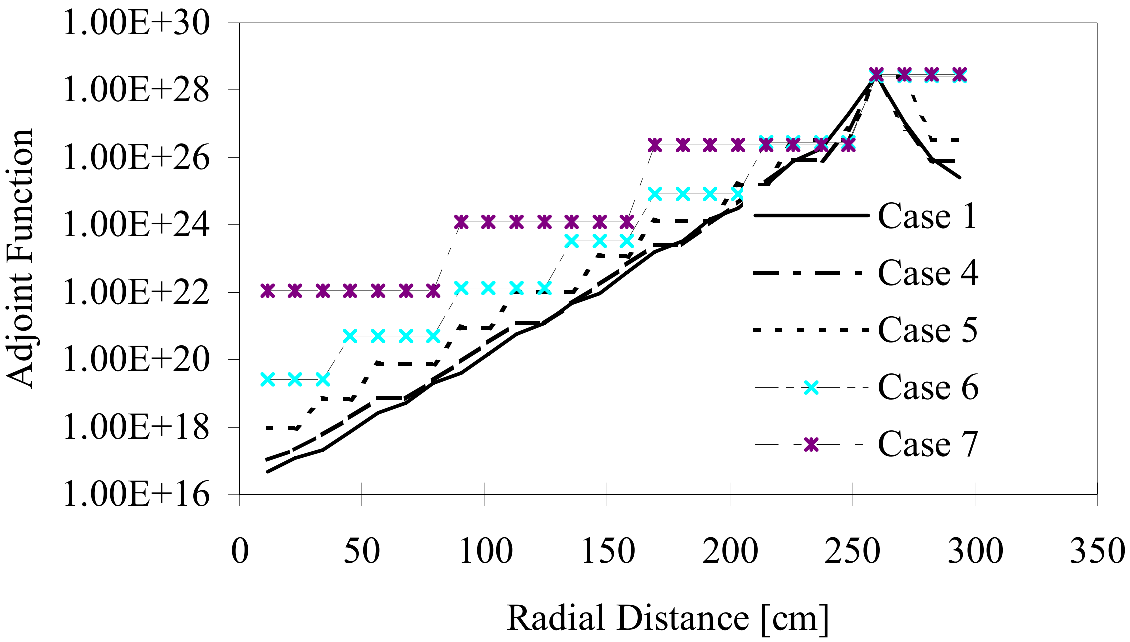
BWR Core-Shroud (continued)

• 3-D Sn TORT calculations: different # of meshes, S8, 47-group/P3, different CPUs

•Detector size (?)

•Sample:

Importance function distributions for different fixed mesh cases



Application

BWR Core-shroud (continued)

Results:

Table 3 - *Estimated DPA and associated statistics after 100 CPU minutes for the unbiased case and cases 1 to 10.*

Case No.	# of meshes (# of axial meshes)	DPA [dpa/sec]	Relative Error [%]	FOM	MCNP Speedup $FOM_{biased}/FOM_{unbiased}$
Unbiased	N/A	3.877E-10*	14.97*	0.022*	1
1	86400 (24)	3.571E-10	1.05	90.7	4123
2	65067 (24)	3.504E-10	1.19	70.6	3209
3	43200 (12)	3.452E-10	1.26	63.1	2868
4	10800 (12)	3.440E-10	1.35	54.9	2945
5	2700 (12)	3.513E-10	2.46	16.5	750
6	1200 (12)	3.512E-10	2.56	15.3	696
7	300 (12)	3.470E-10	5.88	2.89	131
8	38400 (24)	3.517E-10	1.25	64.0	2909
9	32557 (12)	3.469E-10	1.57	40.6	1845
10	18525 (24)	3.593E-10	1.52	43.3	1968

* result after 2000 CPU minutes

Application

BWR core-shroud (continued)

Results:

Table 4 - *Comparison of total CPU time (TORT+A^3MCNP^{TM}) to achieve 1.0% (1σ) statistical uncertainty for the unbiased case and cases 1 to 10.*

Case No.	No. of meshes (# of axial meshes)	TORT [minutes]	A^3MCNP [minutes]	Total [minutes]	Overall Speedup
Unbiased	N/A	N/A	448,201	448,201	1
1	86400 (24)	424.6	110.3	534.9	838
2	65067 (24)	309.0	141.6	450.6	995
3	43200 (12)	257.2	158.8	416.0	1077
4	10800(12)	40.8	182.7	223.5	2005
5	2700 (12)	10.2	604.8	615.0	729
6	1200 (12)	5.0	655.2	660.2	679
7	300 (12)	1.3	3461.4	3462.7	129
8	38400 (24)	256.7	156.3	413.0	1085
9	32557 (12)	205.5	246.5	452.0	992
10	18525 (24)	128.7	231.0	359.7	1246

Application

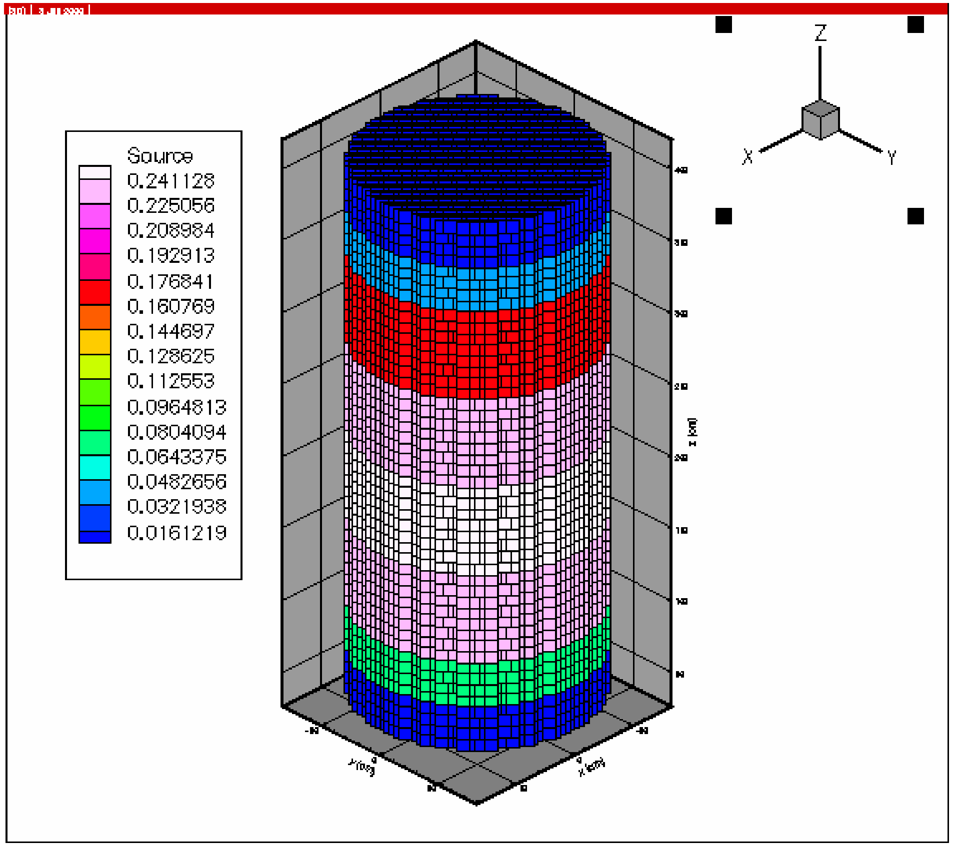
Shipping cask

•Objective: Estimation of Neutron and gamma dose on the cask surface

• Problem Size: 180 x 180 x 840 cm^3

•A Deep penetration problem

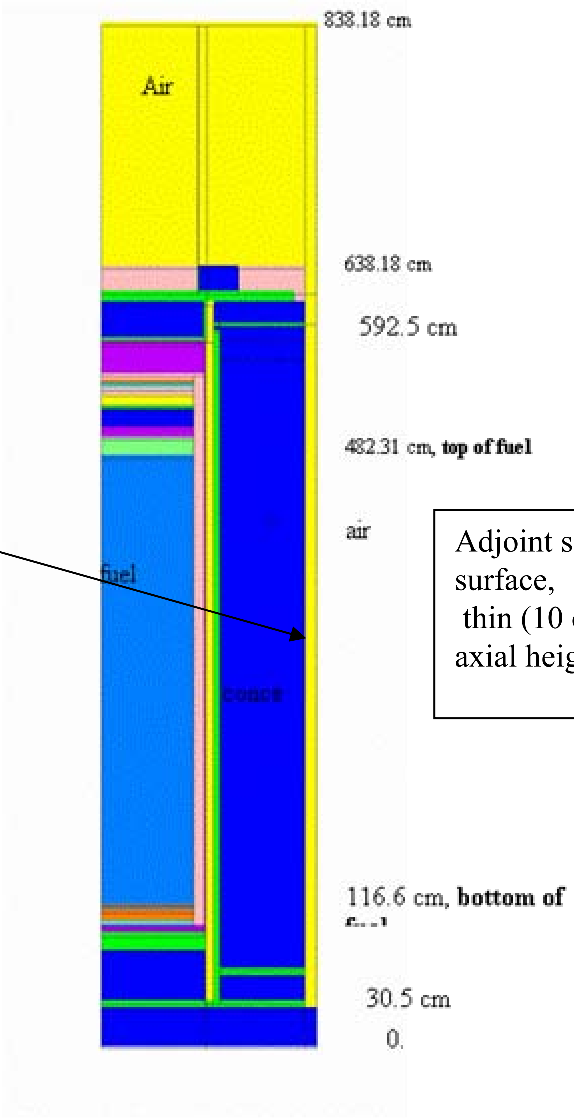
Neutron source distribution



Application

Shipping cask (continued)

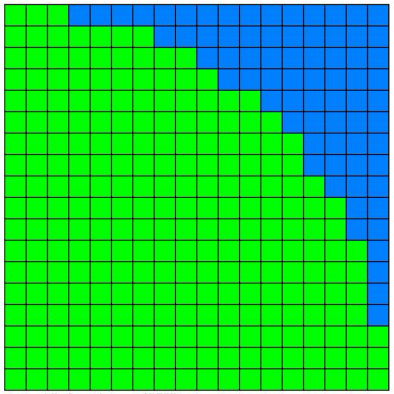
- TORT 3-D Sn calculation: 32256 meshes S8, 18-group/P3, CPU = 20.7 min
- Detector region: a shell over the whole surface of the cask



Adjoint source placed on the surface, thin (10 cm) air region , and axial height of [30.5 – 592.5 cm]

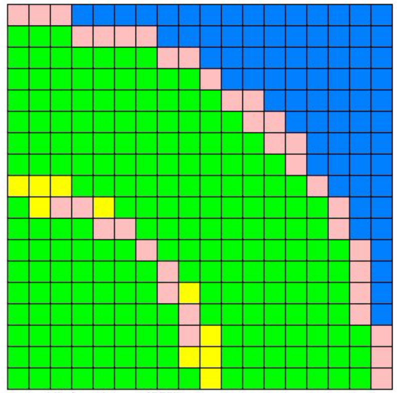
A^{3}MCNP SHIPPING CASK MESHING FOR TORT

Z-level 1



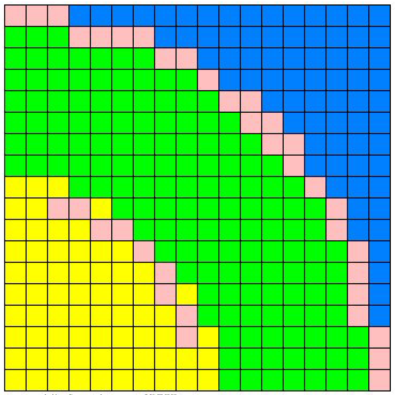
total # of meshes = 13608

Z-level 3



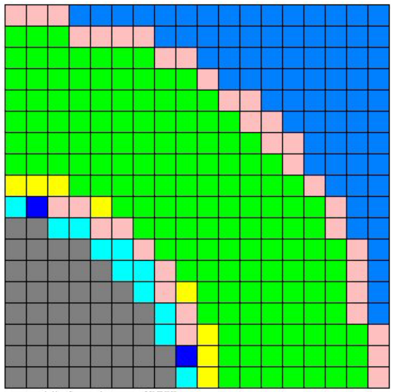
total # of meshes = 13608

Z-level 5



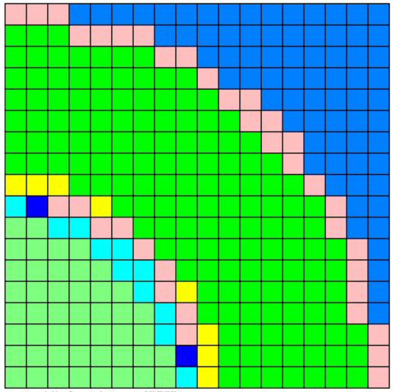
total # of meshes = 13608

Z-level 6



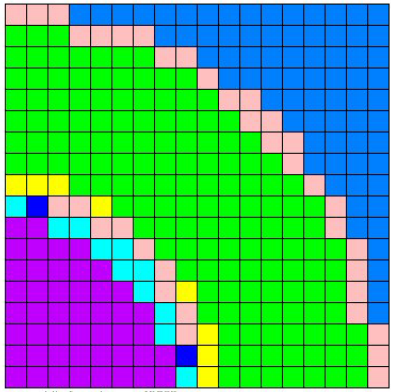
total # of meshes = 13608

Z-level 7



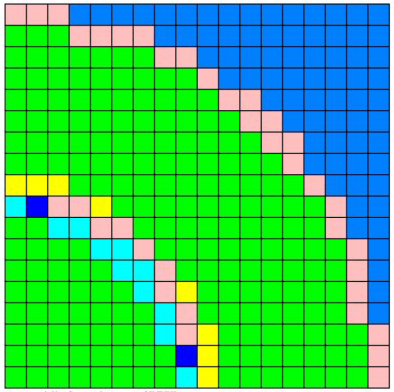
total # of meshes = 13608

Z-level 25



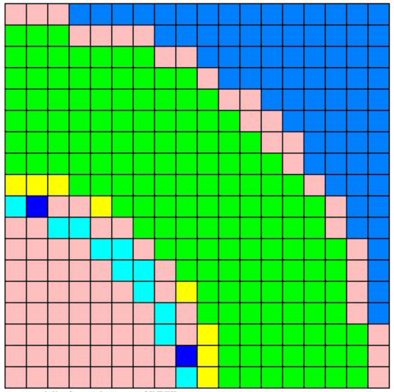
total # of meshes = 13608

Z-level 26



total # of meshes = 13608

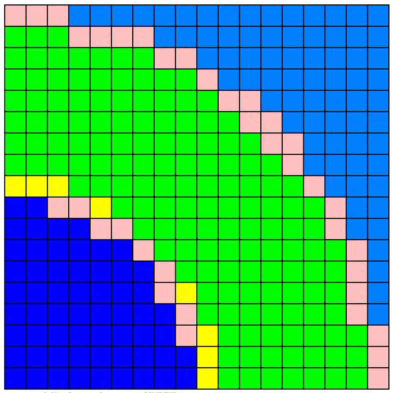
Z-level 27



total # of meshes = 13608

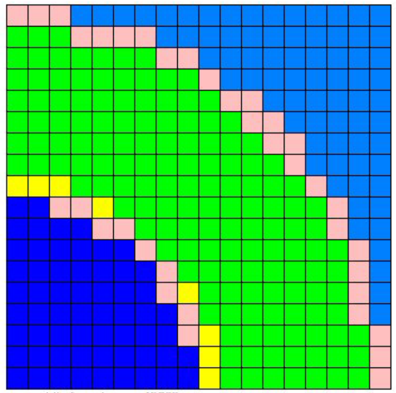
A³MCNP SHIPPING CASK MESHING FOR TORT (continued)

Z-level 28



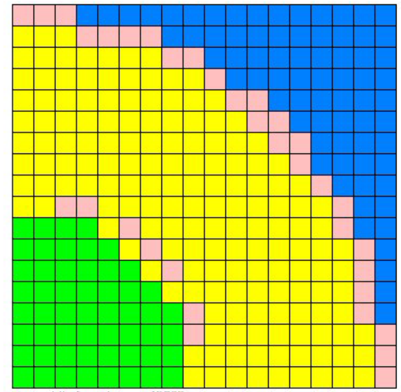
total # of meshes = 13608

Z-level 29



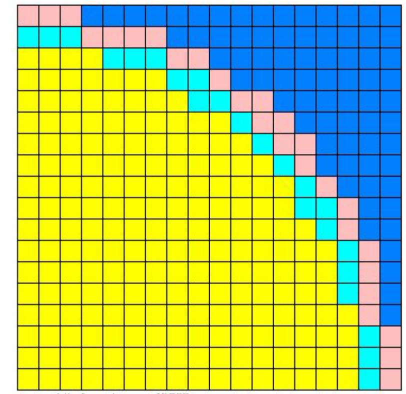
total # of meshes = 13608

Z-level 30



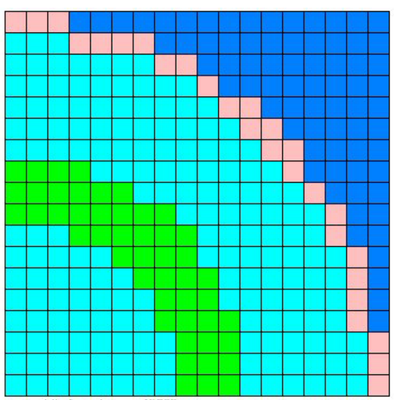
total # of meshes = 13608

Z-level 31



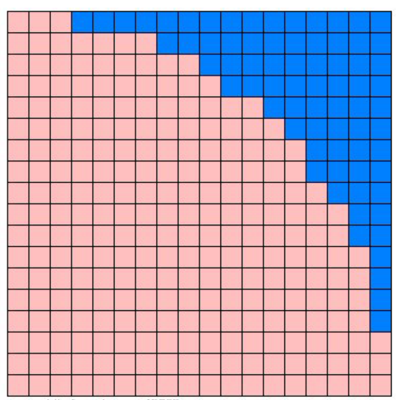
total # of meshes = 13608

Z-level 32



total # of meshes = 13608

Z-level 33

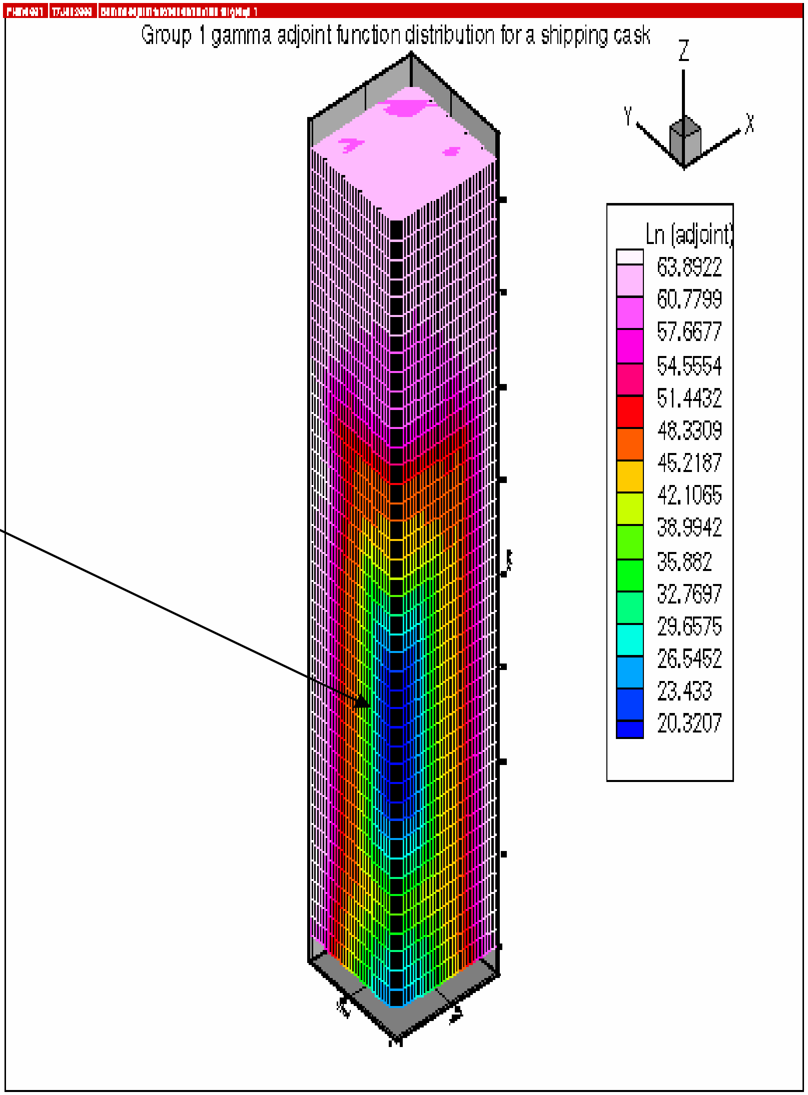


total # of meshes = 13608

Application

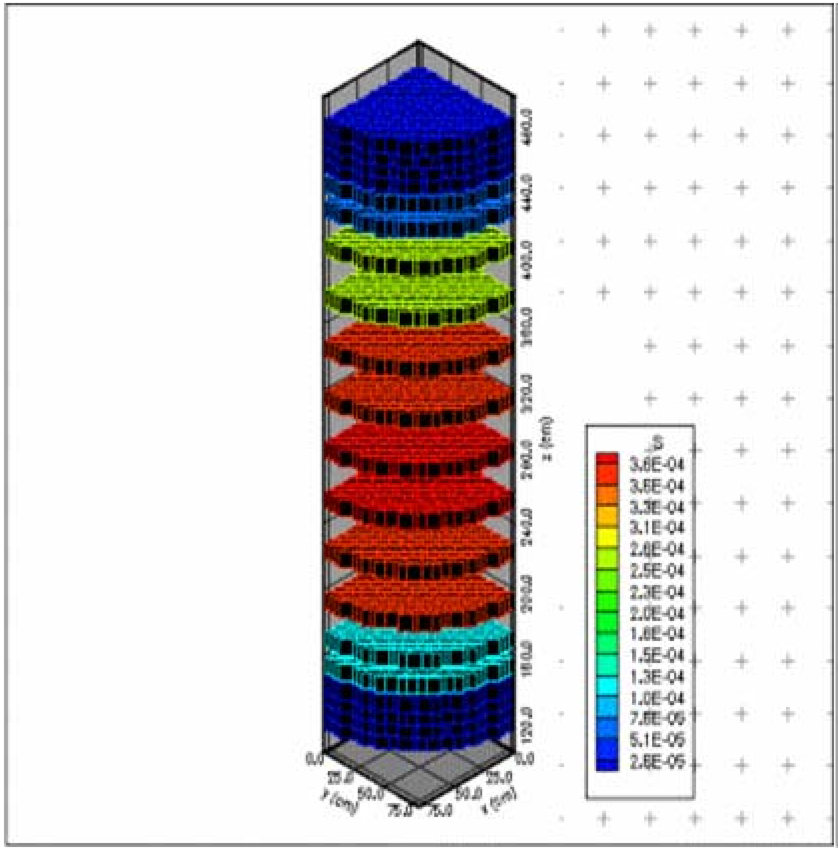
Shipping cask (continued)

Sample: Importance function distribution for group 1 gamma rays

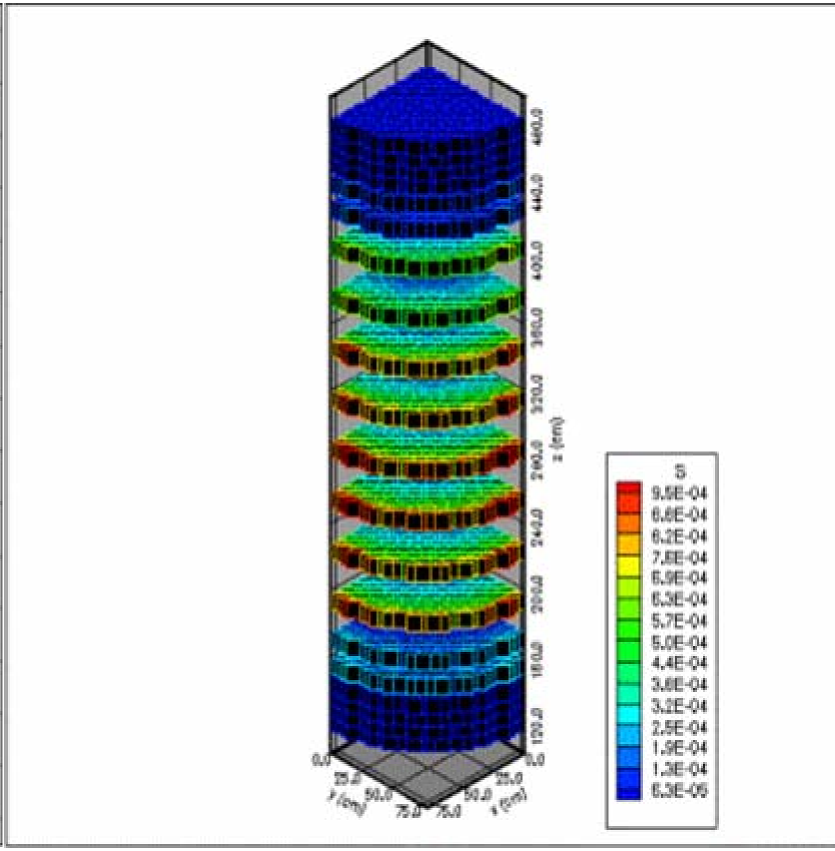


Source Distribution

Unbiased

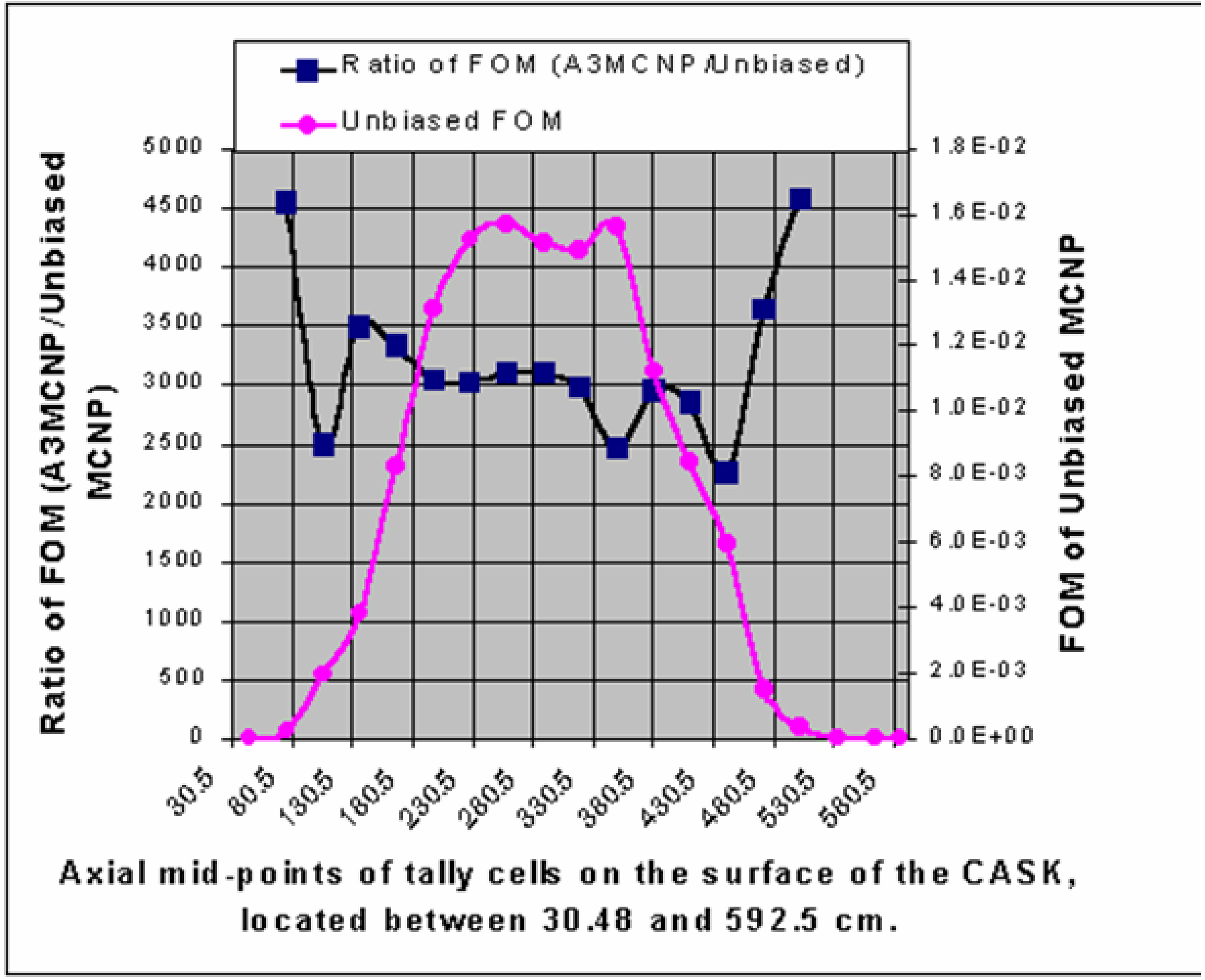


Biased



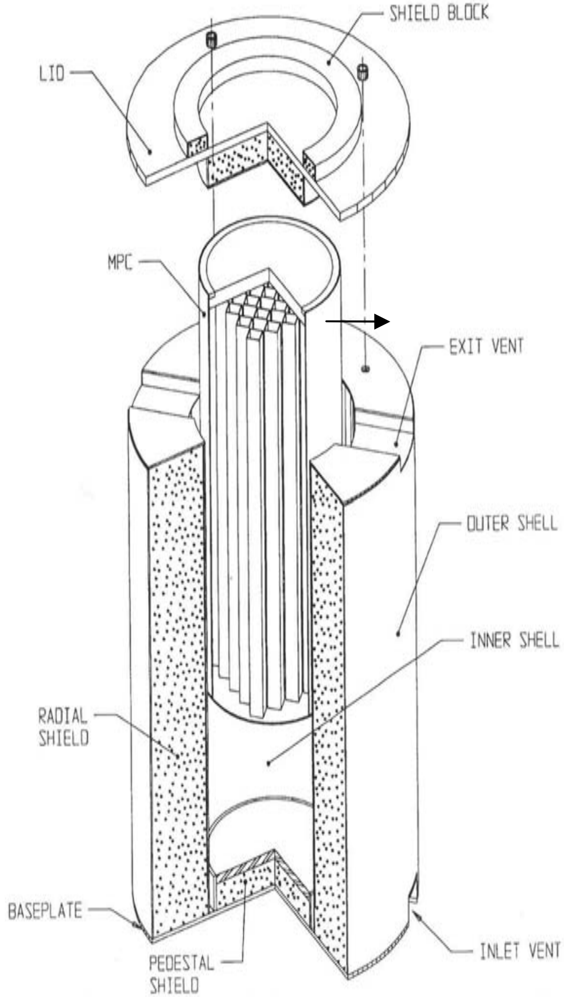
A³MCNP Performance

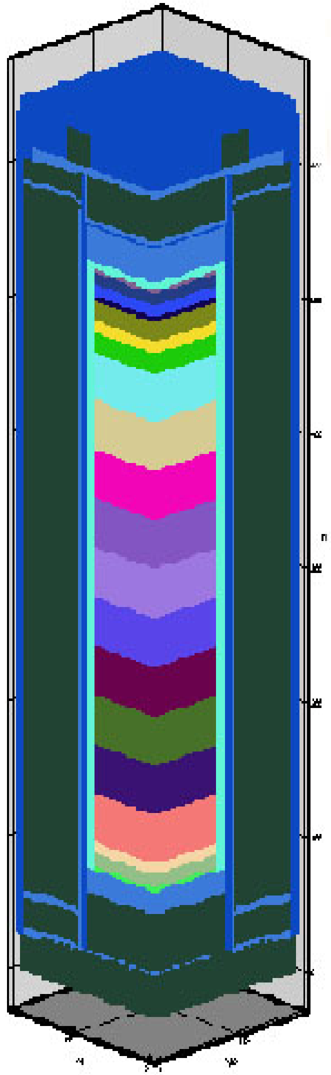
Behavior of FOM for estimation of axial dose



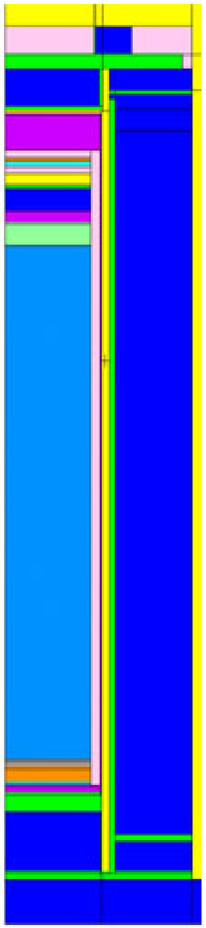
Simulation of a Storage Cask

A^{3}MCNP was used to examine determination of localized regions by performing different calculations



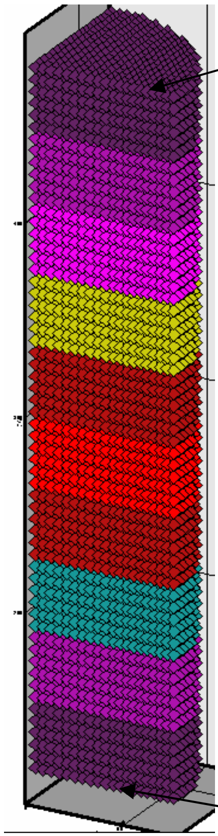


Model



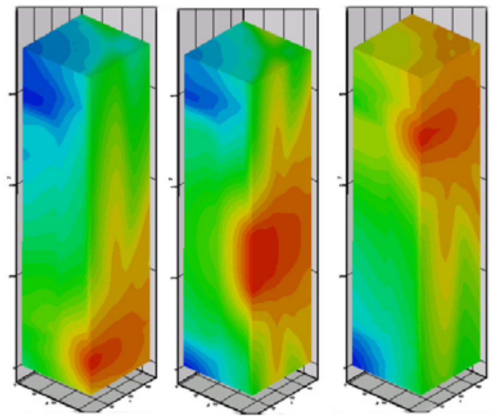
UFTTG

Neutron Source

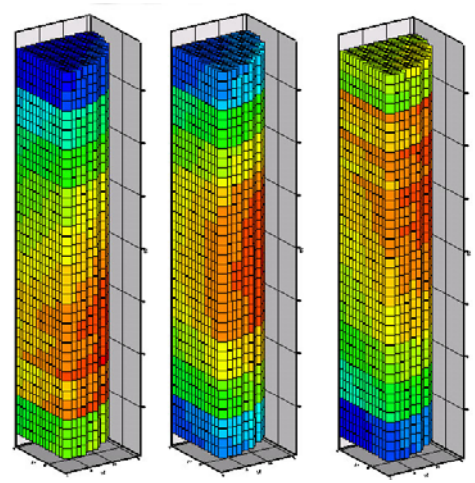


10	5.00E-05
9	4.09E-03
8	3.31E-02
7	1.63E-01
6	2.29E-01
5	2.57E-01
4	2.33E-01
3	7.03E-02
2	9.61E-03
1	5.00E-05

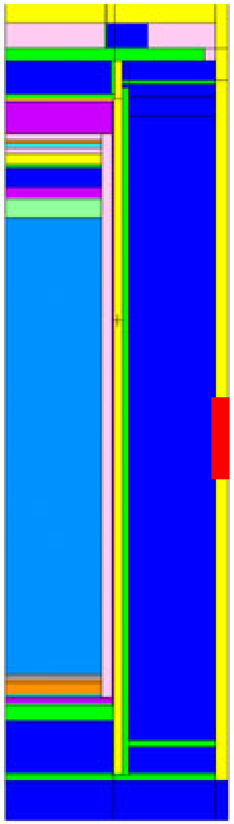
Importance Function Distributions for different adjoint sources



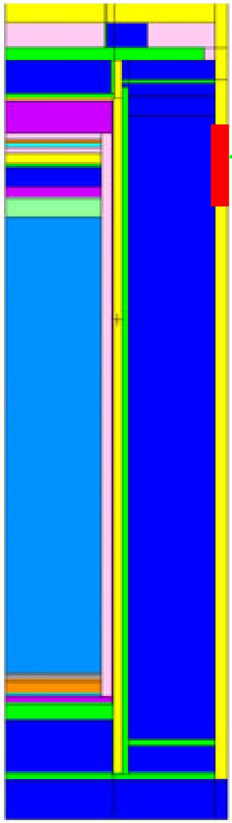
Biased Sources



Determination of surface dose, axial mid-plane (only)
(1-σ Relative Error = 1%)



Model	# CPU	Dose Ratio	FOM	Run Time (hrs)	Speedup	Values/ Hour
Unbiased Cont. Energy MCNP	8	1.00	0.78	214	1.0	19
Unbiased Multigroup MCNP	8	0.70	0.46	362	0.6	30
A^3MCNP Cont. Energy	1	1.00	109	1.5	140	1,856
PENTRAN 'Large' Model	8	0.74		165	1.3	42,100
PENTRAN 'Small' Model	8	0.74		123	1.7	35,000



Tally locations: Four Annular Segments Near Top

(494 cm – 563 cm)

- **<u>No results</u> for the unbiased MCNP case, after 220 hours on 8 processors**

A^3MCNP on 1 processor

[(mRem/hr)/n/cm^2/s]	FOM	PENTRAN/A^3MCNP
3.14E-06 (2.73%)[a]	8.974	0.84
1.70E-06 (3.36%)[b]	1.843	0.82
9.97E-07 (5.08%)[b]	0.806	0.79
5.11E-07 (3.52%)[b]	1.682	0.80

[a] 2.5 hrs, 1 CPU

[b] 8 hrs, 1 CPU

Remarks

•To solve large/complex real-world problems in a reasonable amount of amount, we need to use hybrid methods

•Using deterministic importance function, A^3MCNP can solve large complex problems faster (few orders of magnitudes) than the unbiased MCNP.

•Besides the computation speed, systems like PENTRAN & A^3MCNP significantly reduce the engineer's time and improve confidence in results.