Monte Carlo Methods for Efficient Reactor Analysis

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Bojan Petrovic

- Since August 2007: Georgia Tech
  Professor, Nuclear & Radiological Engineering / Medical Physics
  - Reactor physics, transport theory, shielding
  - Monte Carlo methods for reactor analysis
  - Advanced reactor design
  - Computational medical physics
  - Methods development, numerical simulations

- 1999-2007: Westinghouse Electric Company
  Fellow Scientist, Science and Technology Department (R&D)
  - Advanced reactor design (IRIS, LMR-AMTEC, …)
  - Advanced fuels and fuel cycle
  - Nondestructive waste characterization
  - SNM detection
  - Methods development, numerical simulations

Research group

- Jordan McKillop, M.S. student
  - Variance reduction in MC shielding problems (using MAVRIC/SCALE)
- James Nathaniel, M.S. student
  - Shielding, sensitivity studies using Sn
- Bo Shi, Ph.D. student
  - Improved convergence/diagnostics of MC criticality simulations
- Jeff Ryckman, Ph.D. student
  - Simulations and variance reduction in computational medical physics (proton therapy)
- Vito Memoli, ("part-time" - visiting Ph.D. student from Politecnico di Milano)
  - Fast reactor analysis
- Ph.D. student starting next semester
  - MC depletion, error propagation

Outline/intent of today's talk

- Use of Monte Carlo for reactor analysis
- Present several ongoing research projects
- Identify areas for possible collaboration

Monte Carlo methods for simulation of nuclear systems

- Potentially most accurate
- Computationally intense; inherently: $(1/\sigma) \sim N^2$

- Traditionally used for benchmarking/reference
- Strong interest to make MC practical for routine use

DRIVERS:

- Current reactors: improved safety and/or margin, which translates into economic benefit
- Advanced reactors: complex designs require improved methods to accurately model without extensive testing
- Benchmarking of new methods

ENABLERS:

- Steady increase in computational power
- Improved methods

Monte Carlo methods in reactor analysis

Increasingly more challenging:

SHIELDING (FIXED SOURCE)
- Localized/discrete detector(s)
- Flux/dose distribution “everywhere”

CRITICALITY SIMULATIONS
- Critical systems (reactor)
- Criticality safety

CRITICALITY SIMULATIONS WITH DEPLETION
- Reactor, fuel depletion

INCLUDING CONTROL/FEEDBACK
- Criticality
- Feedback

Monte Carlo methods in reactor analysis

SHIELDING (FIXED SOURCE)

Requires many histories

Independent histories; determining uncertainty/convergence in principle “straightforward”

- Localized/discrete detector(s)

  Automated variance reduction needed – reasonably well understood – e.g. CADIS

- Flux/dose distribution “everywhere”

  Automated global variance reduction needed – e.g. FW-CADIS

CRITICALITY SIMULATIONS [additional “external loop”]

Slow/false source convergence

Stationarity diagnostics

Underestimated uncertainty (correlated batches)

Difficult to accelerate

- Critical systems (reactor) [depletion/feedback]
- Criticality safety [loosely coupled, undersampling]

CRITICALITY SIMULATIONS WITH DEPLETION [additional “external loop”]

- Reactor, fuel depletion

  Uncertainty estimation and propagation

PLUS CONTROL/FEEDBACK [additional “external loop”]

Computer resources

Tools (couple to T/H, variable temperature cross sections, ….)

Ongoing research projects at Georgia Tech

1) SHIELDING (FIXED SOURCE)

- Flux/dose distribution "everywhere"

    Using MAVRIC sequence in SCALE6 (FW-CADIS) to analyze IRIS

2) CRITICALITY SIMULATIONS

    Source convergence / improved stationarity diagnostics

3) CRITICALITY SIMULATIONS WITH DEPLETION

    Uncertainty estimation and propagation

Work in progress…..

(1) Fixed source (shielding)

Dose/flux distribution “everywhere”

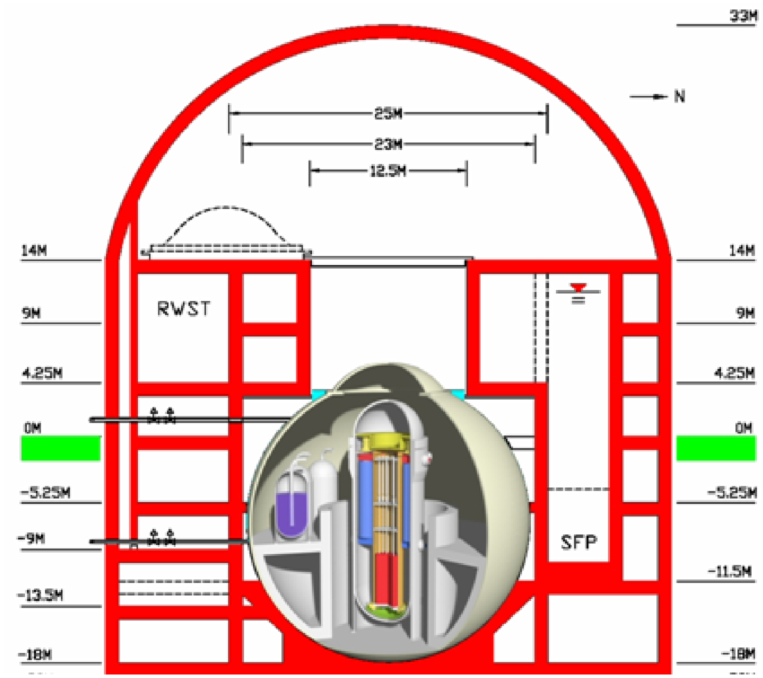
Code/Method: MAVRIC/FW-CADIS

Test problem: IRIS reactor

(Determining radiation environment throughout the plant)

IRIS – International Reactor Innovative and Secure

- Advanced integral light water reactor
- 335 MWe/module
- Innovative, simple design
- Enhanced Safety-by-Design™
- International team
- Potential for deployment as Grid Appropriate Reactor
- Anticipated competitive economics
- Cogeneration (desalination, district heating, bio-fuel)
- NRC pre-application underway
- Design Certification testing program underway
- Interest expressed by several countries
- Projected deployment target: 2015 to 2017
- Compact design - single building integrates containment, reactor and auxiliary building

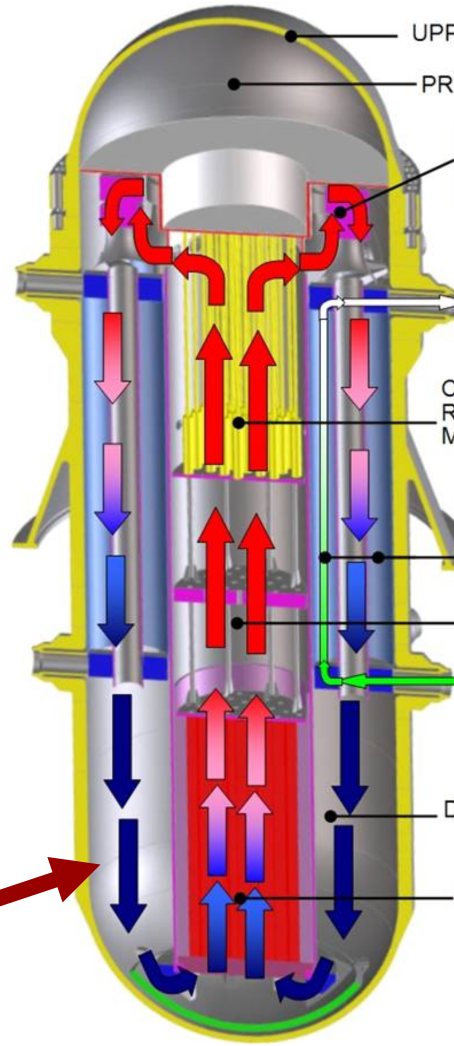


IRIS Integral Reactor Vessel

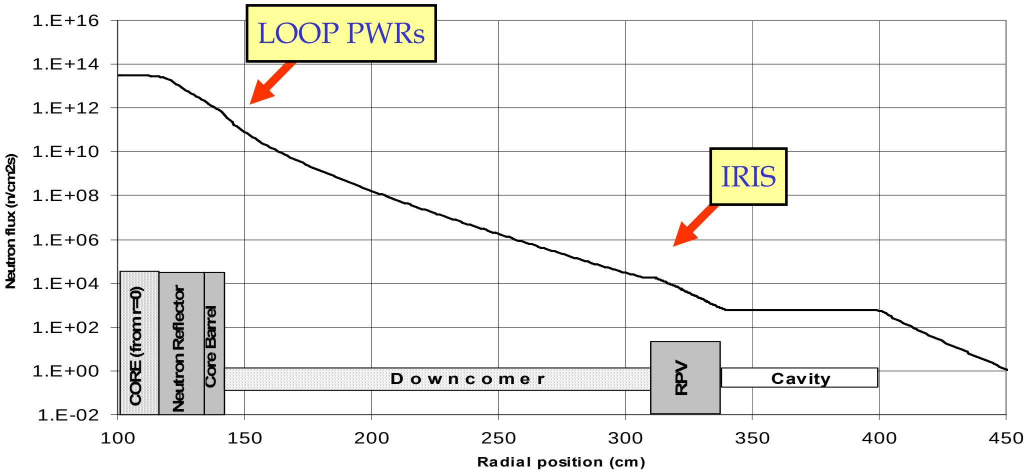
No external primary loops, all primary components inside the vessel

- 8 helical-coil steam generators
- 8 axial flow fully immersed primary coolant pumps
- Internal control rod drive mechanisms
- Integral pressurizer with large volume-to-power ratio

Thick (1.7m) downcomer provides extra shielding compared to loop PWRs



Benefits of (inherent) additional shielding

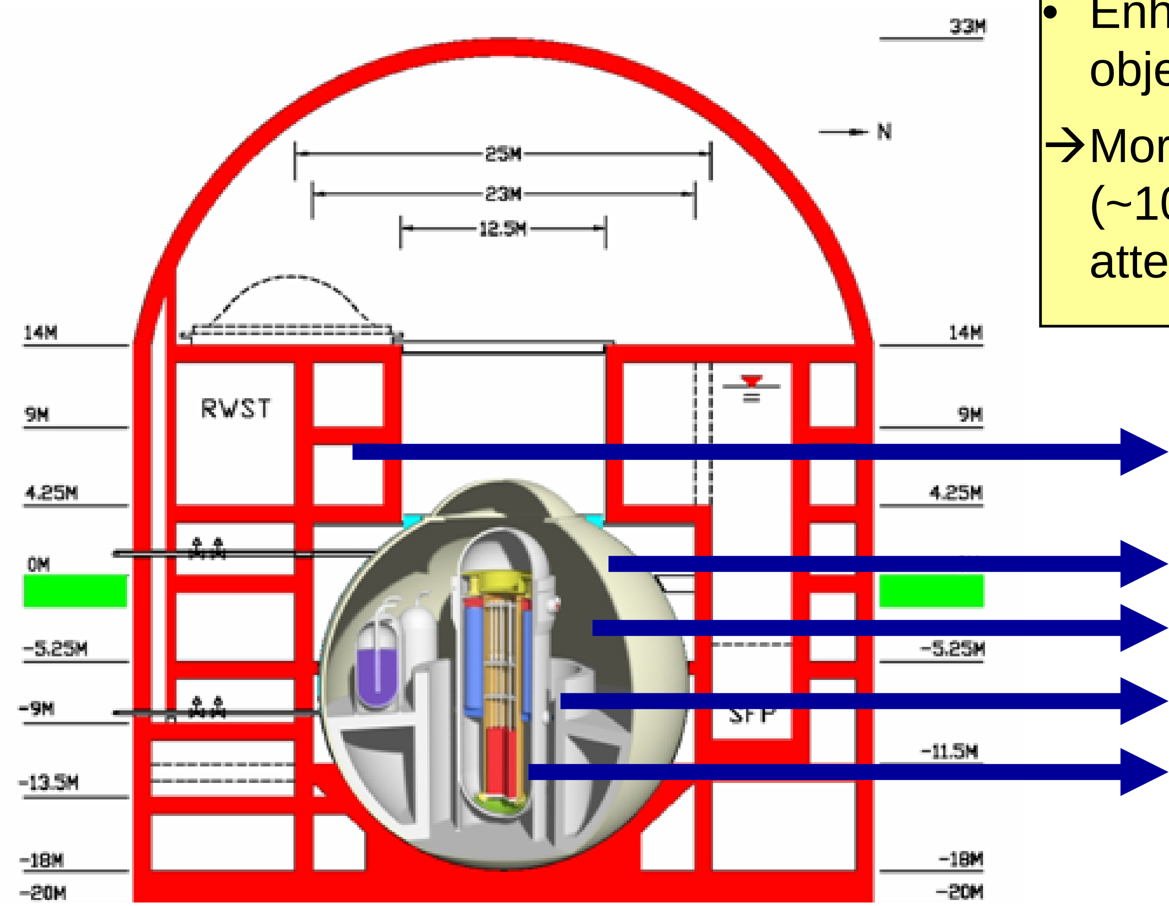


- Fast neutron fluence to RV drastically reduced (~6 orders of magnitude)
- Practically no embrittlement
- RV surveillance program not needed (O&M cost reduction)
- Strongly reduced activation
- “Cold” outer RV surface
- Reduced dose for maintenance operations
- Reduced dose/simpler ultimate decommissioning
- Vessel could act as sarcophagus for ultimate disposal

IRIS Shielding Analysis - Challenges

- Integral configuration, extra shielding
- Enhanced dose reduction objectives

→More complex shielding analysis (~10 orders of magnitude fast flux attenuation to vessel outer surface)



Dose in accessible areas = ?

Dose at CV boundary = ?

Dose in maintenance = ?

Concrete activation = ?

RV fluence =?

IRIS Shielding Analysis - Approach

- Core physics (Westinghouse) → Fission source distribution

MC + S_N

- Improved confidence in results
- Exploit advantages of each method

Shielding analysis (employing expertise within the IRIS team)

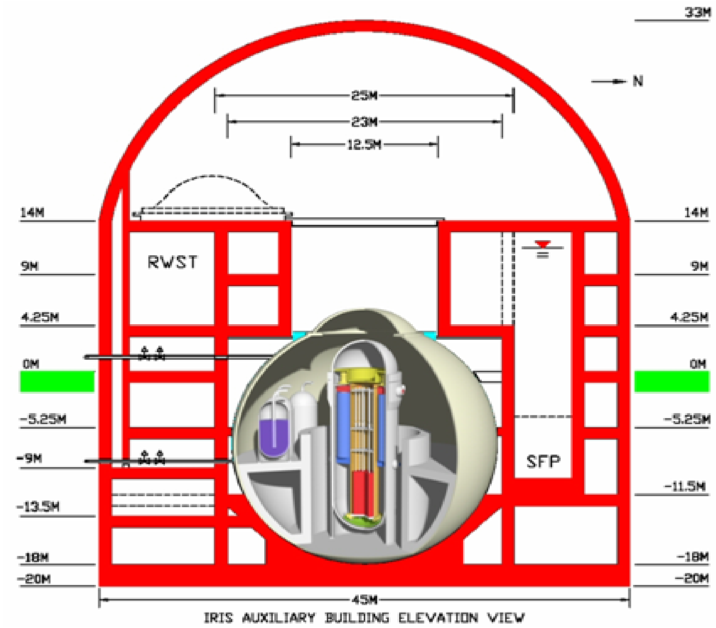
- Monte Carlo – MCNP + DSA (K. Burn, ENEA)
- Deterministic – 3D TORT (M. Sarotto, M. Ciotti, ENEA)

And

Investigate using SCALE/MAVRIC
to facilitate obtaining MC solution over the large domain

IRIS Reactor Vessel + Containment + Building

- Large spatial domain:
  Building – cylindrical, ~50m diameter
- Complex geometry:
  Shields (walls) and cavities

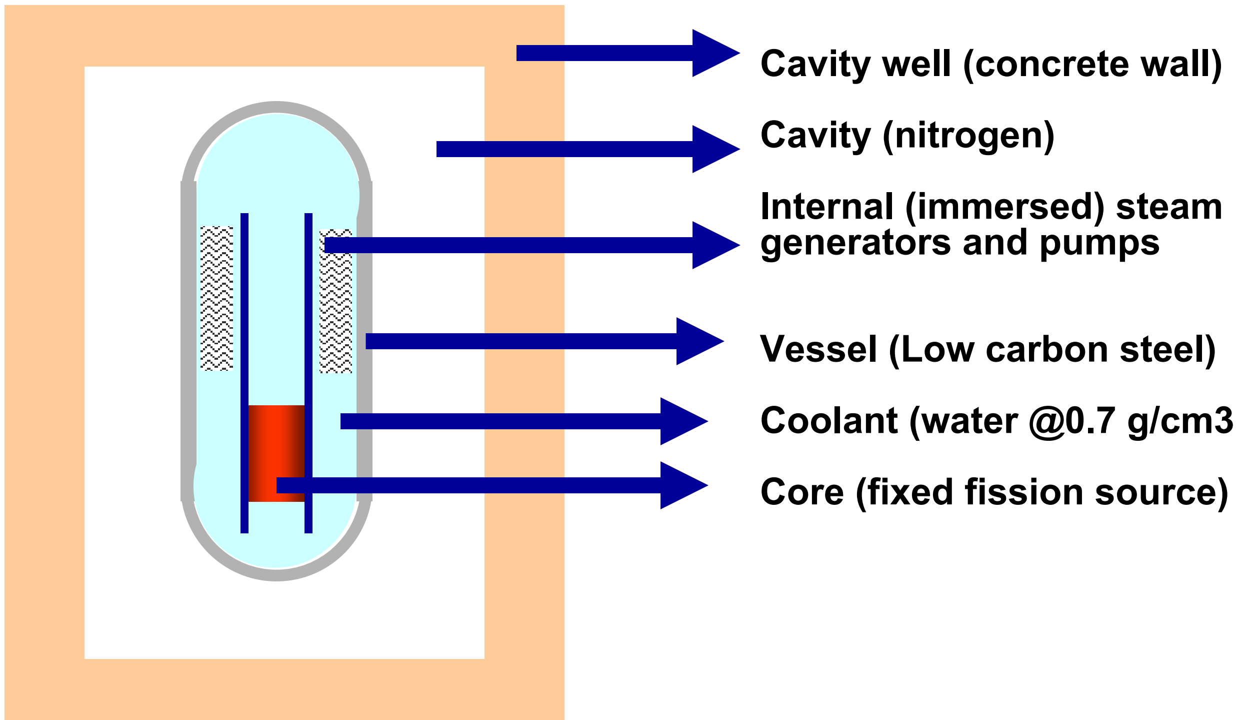


Focus of MAVRIC studies:

Obtain an indication of the flux/dose distribution "everywhere" in the containment (initially) and building (later) to guide detailed studies

Initially –use very simplified model(s) to obtain approximate results

Preliminary / Simplified Geometry for Initial Evaluation



- Very simplified geometry, still 14m x 14m x 30m
- Nevertheless, preserved essential features and difficulties of the actual geometry
- Suitable for investigating the capability to generate global flux/dose distributions throughout a large spatial domain

Preliminary Results

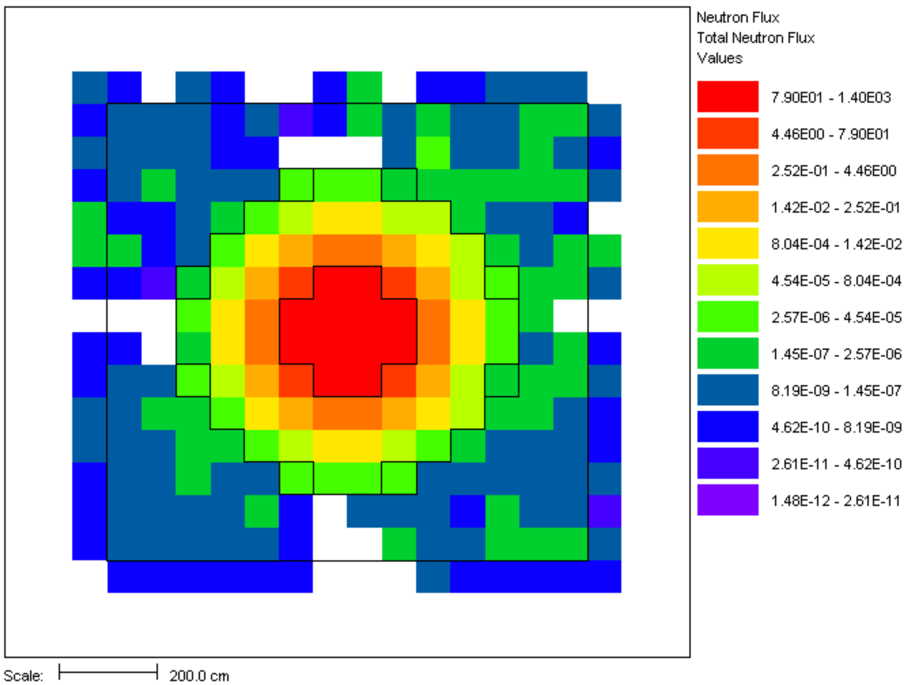
>1MeV: flux and relative uncertainties distribution

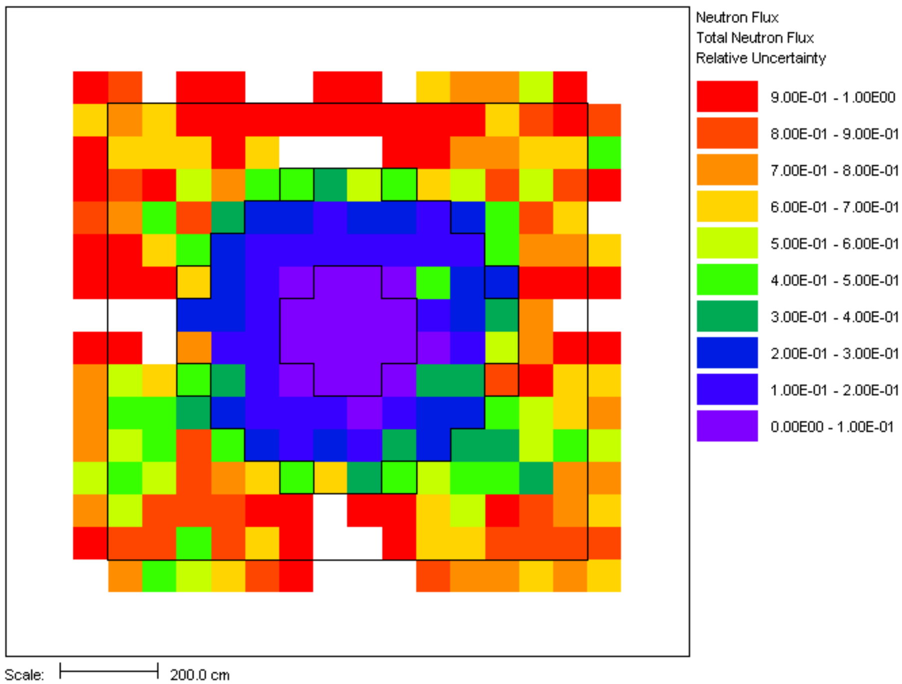
~15 min adjoint+forward S_N

~2 min MC

(on a Dell PC)

radial distribution (at core midplane) – fast flux and uncertainties

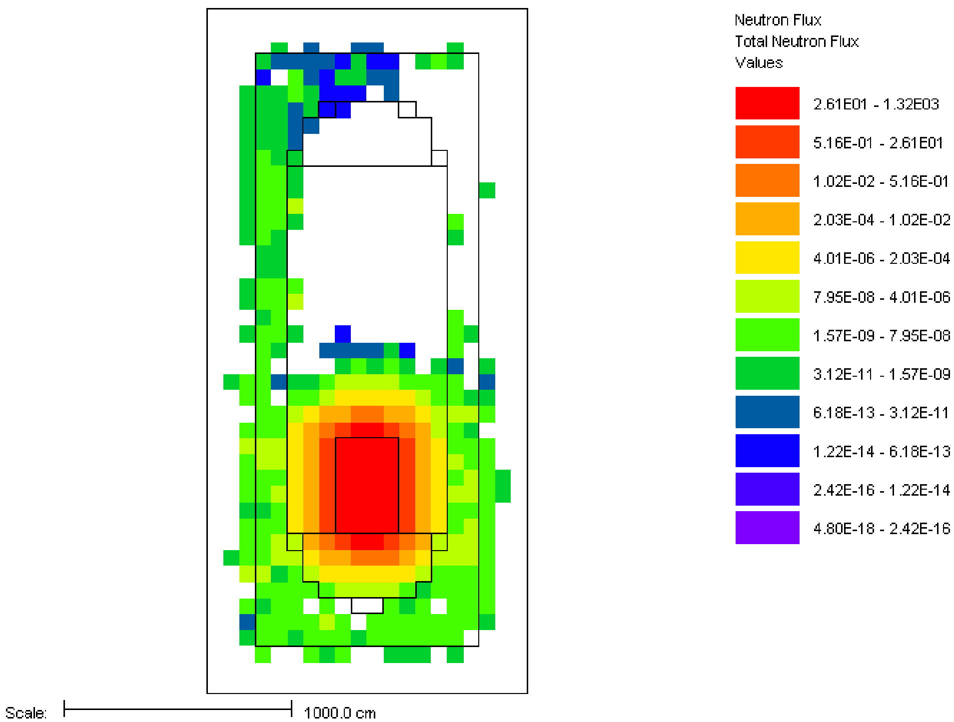


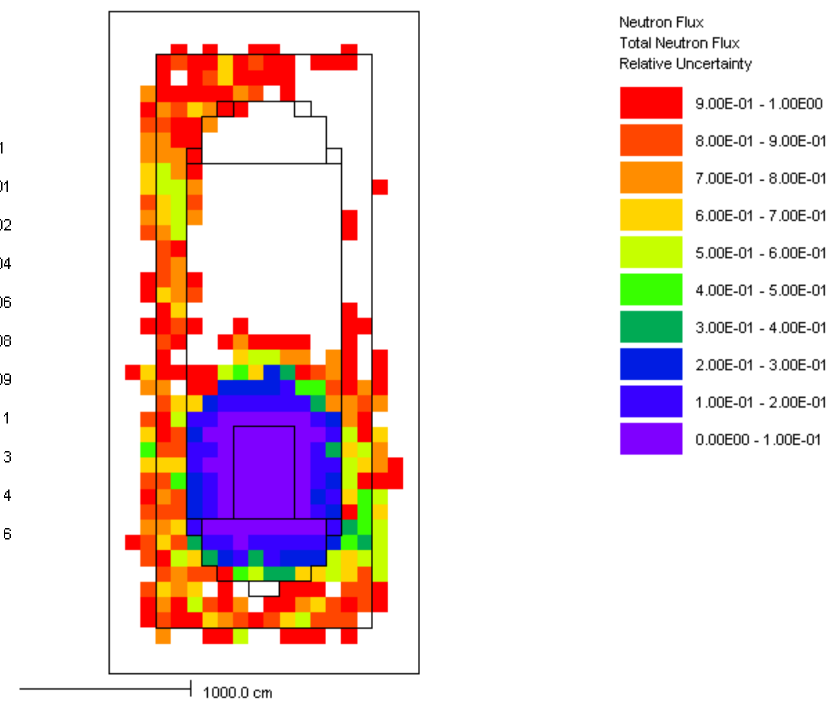


Preliminary Results

>1MeV: flux and relative uncertainties distribution

~15 min adjoint+forward S_N + ~2 min MC

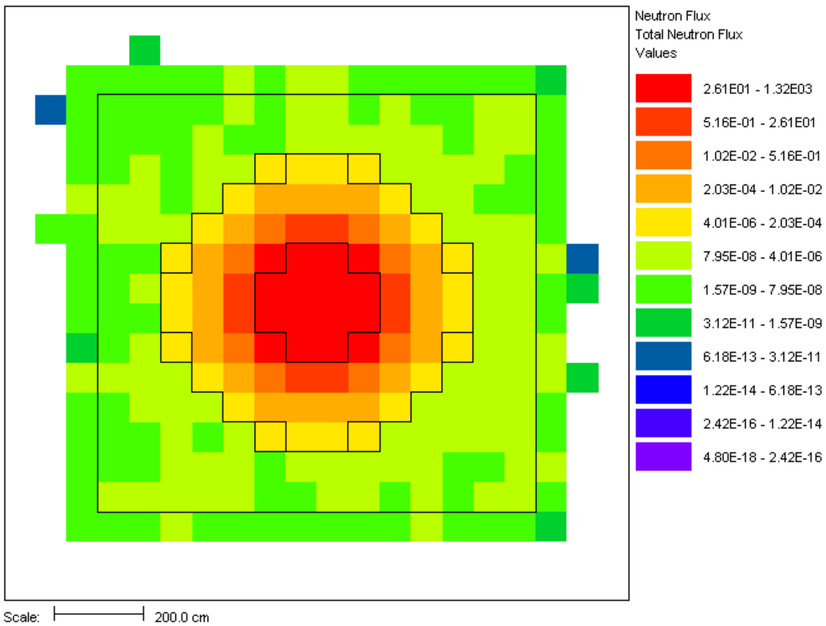


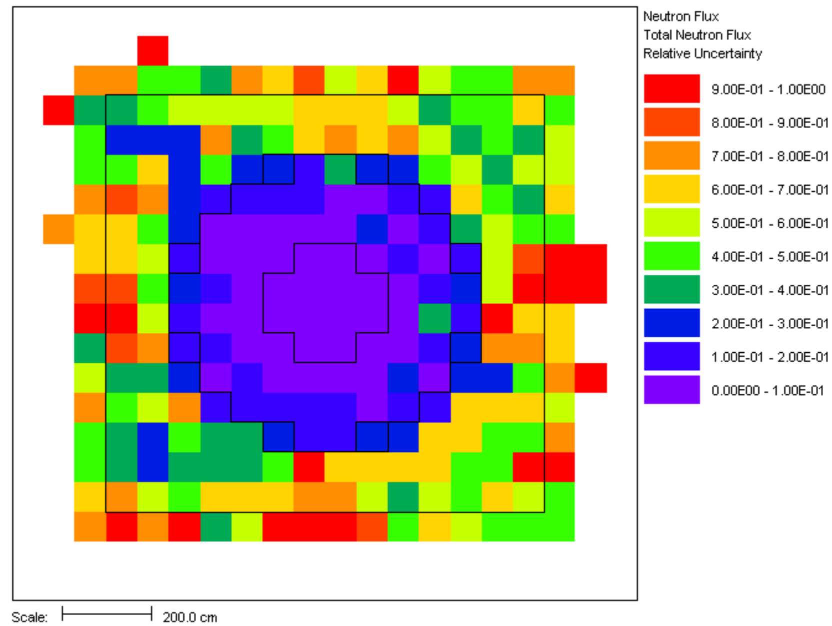


Preliminary Results

>1MeV: flux and relative uncertainties distribution

- ~15 min adjoint+forward S_N
- ~70 min MC (red to green → 12 orders of magnitude)
  [not bad, but noisy in spite of large voxels]



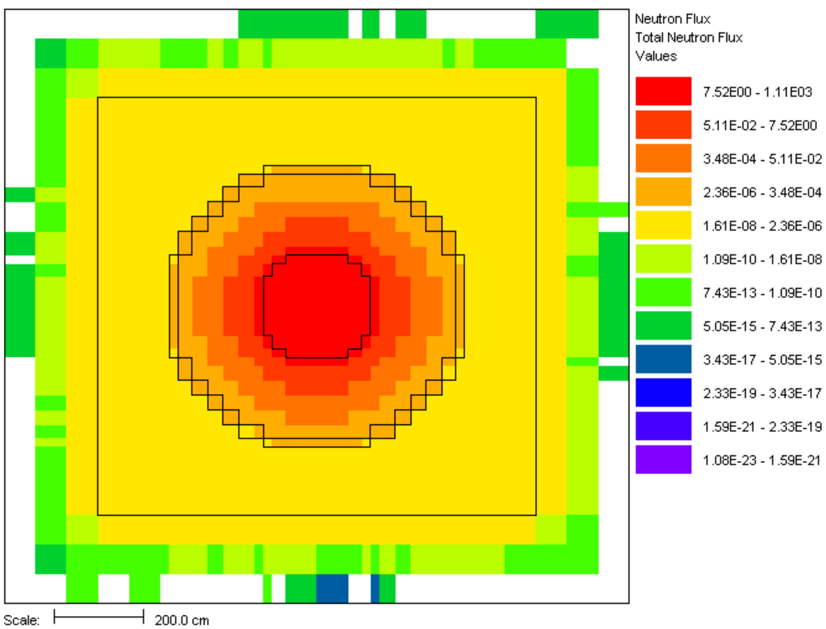


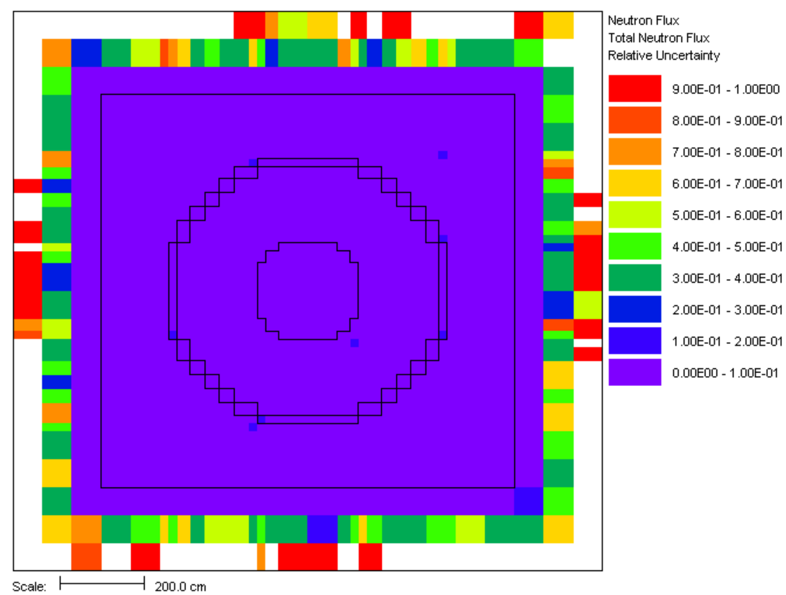
Preliminary Results

Finer mesh at core and RV boundary

>1MeV: flux and relative uncertainties distribution

~18+6 min forward+adjoint S_N + ~471 min MC = 8.25 h



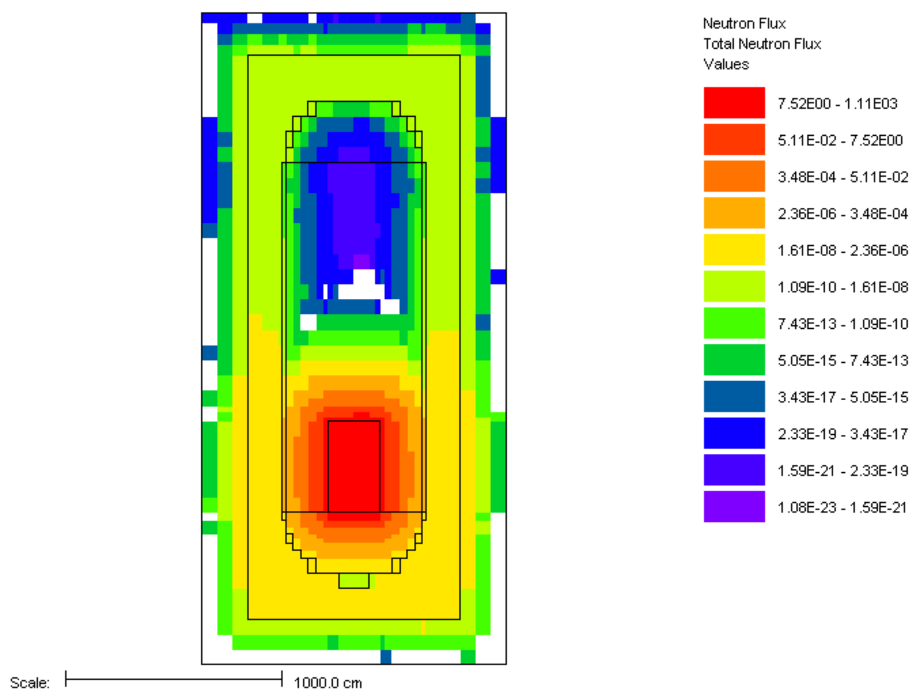


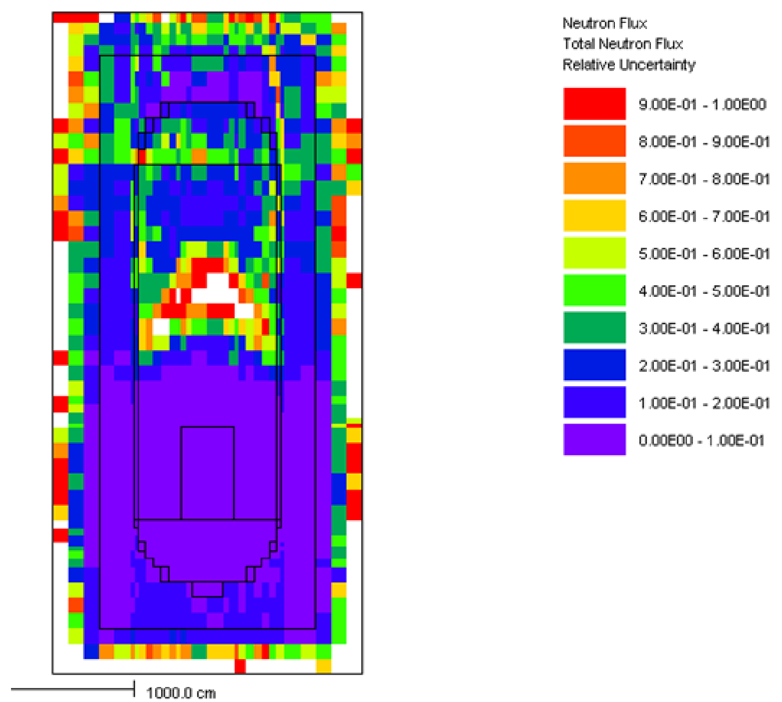
Preliminary MAVRIC/FW-CADIS Results of IRIS Shielding Analysis

>1MeV: flux and relative uncertainties distribution

~18+6 min forward+adjoint S_N + ~471 min MC = ~8.25 h

Useful results (over the ~12 orders of magnitude attenuation)





Initial findings/experience with MAVRIC

- Obtained indication of the global flux/dose distribution in large, deep penetration problem (IRIS – large integral vessel + containment + building)
- Relatively easy to set up and run
- Automated VR
- Obtained global distribution with reasonably reduced uncertainty over the large domain with limited use of both engineering and CPU time

- Further, examining:
  – Impact of Sn solution quality
  – Flux (fast, thermal), dose, activation …..

Impact of S_N solution quality

- Initial results: ~52K meshes, P_3S_8
- 100 batches @ 1M
- 18+6+471 min = ~8.25h

- Refined mesh: ~440K meshes, P_1S_6
  (reduced P_LS_N to enable finer mesh was necessary on PC)
- 20 batches @ 1M
- 43+17+798 min = ~14.3 h

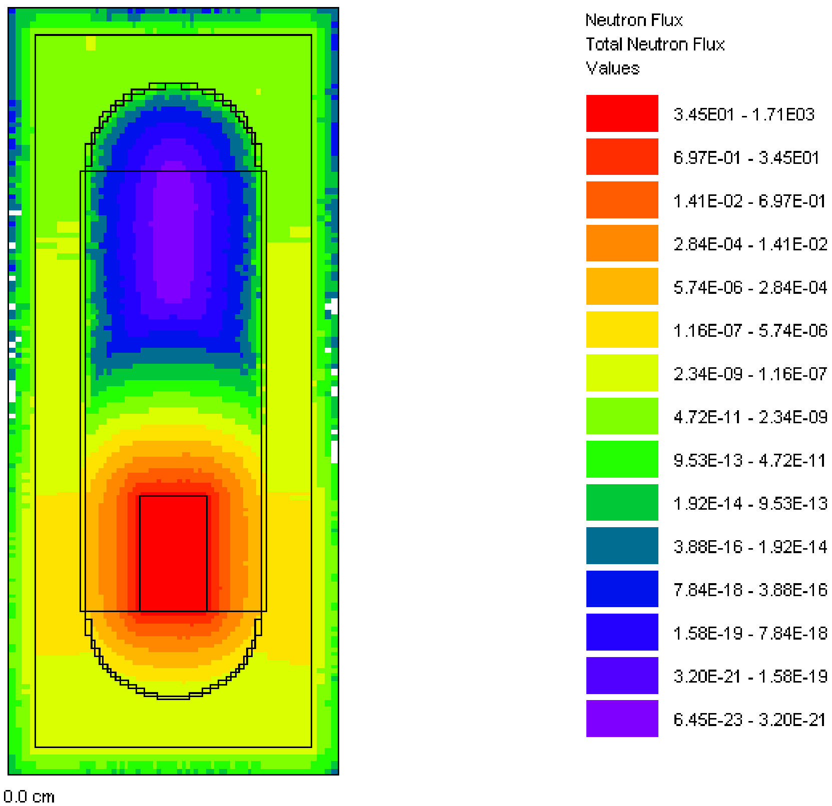
(Dell Latitude D630 CPU time quoted. About 3x faster on a workstation)

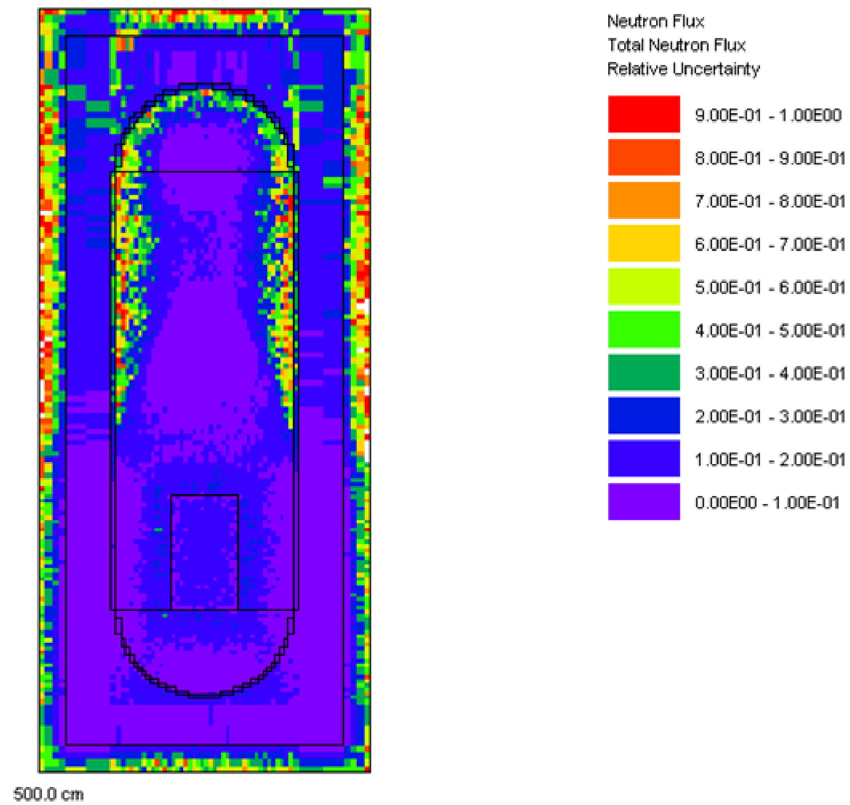
Refined S_N mesh results

>1MeV: flux and relative uncertainties distribution

~43+17+798 min = ~14.3 h

Very good performance (covers >15 orders of magnitude)





Impact of refined mesh / improved S_N

- ~52K meshes, P_3S_8
- 100 batches @ 1M
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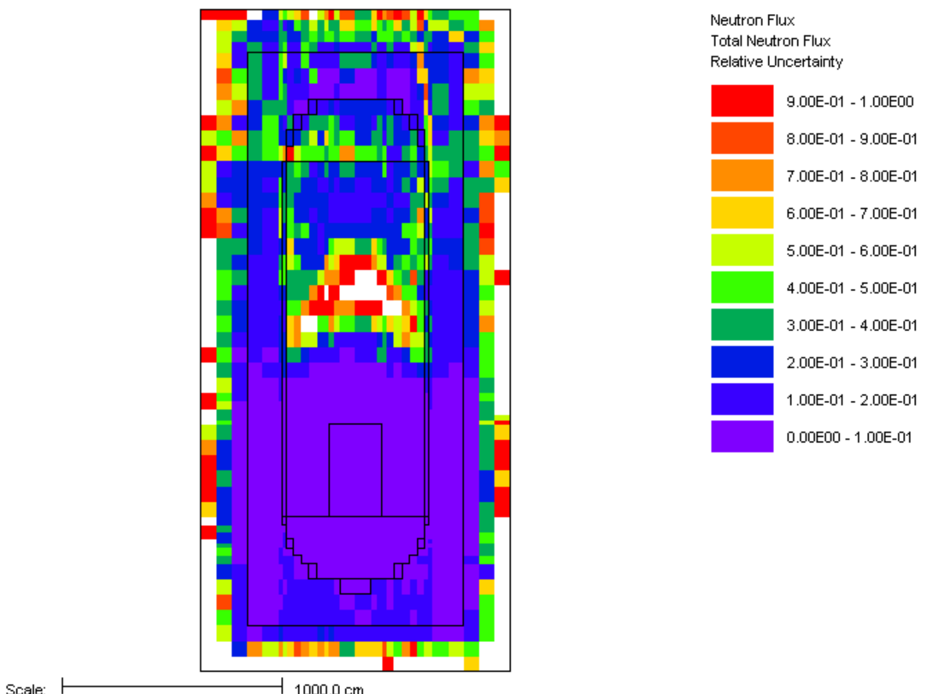

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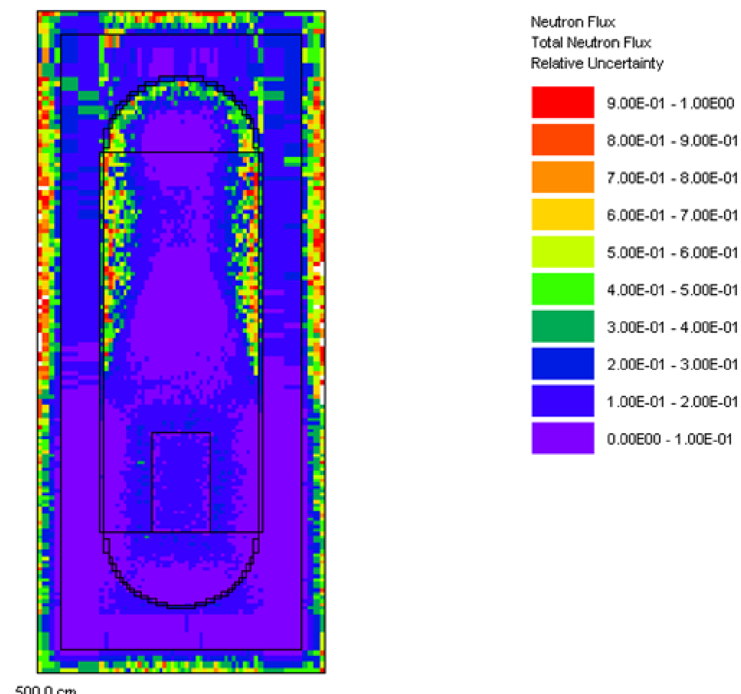
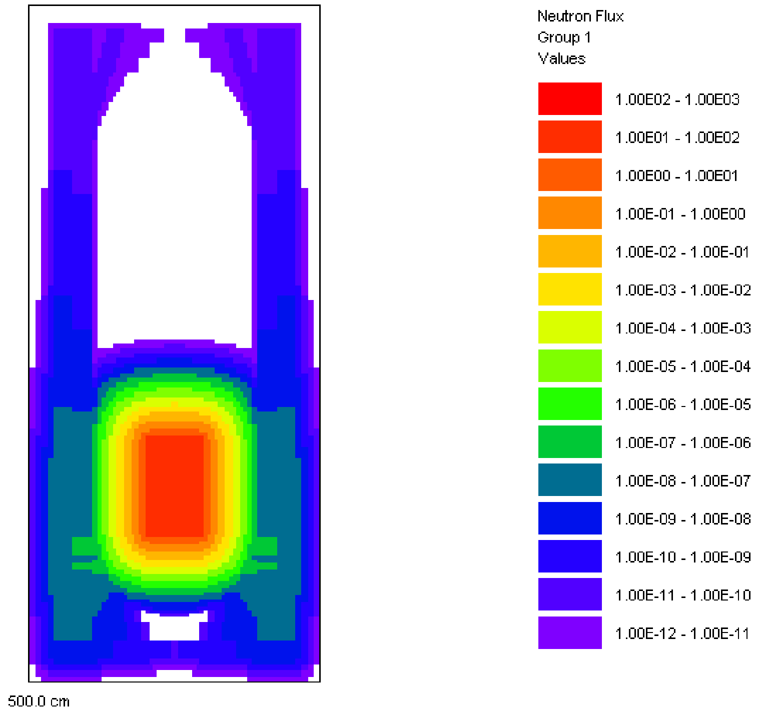


- Finer mesh – smoother/better MC convergence
- Less histories ~twice CPU, but more than compensated by gain in variance reduction

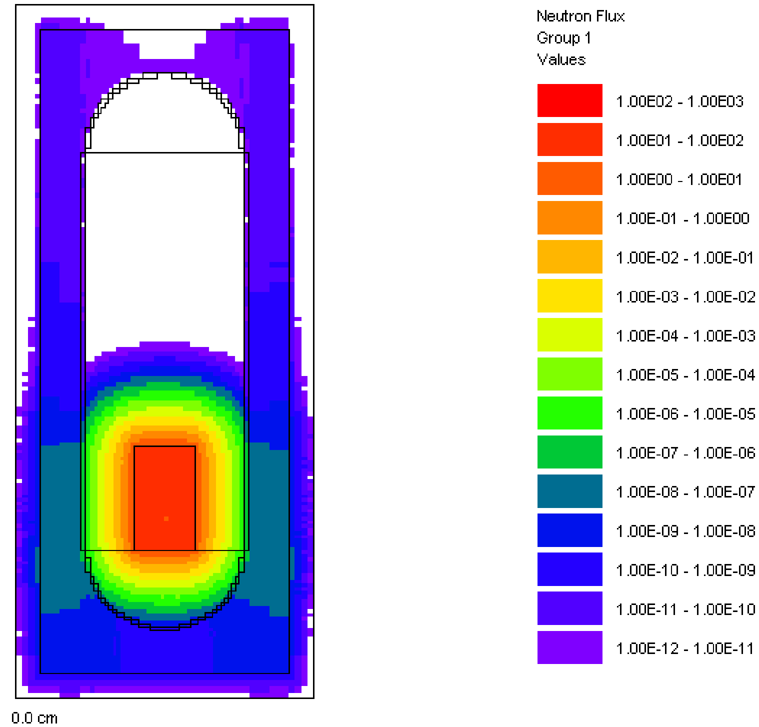
Impact of refined mesh / improved S_N

~440K meshes, P_1S_6, 20 batches @ 1M [43+17+798 min = ~14.3 h]

Forward Gr1 – S_N



Forward Gr1 - MC



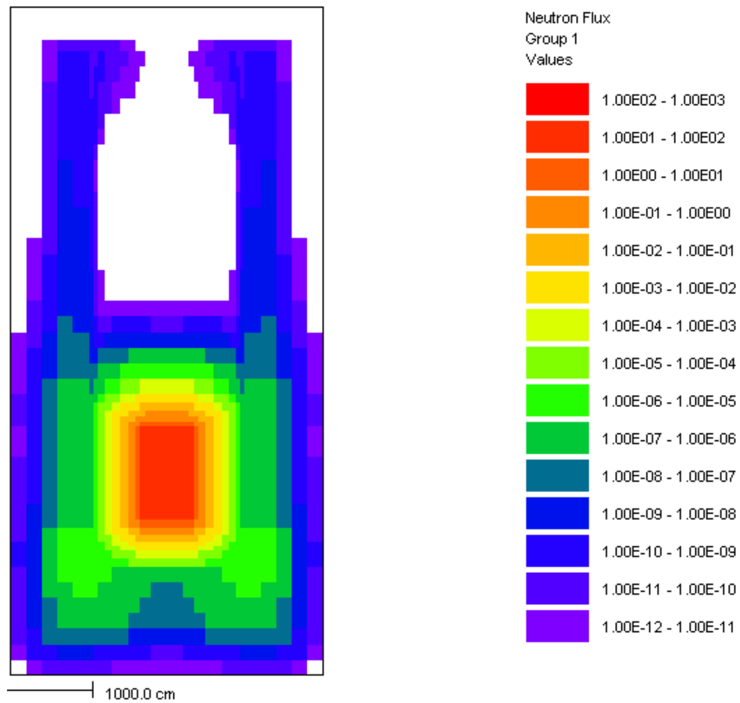
- Relatively accurate S_N (~ within order of magnitude)

  [consistent contour levels, defined to cut off below 1×10^{-12}]

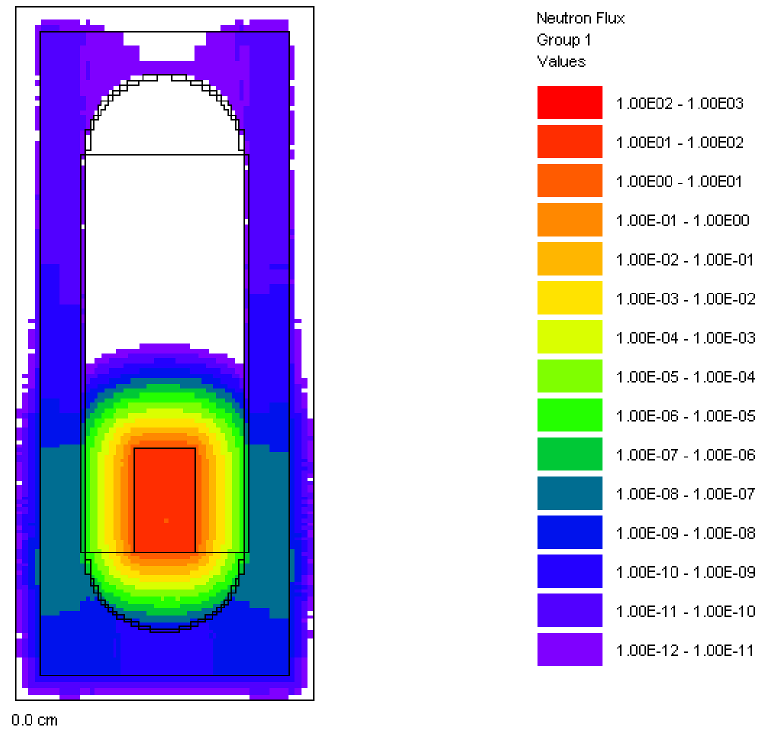
Impact of refined mesh / improved S_N

~52K meshes, P_3S_8 100 batches @ 1M [18+6+471 min = ~8.25h]

Forward Gr1 – S_N



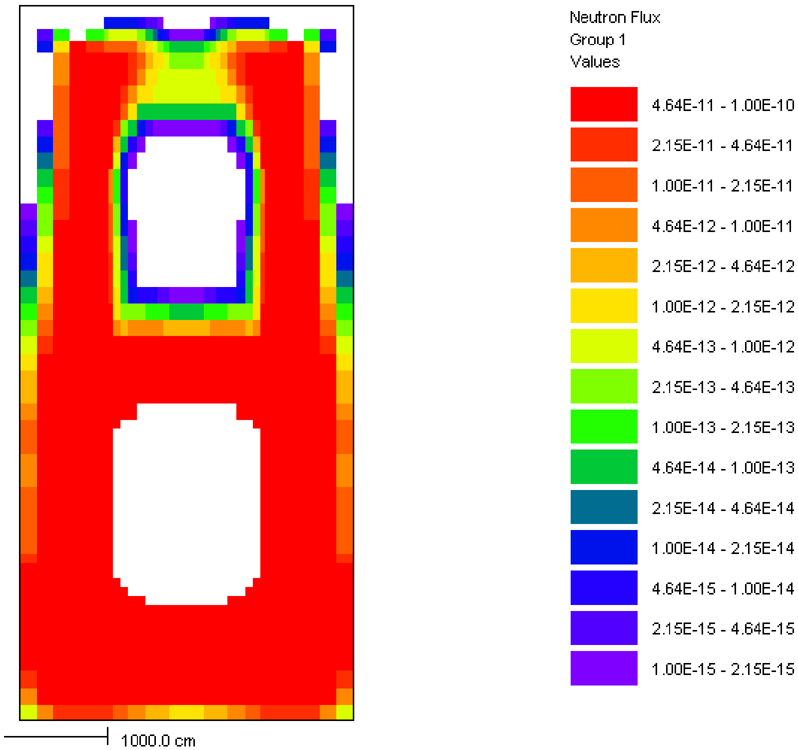
Forward Gr1 - MC



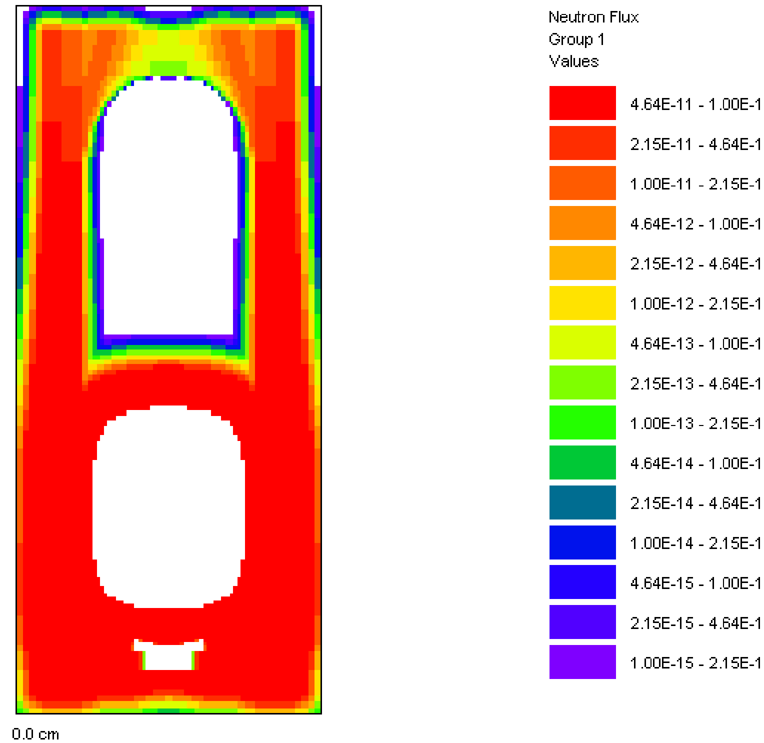
- Less accurate S_N
- Difference grows to exceed 2 orders of magnitude

Impact of refined mesh / improved S_N

- ~52K meshes, P_3S_8
- 100 batches @ 1M
- 18+6+471 min = ~8.25h



- ~440K meshes, P_1S_6
- 20 batches @ 1M
- 43+17+798 min = ~14.3 h



- Qualitatively similar, but difference several orders of magnitude upon closer inspection

(shows same results as previous VG but different contours)

Impact of S_N solution quality

- The approximate shape for S_N flux provides acceleration by orders of magnitude
- However, VR parameters directly depend on S_N (e.g., adjoint source weighted by inverse forward S_N flux)

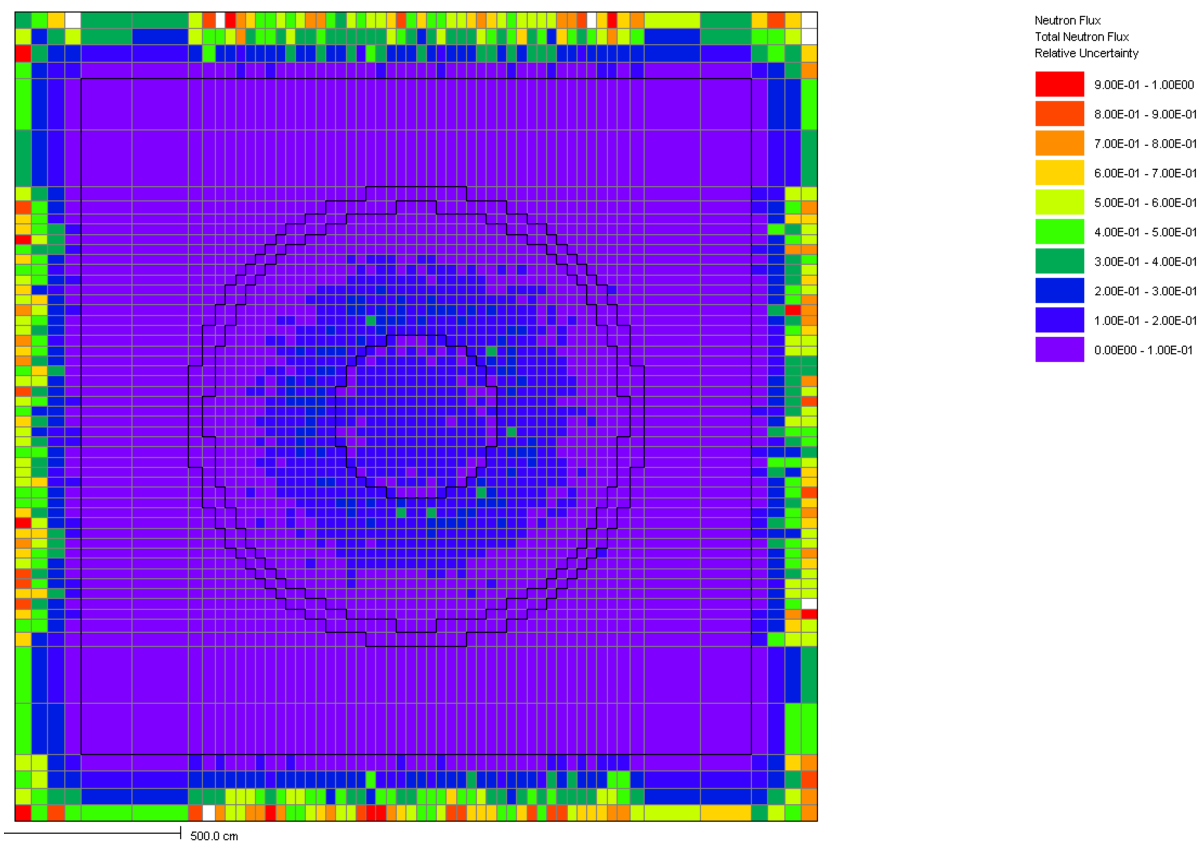
- Inaccuracy in S_N flux will lead to equally large region-wise "over/under-population" in MC simulation, requiring longer run time to compensate for weak spots (if we really mean that we need uniform uncertainties throughout)
- The desired MC uncertainty will dictate the optimum trade-off between the speed and accuracy of S_N solution

- How to maximize the overall efficiency? (difficult to quantify a priori the quality of S_N solution)

Detailed / group-wise flux distribution and uncertainty

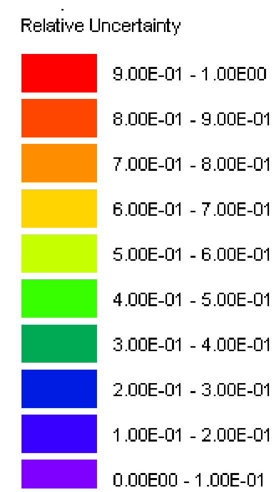
~440K meshes, P_1S_6, 20 batches @ 1M [43+17+798 min = ~14.3 h]

Total flux uncertainty (optimized for)

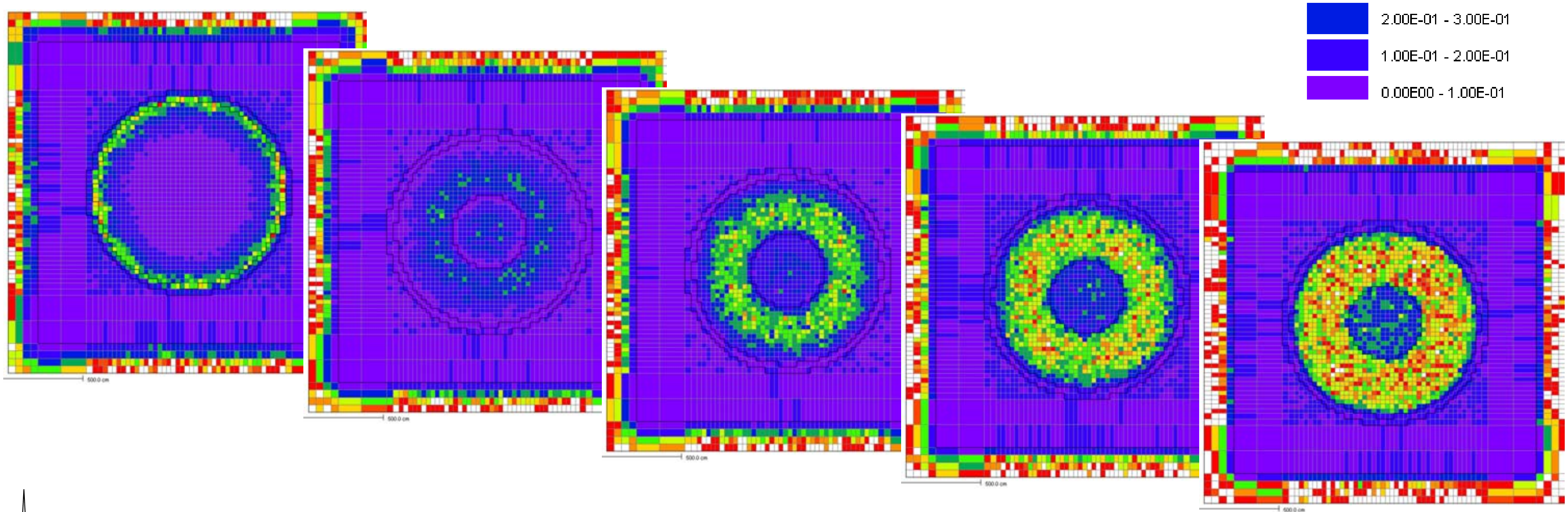


Detailed/group-wise flux distribution

- Note: MC VR is optimized for integral fast flux (total >1MeV) distribution
- Group-wise neutron flux distribution?
- Look at the relative uncertainty distribution – is it uniform?

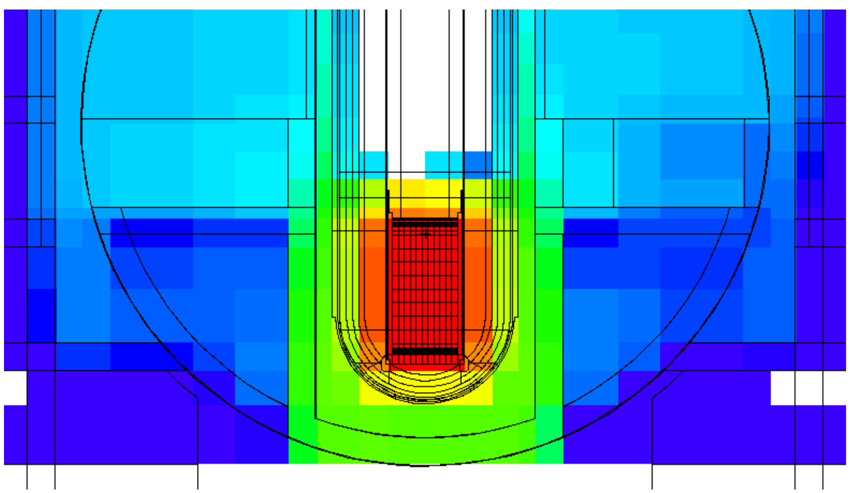


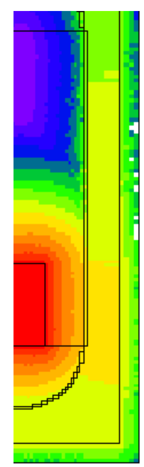
~440K meshes, P_1S_6, 20 batches @ 1M
Uncertainty group-by-group (1-5)

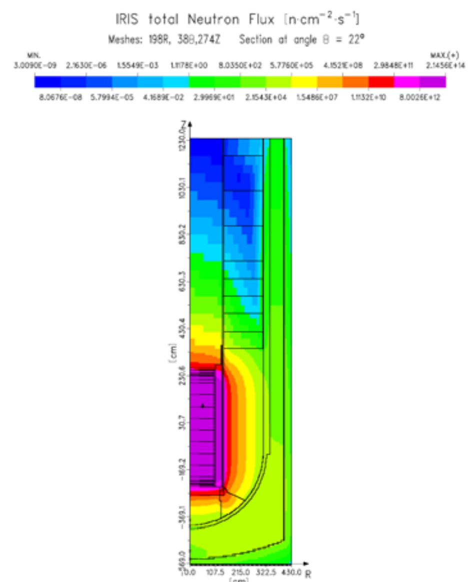


Work in progress and future work related to using MAVRIC/SCALE

- Trade-off between S_N and MC
- Detailed (group-wise) distribution
- Practical issues for fast/thermal flux, activation, dose, …
- Detailed IRIS power plant model
- Comparison to MCNP, TORT







(2) Criticality simulations

In search of improved stationarity diagnostics

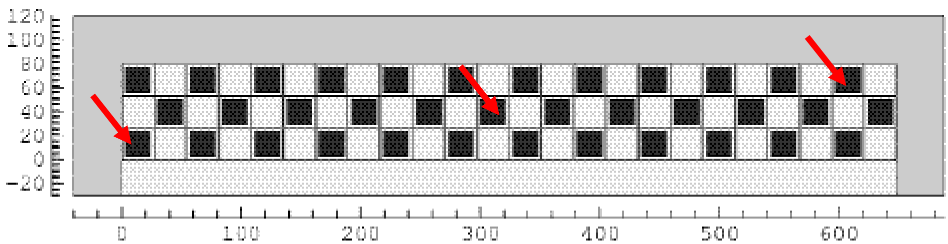
Monte Carlo criticality simulations

- Slow convergence
- False convergence
- Difficult to establish convergence criteria
- Underestimated statistical uncertainty (correlated histories)
- Under-sampling
- Potentially inaccurate fission source (flux, power) distribution
- Potentially significant reactivity underestimate (NCS)
- Computationally challenging
  (one more implicit level to resolve – eigenvalue/mode)

OECD Benchmark #1 - Spent fuel pool, checkerboard pattern of assemblies (more loosely coupled than core)

EXAMPLE OF A REAL-LIFE APPLICATION
WITH POTENTIAL FOR UNDERSETIMATING Keff

15x15 FAs, 5%U235
Concrete on 3 sides
on the fourth side
Initial source uniform and
at different positions
36 prescribed cases
Almost completely decoupled FAs
Extremely slow source convergence
Somewhat similar to an exaggerated
case of a large core, checkerboard
pattern, with very low-reactivity
twice-burnt fuel



Groups/Codes and basic results Water
(Trans. ANS)

Group	Code	Data	Contributor(s)
ANL	VIM	ENDF/B-V	Roger Blomquist
JAERI	MCNP 4B	JENDL3.2	Takeshi Kuroishi
JNC	Keno	SCALE4.4	Shirai Nobutoshi
KFKI	MCNP 4C	ENDF/B-V&VI	Gabor Hordosy
LANL	MCNP 4C	ENDF/B-VI	Forrest Brown
ORNL	KenoV	ENDF/B-V	John Wagner, Lester Petrie
ANSWERS	MONK8A	JEF2	Dave Hanlon

	Min	Max	Case 27
ANL	0.8508 (0.0006)	0.8548 (0.0015)	0.8538 (0.0006)
JAERI	0.8870 (0.0005)	0.8920 (0.0008)	0.8895 (0.0005)
JNC	0.8773 (0.0013)	0.8836 (0.0013)	0.8825 (0.0006)
KFKI	0.8800 (0.0011)	0.8838 (0.0008)	0.8828 (0.0005)
LANL	0.8773 (0.0011)	0.8826 (0.0004)	0.8803 (0.0004)
ORNL	0.8782 (0.0007)	0.8825 (0.0007)	0.8825 (0.0007)
ANSWERS	0.8837 (0.0010)	0.8884 (0.0006)	0.8867 (0.0006)

Simple problem to demonstrate source convergence issues

(B. Petrovic, 2001, Trans. ANS)

Thick slabs (400 cm),
alternating, high-low reactivity

PWR-like:

- 40% UO_2, 10% Zr, 50% water
- homogeneous mixture

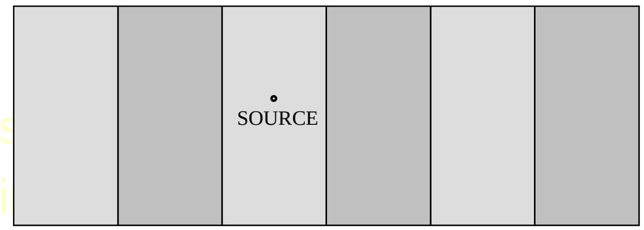
U235 enr.: 1% - 2% - 1% - 2% ….

INITIAL SOURCE
Center of 1% ^{235}U (low-reactivity) slab

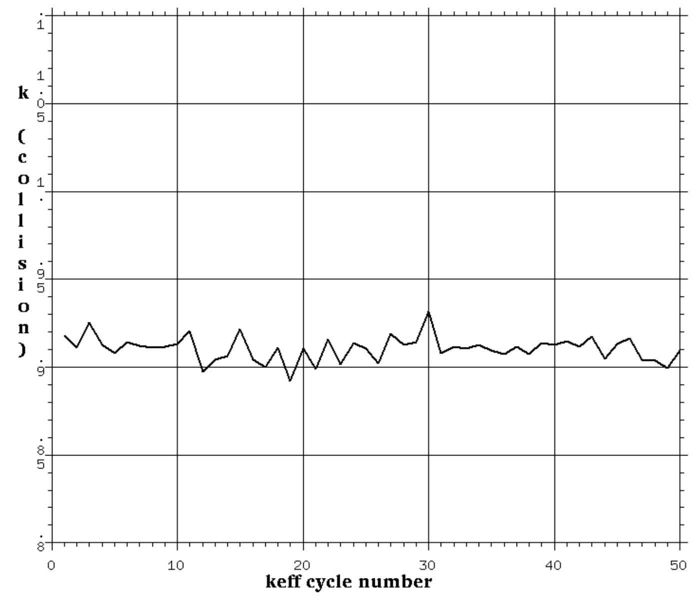
MCNP, 50 generations (cycles)
5,000 neutrons/generation

All 10 statistical checks OK
(no entropy test)
No warnings/indications

Converged to k~0.91
CORRECT RESULT IS k~1.08 !!



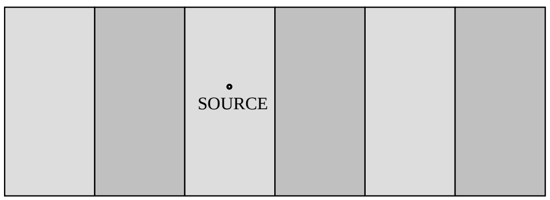
Kinf1.xls
inf01b, i
info2b, inf03b,...

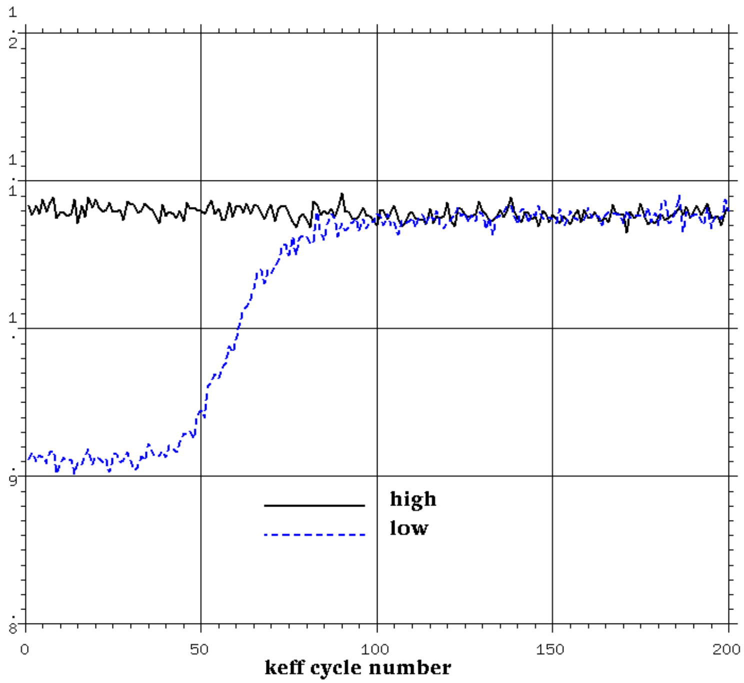


VG 36

Issue – convergence to eigenmode
Bracketing k

HIGH-LOW REACTIVITY ALTERNATING SLABS (200 generations, 20,000 n/gen)





Initial source very different from eigen-distribution if started in low-reactivity slab, but it does not initially impact k

Need to skip more cycles
(~100 if start in low reactivity region)

Initial source position
- High-reactivity slab (black)
- Low reactivity slab (blue)

Here, k-eff "bracketed" from below/above
But, difficult to bracket in real-life problems

Entropy criterion more likely to detect the unconverged source?

Use of entropy for stationarity diagnostics

- Entropy in Information theory (Shannon Entropy) is a measure of the uncertainty associated with a random variable
- Introduced into MC criticality simulations to check the stationarity of fission source distribution

$$H(S^B) = -\sum_{i=1}^{B} S^B(i) \log_2 \left(S^B(i)\right)$$

Simple example:

- N-mesh system
  - Uniform source distribution: maximum H;

    P=1/N

    H_{max}=-N*1/N*$\log_2(1/N)=\log_2(N)$
  - Source in one mesh only: minimum H

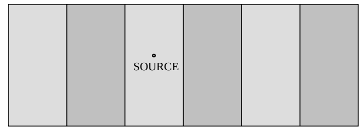
    $H_{min}=0$

Entropy diagnostics – examined in many recent studies

Still, it is an integral parameter…..

Entropy diagnostics applied to slab problem

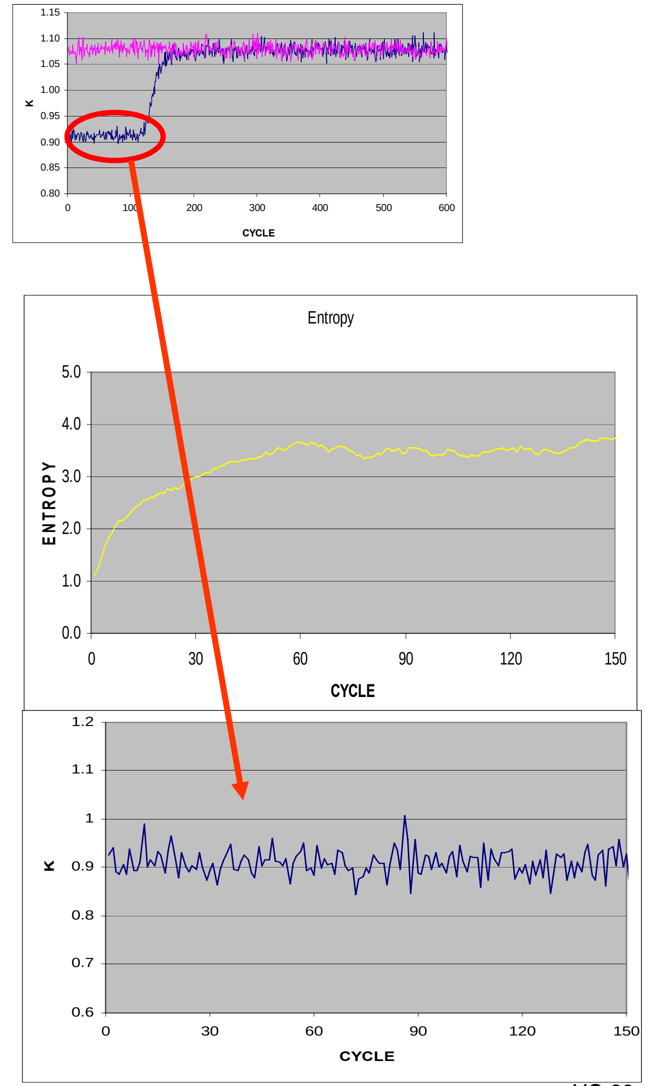
- If the source is initialized in low-reactivity slab
  - 150 cycles
  - Skip 60



- Passes both the k convergence and entropy check…..
  Still with completely incorrect answer k=0.92

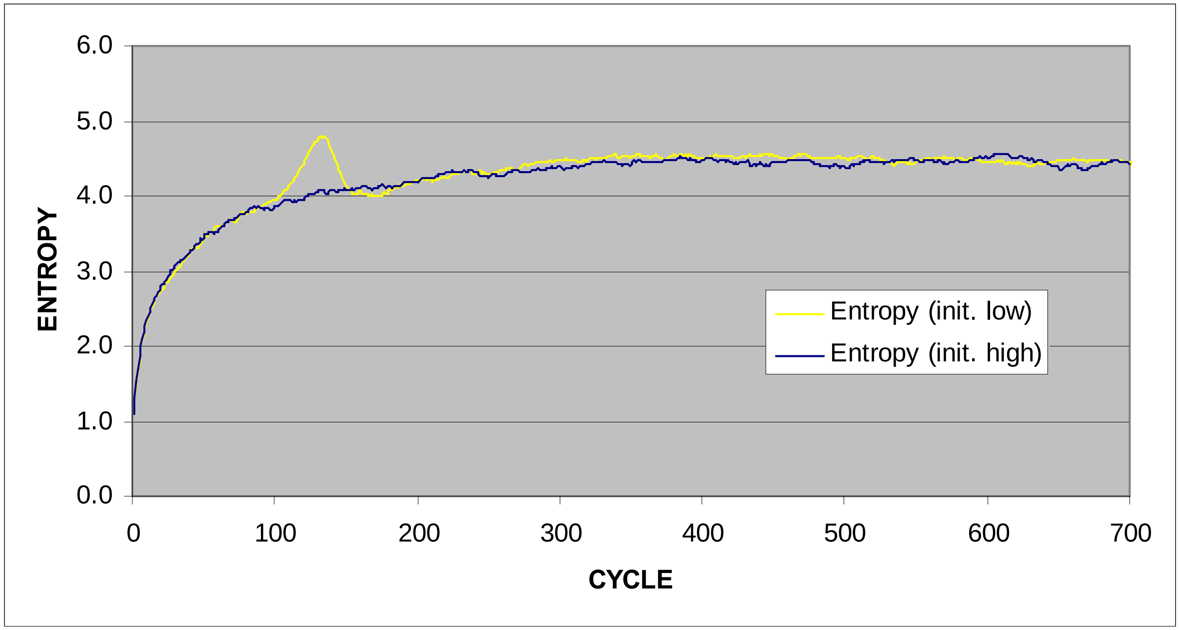
```
Average fission-source entropy for the last half of cycles:
H=  3.77E+00  with population std.dev.=  2.63E-01
Cycle   53 is the first cycle having fission-source
entropy within 1 std.dev. of the average
entropy for the last half of cycles.
At least this many cycles should be discarded.
Source entropy convergence check passed.
```

Entropy – a single number (like k).
Two different (not converged) source distributions may have similar entropy



Entropy diagnostics applied to slab problem

- In both cases, entropy initially primarily reflects spreading of the initial delta source, even though very different k (~0.92 vs 1.08) and distribution



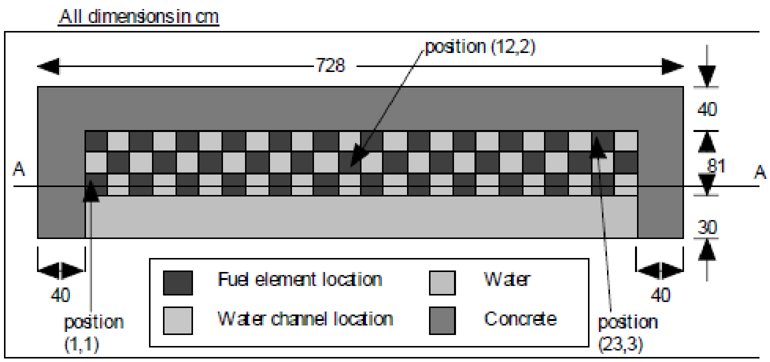
Entropy bracketing (convergence from above/below)

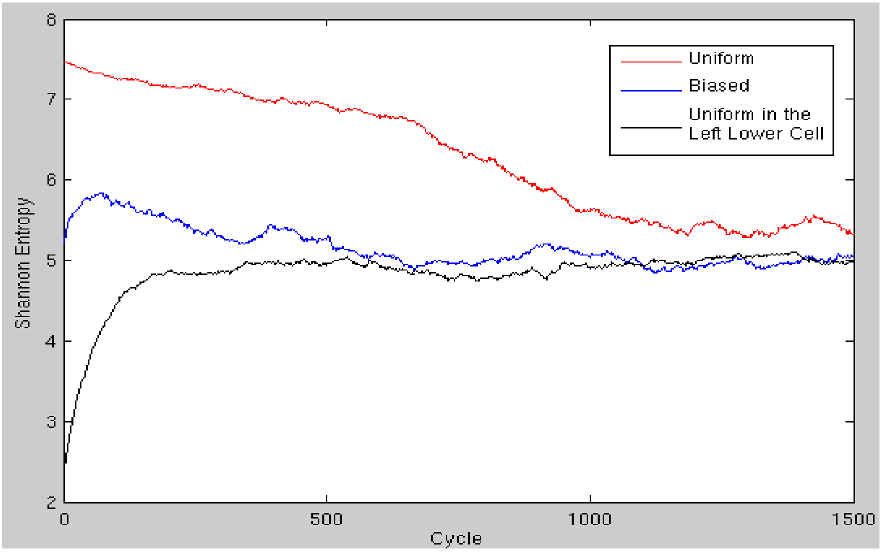
Similar problem with entropy as with k-eff: deciding when it has converged

Attempt to bracket entropy from above/below – applied to OECD Bench#1

- Uniform source;
- Biased source, upper left lattice position (high reactivity) has 81% of initial source (90% for both X and Y direction)
- Uniform source in lower left lattice position (low reactivity)

Here, seems to provide good indication
Is it useful/practical in general cases?





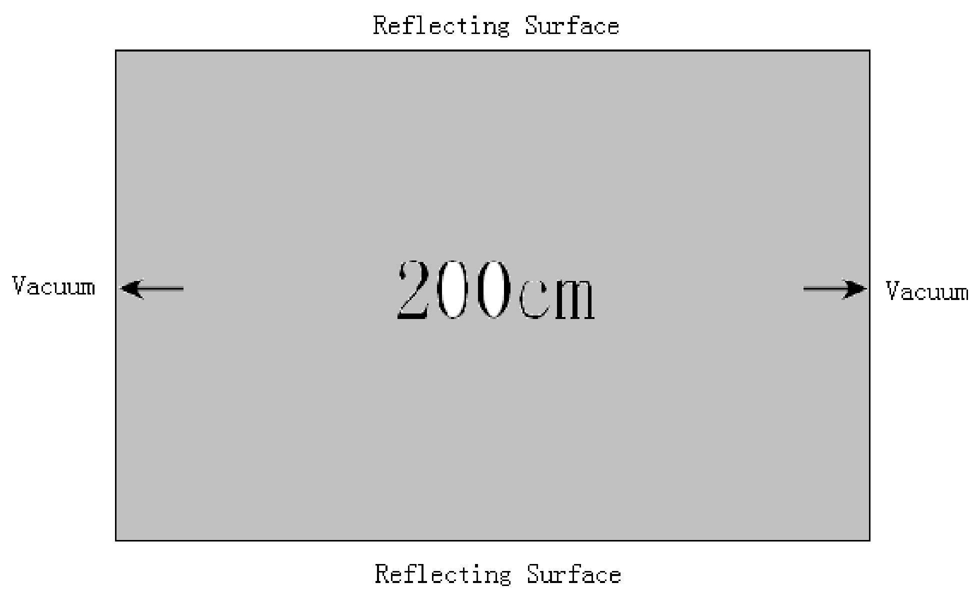
Collision entropy

- The current use of entropy is based on source sites ("Source Entropy")

- Introduce "Collision Entropy" (based on the collision sites)
  - The collision rate is related to the flux distribution, and thus can also represent the flux (and source) convergence.
  - Every collision contributes, and since several collisions precede a fission, it could provide a better statistics than the source sites. (However, these events are correlated.)
  - Non-multiplying regions are included in collision entropy, thus could capture more information than source entropy

Collision entropy – example – fissile region

- Homogeneous slab
- 1-group problem
- Width=200 cm in z direction
- Σ_{tot}=1.000 /cm
- Σ_{capt}=0.084 /cm
- Σ_f=0.060 /cm1
- Σ_s=0.856 /cm, isotropic
- v=2.4

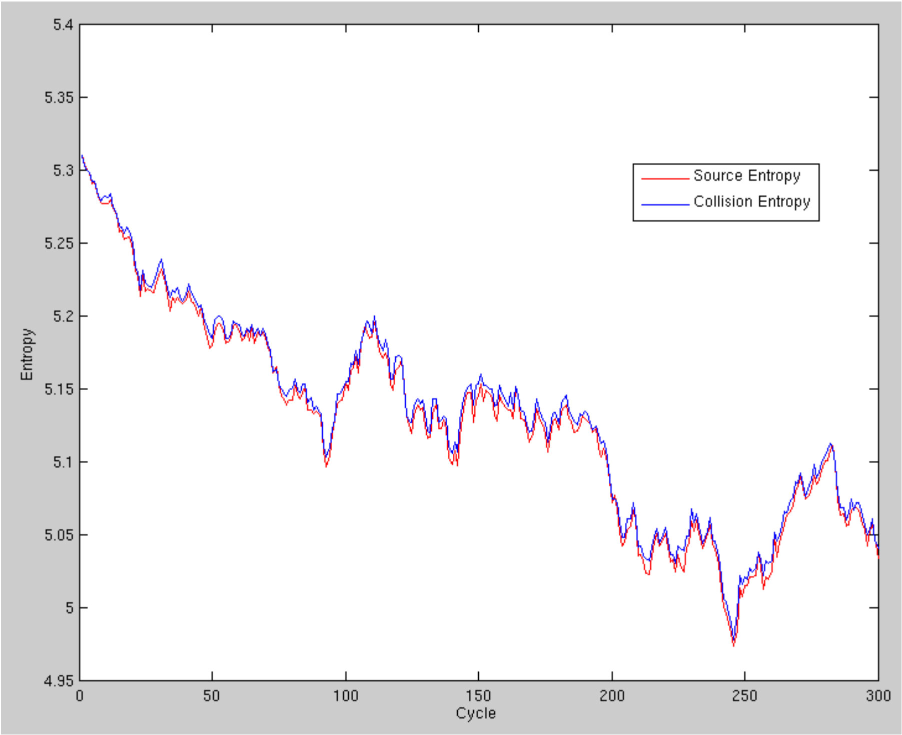


- 5000 particles/cycle
- 300 total cycles
- Z direction is divided into 40 meshes evenly
- Initial uniform source distribution

- Fissile-only regions, expected to obtain essentially identical results from source and collision entropy

Collision entropy – example – fissile region (cont.)

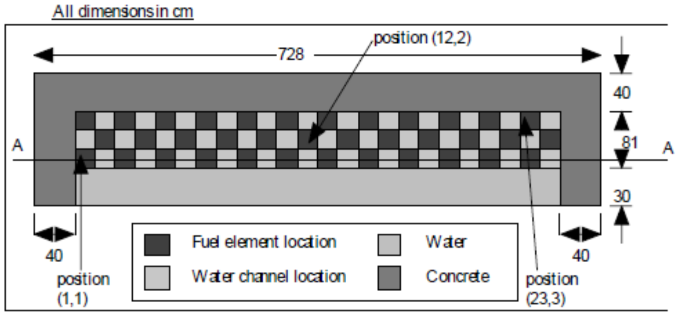
- In this case, essentially the same (as expected).



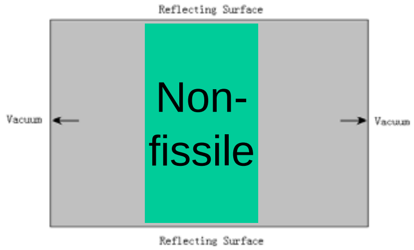
	Mean Value	σ
Source Entropy	5.13	0.07
Collision Entropy	5.13	0.07

Collision entropy – with non– fissile region(s) [work in progress]

- OECD Benchmark#1
  Checkerboard – “half” the space/information not used
  (not clear how much additional information, however)



- Modified 1-group slab problem
  similar to OECD Benchmark#3 (uranyl nitrate slabs separated by water)



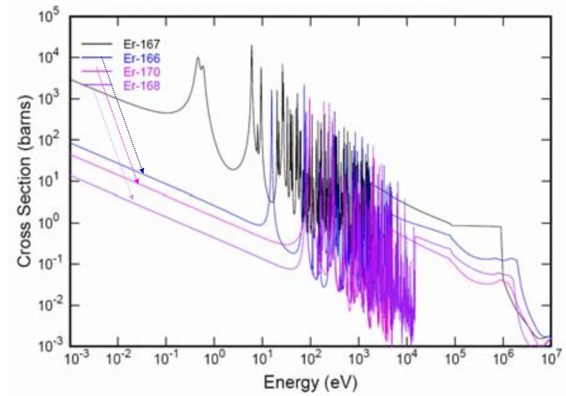
(3) Criticality simulations and depletion

MC Depletion

- One additional level of uncertainty
- Difficult to analyze and separate various effects

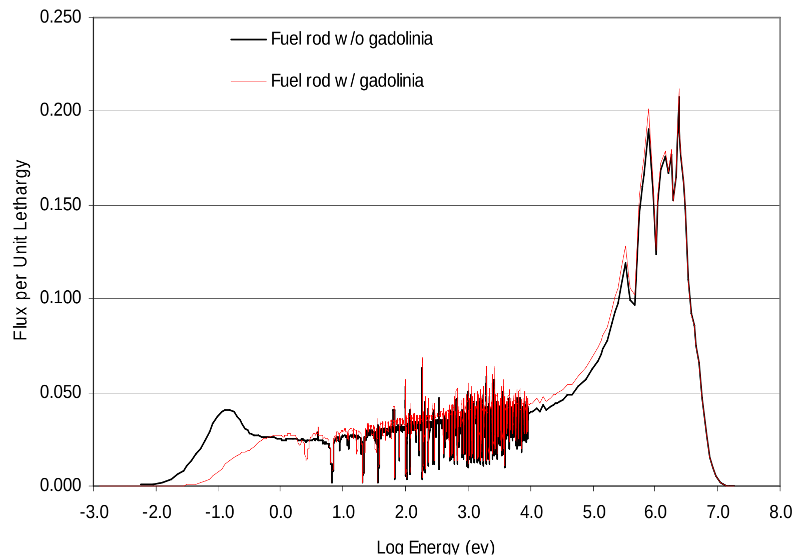
Project being initiated

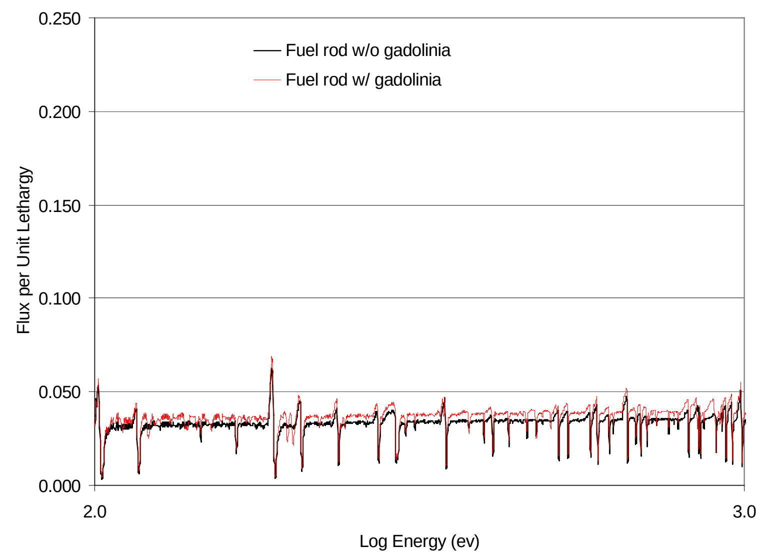
- Will employ deterministic with ultra-fine “continuous” library (6,000+ groups) to filter out MC statistical effects
- Collaborative research with Westinghouse



Resonances in erbium (burnable absorber)

Example of detailed spectrum obtained by deterministic / ultra-fine library

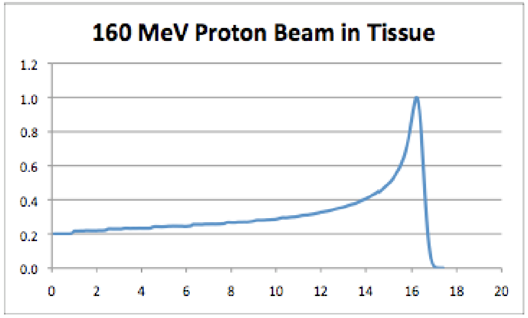


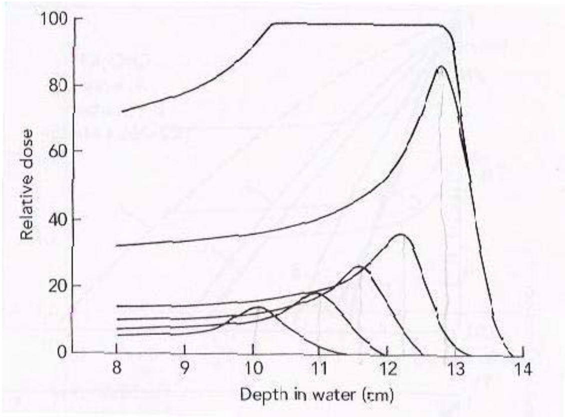


(4) Computational Medical Physics

Proton therapy and secondary (neutron) dose

- Proton therapy - promising treatment modality
- Can adjust depth (Bragg's peak) to minimize primary dose to healthy tissue
- Can optimize tumor coverage (spread out Bragg's peak)
- Secondary (neutron) dose to healthy tissue may be of concern
- Simulations - computationally intense
- Developing a methodology for efficient simulations





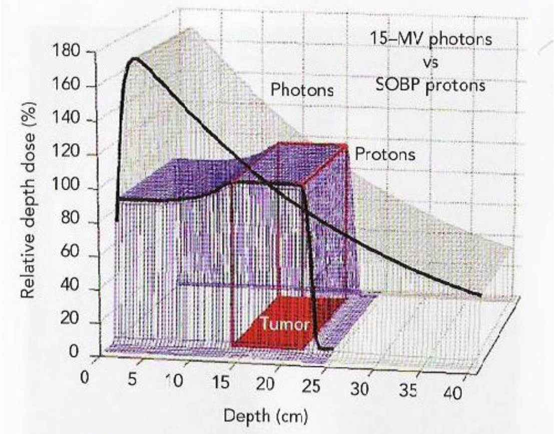


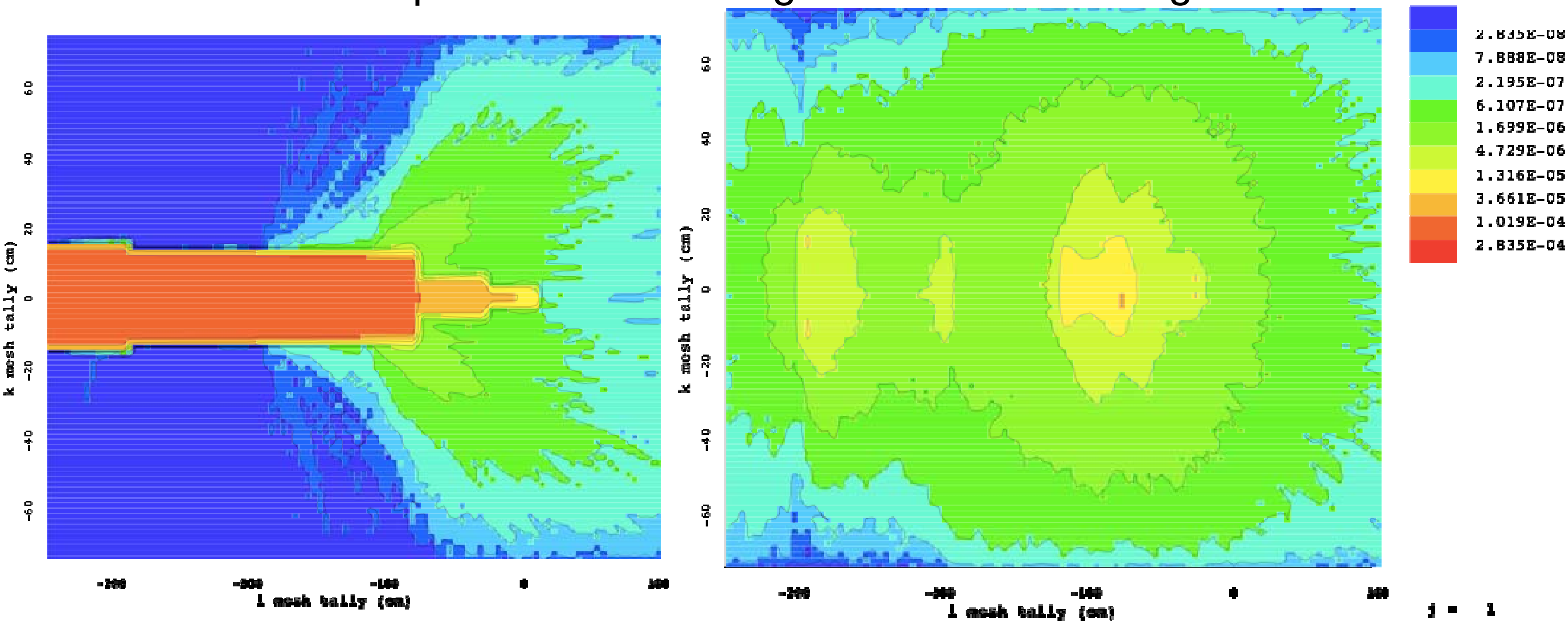
Figure 1.3 Depth-dose distributions for a single field of 15-MV photons and an spread-out Bragg peak (SOBP) of 23-cm range and 12-cm modulation.

Thomas F. DeLaney, Hanne M. Kooy, Proton and Charged Particle Radiotherapy, Philidelphia: LWW, 2008

Computational medical physics - proton therapy

- Work in progress: establishing beam-nozzle-patient model

160 MeV proton beam through a 6.9cm thick range shifter



Objective: effective variance reduction for coupled p-n

Summary and Future Work

Work in progress on Monte Carlo methods in reactor analysis, with the objective of making them more practical for routine use:

- Fixed-source MC: Investigating use of MAVRIC/FW-CADIS for global flux/dose distribution in large deep penetration problem:
  - Good results/experience so far
  - Further study in progress (fast-thermal-flux-does-activation; uniform variance for individual fluxes)
- Improved diagnostics for MC criticality
  - Modified entropy
  - Use of different criteria
- MC criticality simulations with depletion
  - Error determination and propagation
  - Supported by “pointwise deterministic” (ultrafine 6,000+ group library)

Computational medical physics:

- Variance reduction for MC coupled proton-neutron-gamma simulations

Thank you for your attention

Questions?