Applications of PENTRAN using Parallel Clusters For Selected Medical Physics Problems

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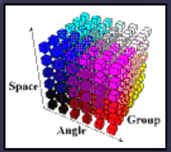


Overview

- Introduction
- PENTRAN features and current status
- Code Benchmarks & Parallel Performance
- Medical Physics Applications
- Brachytherapy, CT, X-ray room simulations
  - Discussion of Models, approach, etc
  - Ordinate splitting (OS)
- Medical Physics Transport Research
- Closing Remarks

3-D Boltzmann Equation

$$(\mu\frac{\partial}{\partial x}+\eta\frac{\partial}{\partial y}+\xi\frac{\partial}{\partial z})\,\psi_g(x,y,z,\mu,\varphi)+\sigma_g\,(x,y,z)\,\psi_g(x,y,z,\mu,\varphi)=$$

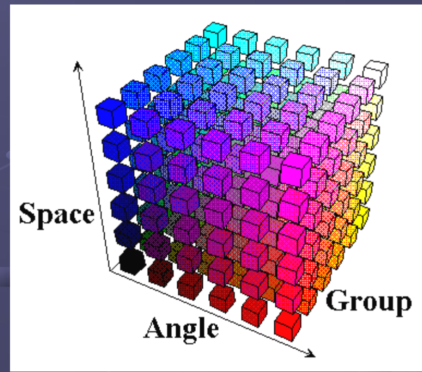
$$\sum_{g'=1}^{G}\sum_{l=0}^{L}(2l+1)\,\sigma_{s,g'\to g,l}(x,y,z)\,\{P_l(\mu)\phi_{g',l}(x,y,z)+2\sum_{k=1}^{l}\frac{(l-k)!}{(l+k)!}P_l^k(\mu)\,\cdot$$

$$\left[\phi^k_{C\,g',l}(x,y,z)\cos(k\varphi)+\phi^k_{S\,g',l}(x,y,z)\sin(k\varphi)\right]\}+\frac{\chi_g}{k0}\sum_{g'=1}^{G}\nu\sigma_{fg'}(x,y,z)\;\phi_{g',0}(x,y,z)$$

- Boltzmann Transport Equation
  - Track particles traveling in different
    - *directions*
    - over a range of *energies*
    - in different *spatial locations* in 3-D

Parallel Environment Neutral-particle TRANsport

- **3-D Parallel Sn Code**
  - by Sjoden & Haghighat
  - X-Y-Z Geometry, anisotropic scatter

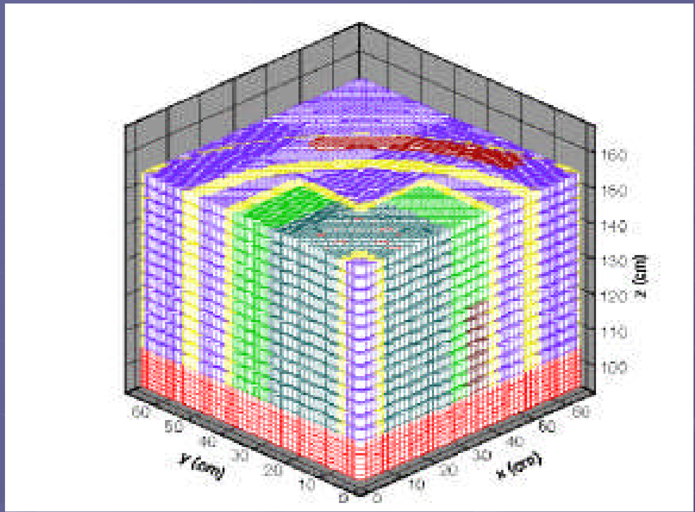


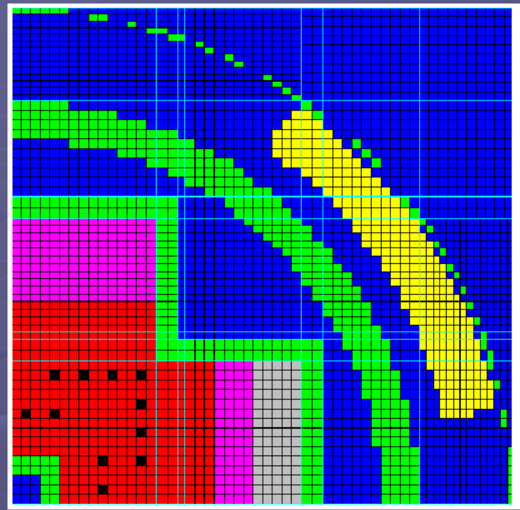
- **Complete Parallel Decomposition**
  - Angular, Energy, Spatial
  - Memory is parallel & tuned, minimized (scalable)
  - Arbitrary Sn order, Pn order
- **Adaptive differencing schemes : DZ -> DTW -> EDW**
  - Differencing "adaptive", adapts to spatial mesh
- **Discontinuous grids**
  - Taylor Projection Mesh Coupling (TPMC)
- **Numerous Benchmarks performed...**

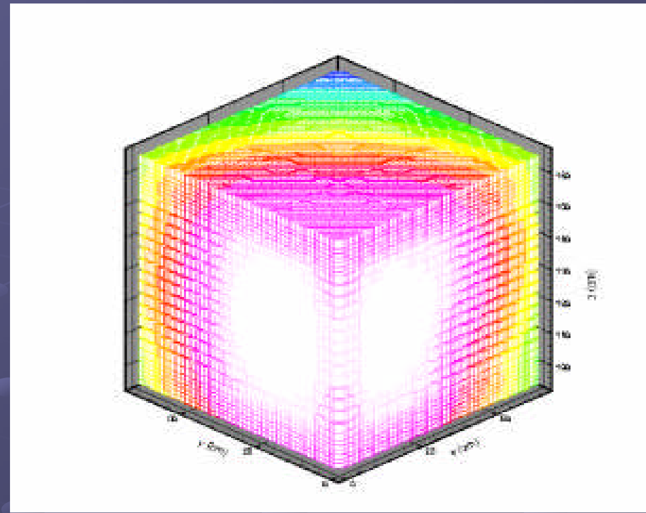
Code Benchmarks and Parallel Performance Metrics

- OECD/NEA Venus-3 3-D PWR Benchmark
- OECD/NEA Kobayashi Benchmark
- Fuel Storage Cask
- Prompt γ-Neutron Activation Analysis (PGNAA) device
- BWR Reactor Simulation
- He-3 Detector System
- HEU Criticality Benchmark
- OECD/NEA MOX 2-D & 3-D Benchmarks
- WG-Pu Homeland Security Detection problem
  - **Benchmark in development**

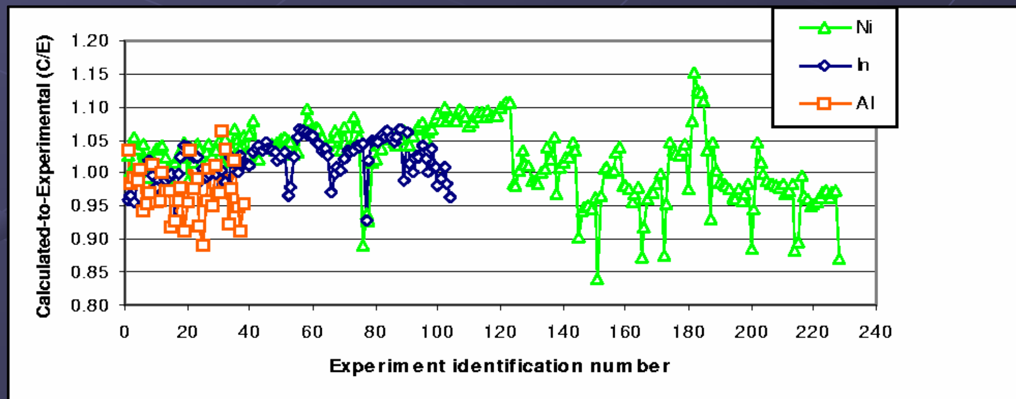
OECD/NEA Venus-3 Benchmark



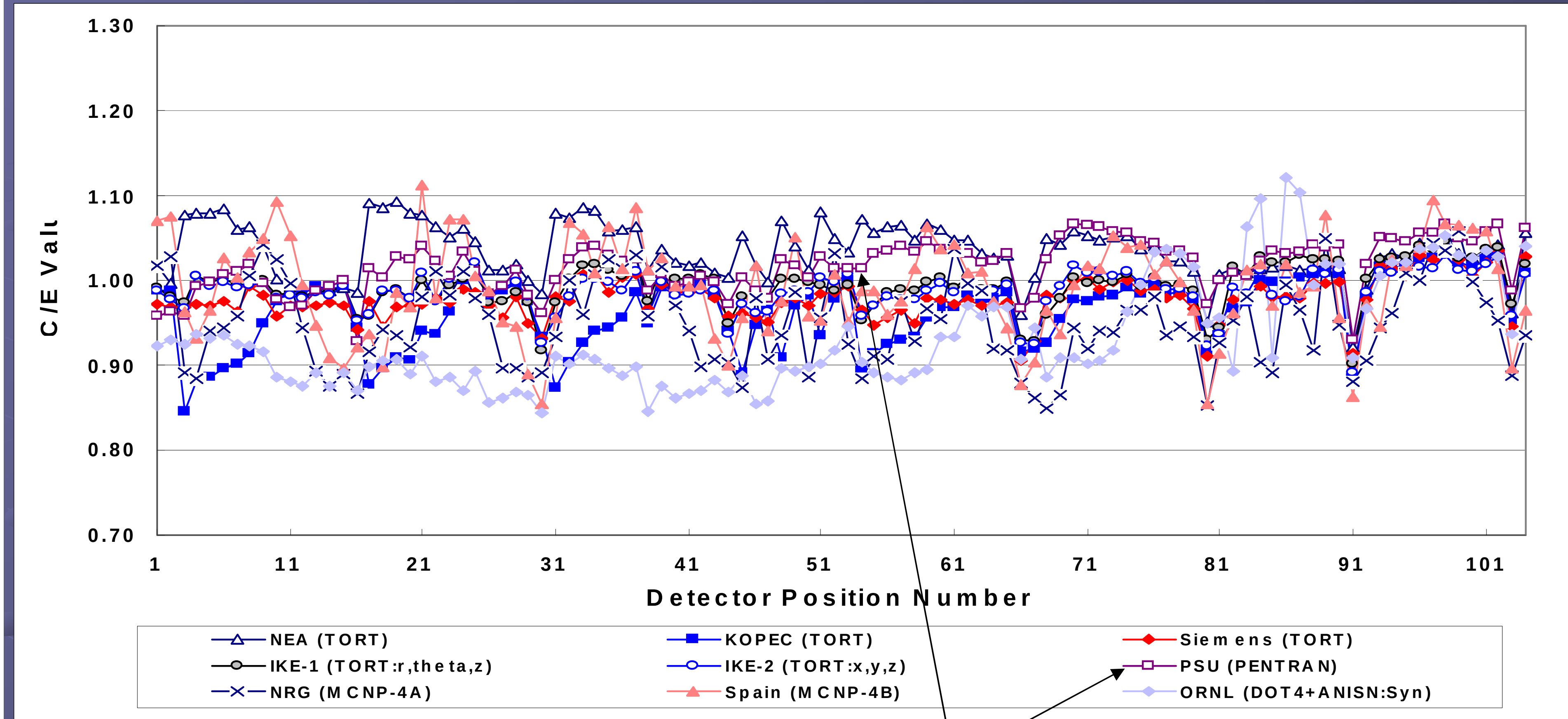




- VENUS-3 Calculation to Experiment (C/E) of 370 <u>experimentally measured</u> neutron reaction rate foils using Ni, In, Al dosimeters
- Reaction rates computed using PENTRAN (P3-S8 26 group-dependent) fluxes
- 95% of C/E's within +/-10%
- 5% of C/E's within +/-15%



OECD/NEA Venus-3 Benchmark



- **PENTRAN results in good agreement with others**
- **26 Groups, P3-S8, in 84.3 min on 32 SP2 procs**

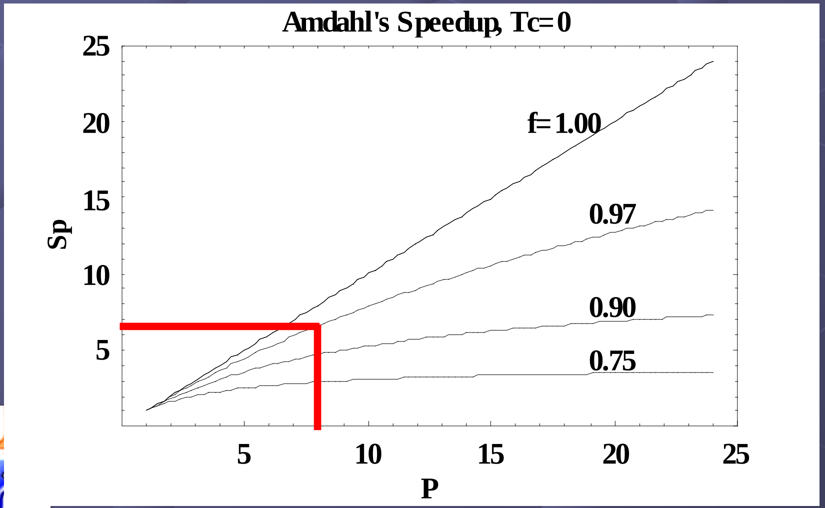
OECD/NEA Nuclear Science Publication: "Venus-1 and Venus-3 Benchmarks", 2000)

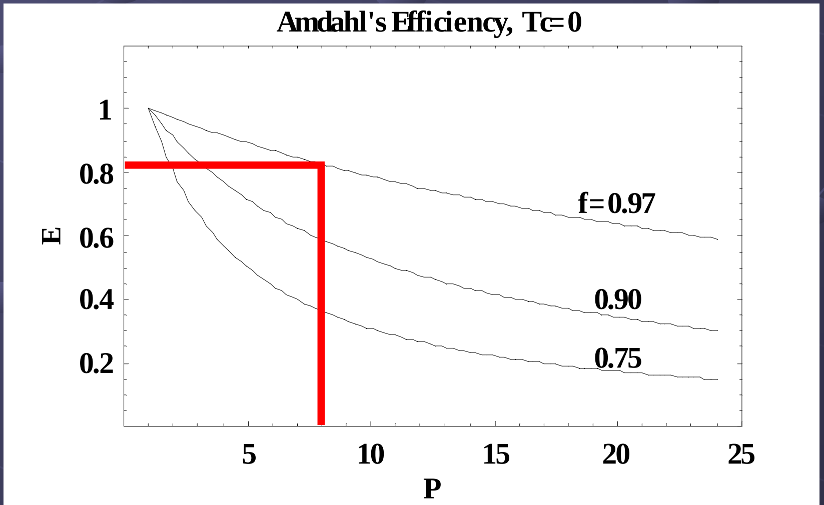
OECD/NEA Venus-3 Benchmark

- Parallel Performance Values

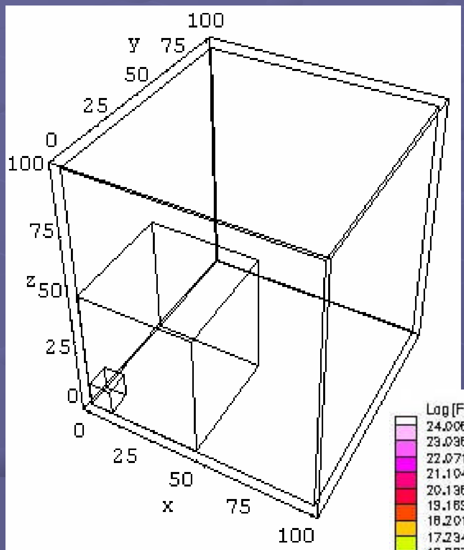
VENUS-3 *PENTRAN* Parallel Performance study					
Case	No. of processors	Domain Decompostion Algorithm (A/G/S)[1]	Wall-Clock time (min)[2]	Speedup	Efficiency (%)
1	4	4/1/1	551.8	1.00	-
2	8	8/1/1	311.9	1.77	88
3	16	8/1/2	153.3	3.60	90
4	32	8/1/4	84.3	6.54	82

[1] *(A/G/S) refers to the number of angular, group, and spatial subdomains*
[2] *Time is obtained in a BATCH mode*

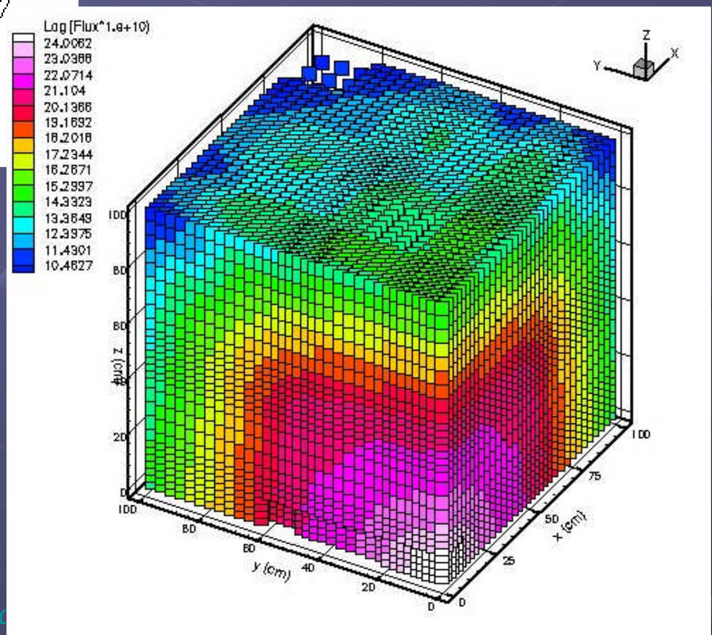


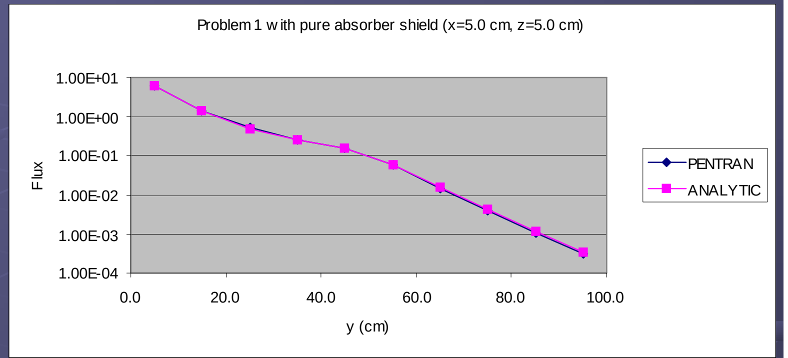


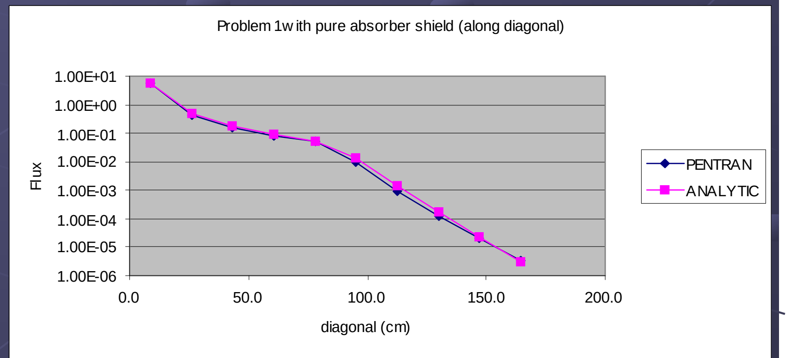
OECD/NEA Kobayashi Benchmarks

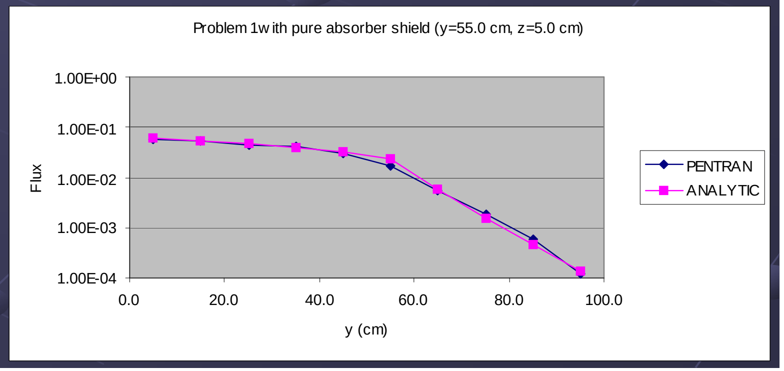


Problem 1i: Pure Absorber

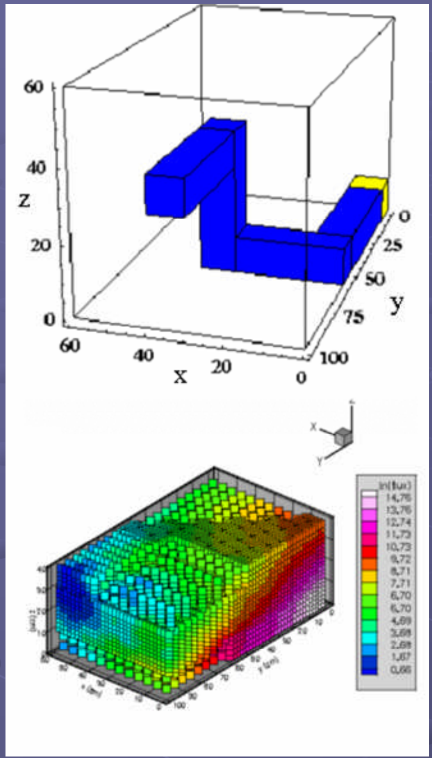


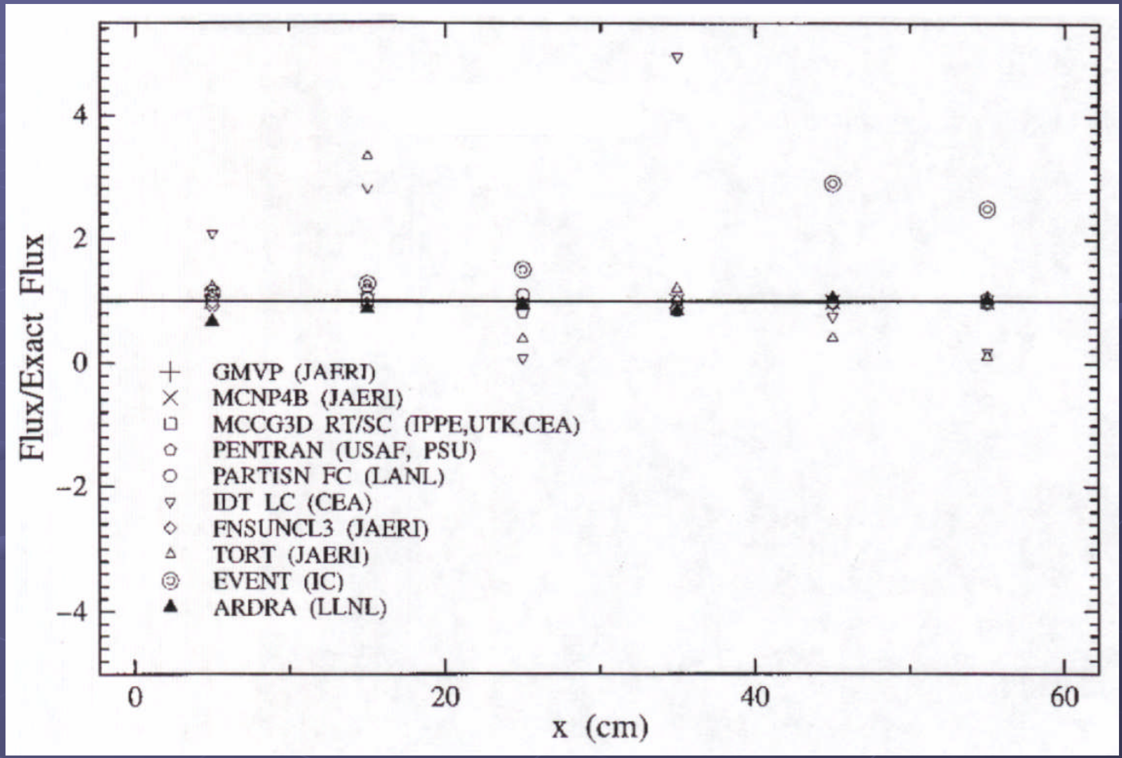






OECD/NEA Kobayashi Benchmarks

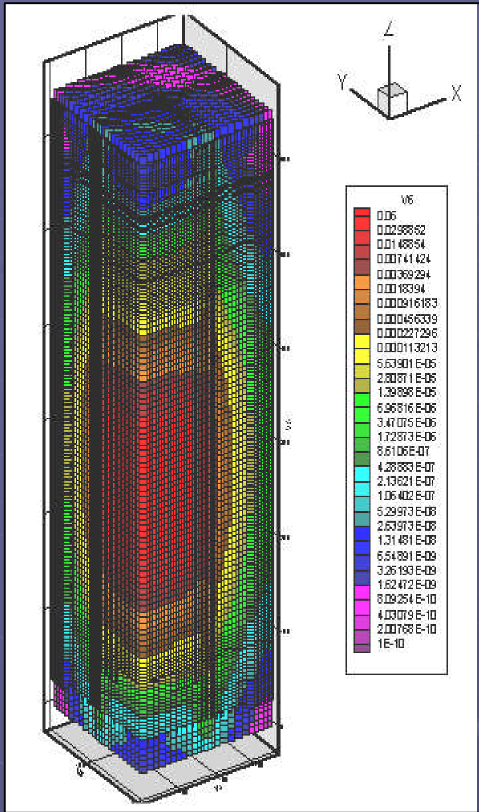


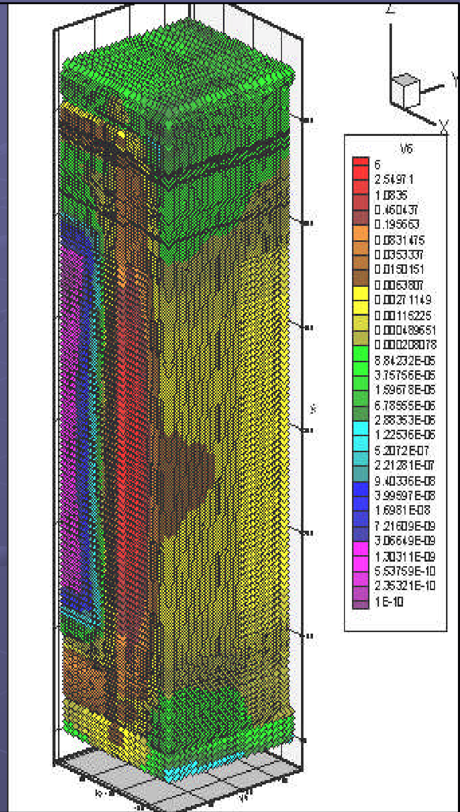


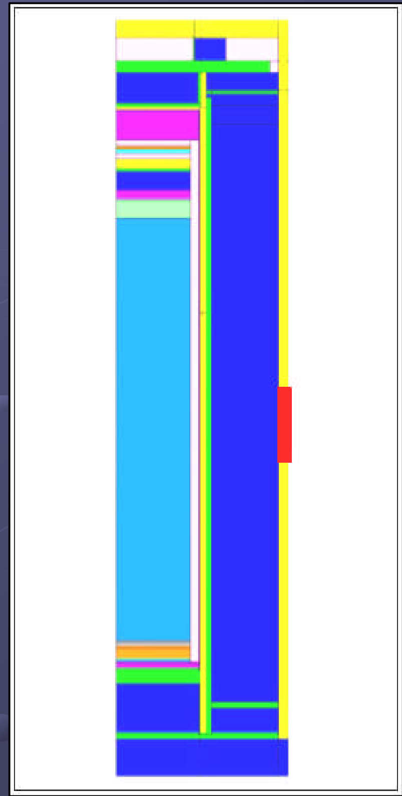
- Dog-Leg Void Problem, Zero Scattering solutions at y=95 cm, z=35 cm (Right)
- Benchmarks: 3-D Pure Absorber, 50% Scatter Cases
- Excellent agreement with benchmark solutions…

Haghighat, Sjoden, and Kucukboayci, 2001

Fuel Storage Cask

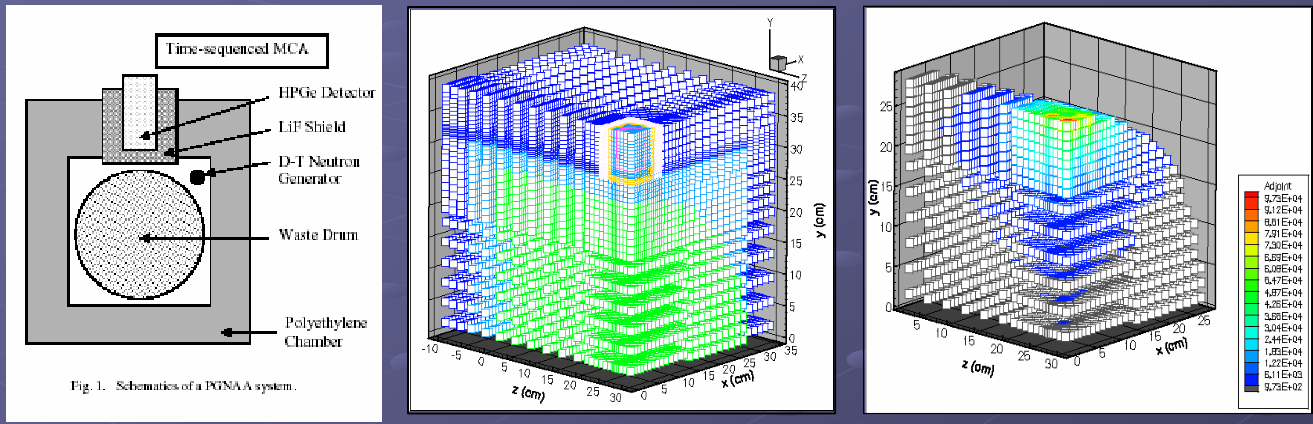






- Height 610 cm, O.D. 340 cm, Shell I.D. 187 cm, 162.4 MT, 318,426 fine meshes solved with P3-S12, coupled 22 n/18 γ
- PENTRAN Solution, CASK Group 1 (Left), CASK Group 22 (Center), and (Right) A^{3}MCNP model of Cask
- PENTRAN, MG-MC dose results differed <5% at tally points

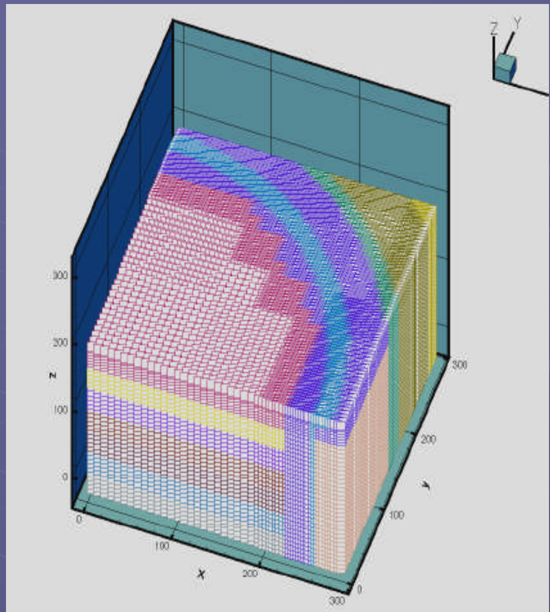
Prompt-γ Neutron Activation Analysis (PGNAA) device

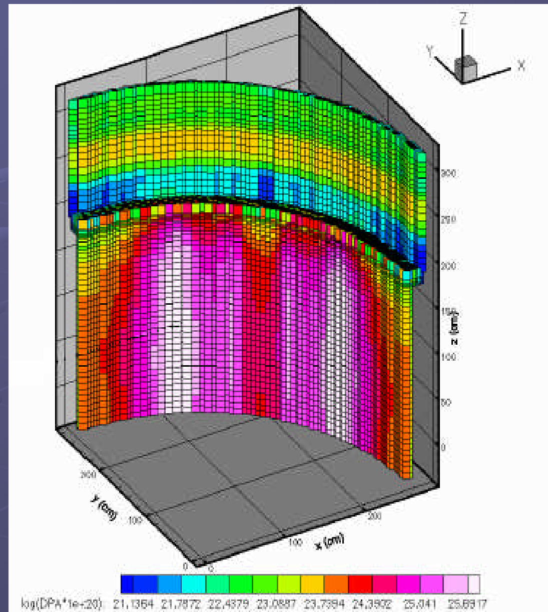


Contaminant (Metal)	Max. Relative Difference (calculated-to-experiment)	Estimated Experimental Uncertainty	Low Limit of Detection (LLD)
Hg	12%	14%	9 ppm
Cd	6%	10%	115 ppm
Pb	19%	20%	4,400 ppm

- PENTRAN adjoint used to fold (n,γ) source to predict HPGe detector response ...
- … Results agree with experimental data within the limit of the experimental uncertainty

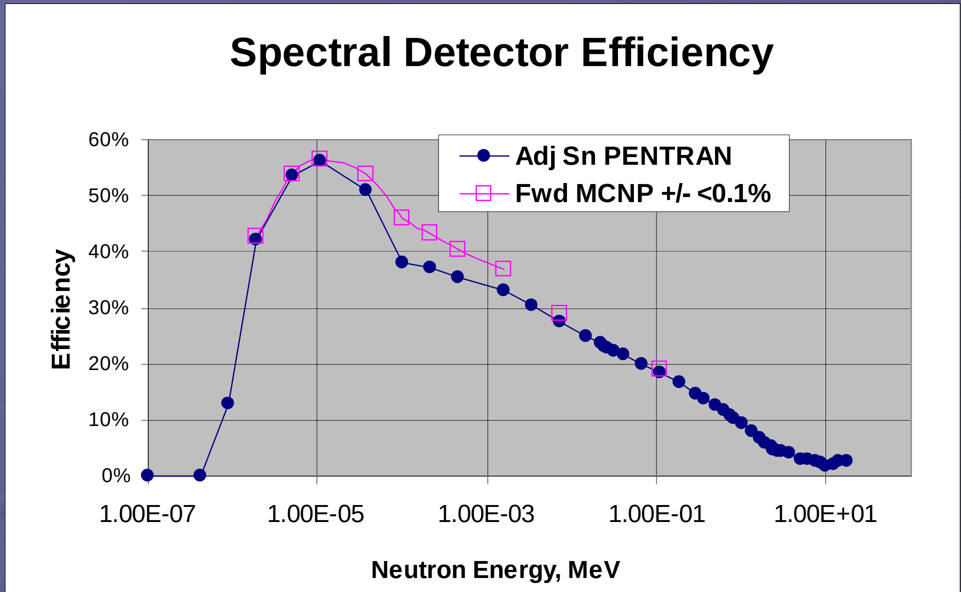
BWR Simulation (for Core Shroud)

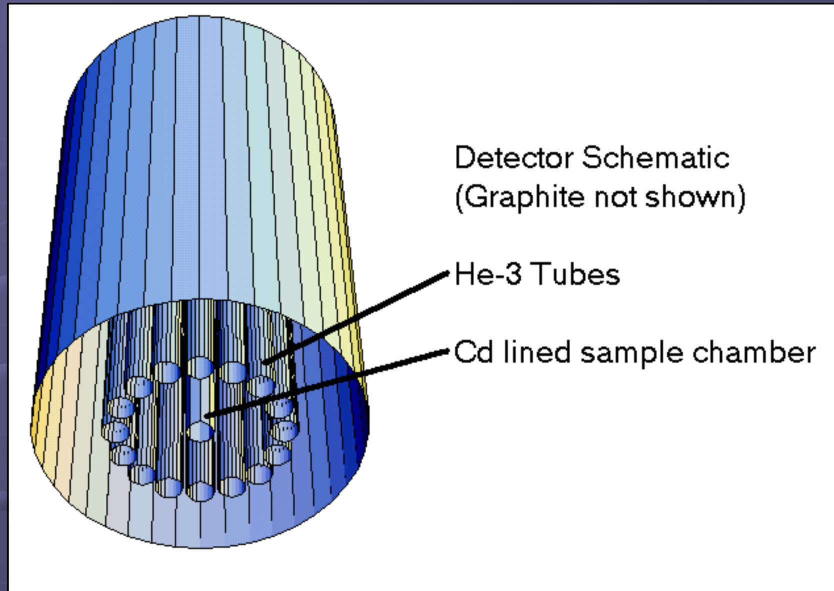




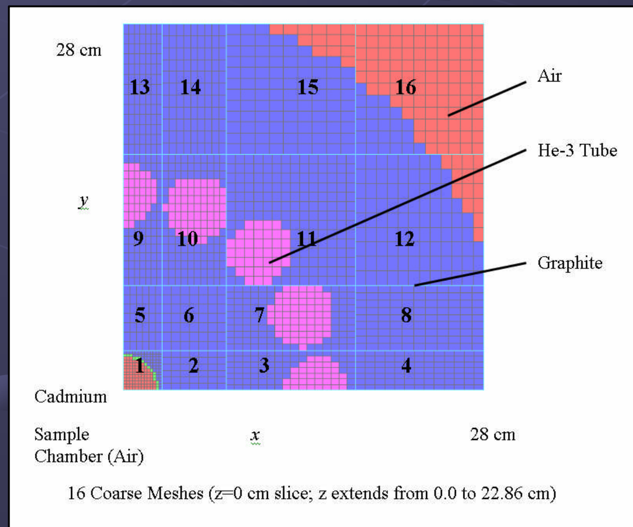
- PENTRAN BWR reactor/Core Shroud Assembly Model (Left)
- 67 Group P3-S8 coupled n-γ calculation
  - 265,264 fine mesh cells, 12 hours on 48 IBM-SP2 processors
  - Decomposition: 8 processors Angular, 6 processors Spatial
- Displacement per Atom (DPA) in core shroud (Right)
- Multigroup (BUGLE-96) PENTRAN values within 5-15% of continuous energy MCNP values (Kucukboyaci, et. al, 2000).

He-3 Detector System (adjoint app)



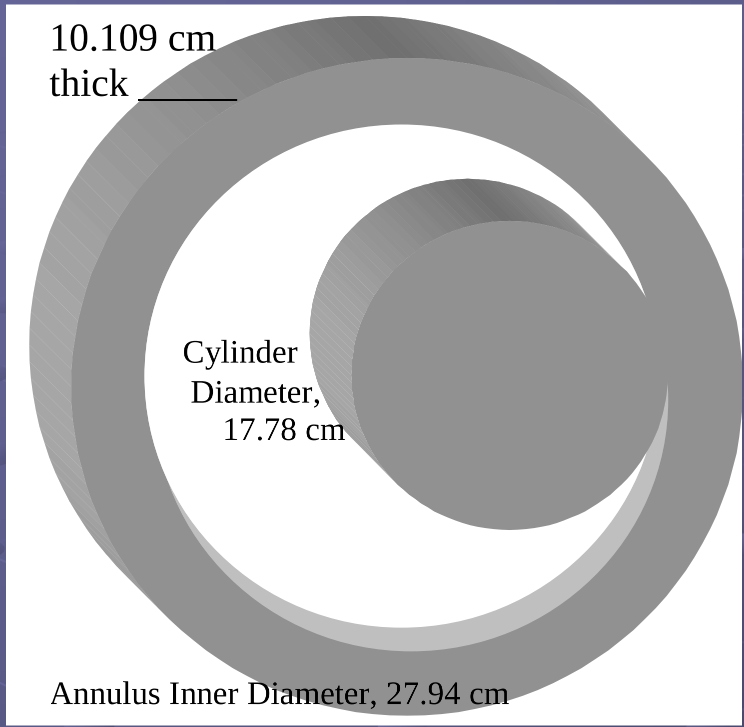


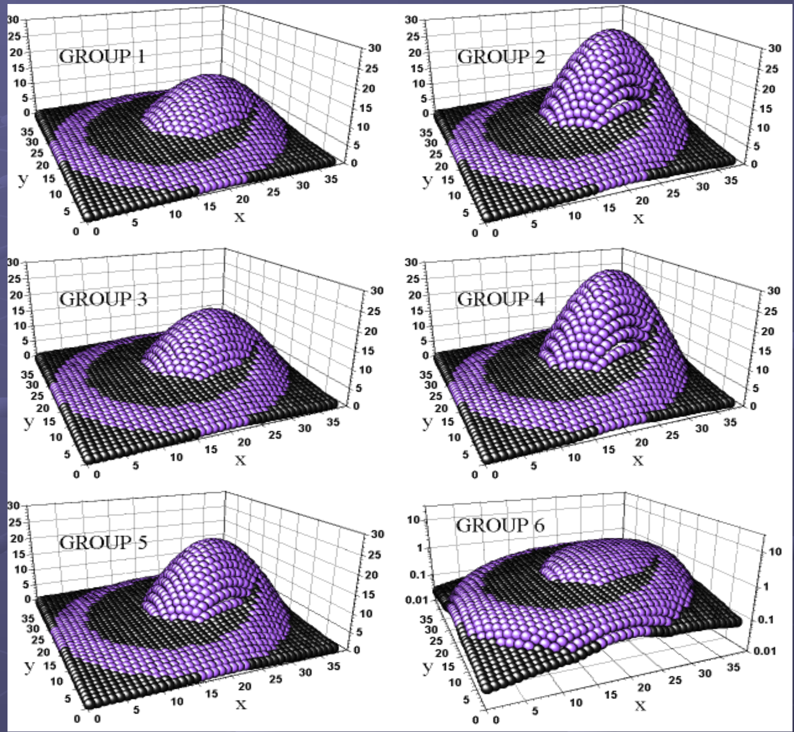
- Computational He-3 Detector Design
- Objective: Predict neutron detector response using PENTRAN Sn adjoint
- Continuous Energy MCNP agreement
- Limitations of BUGLE-96



(Sjoden, 2002)

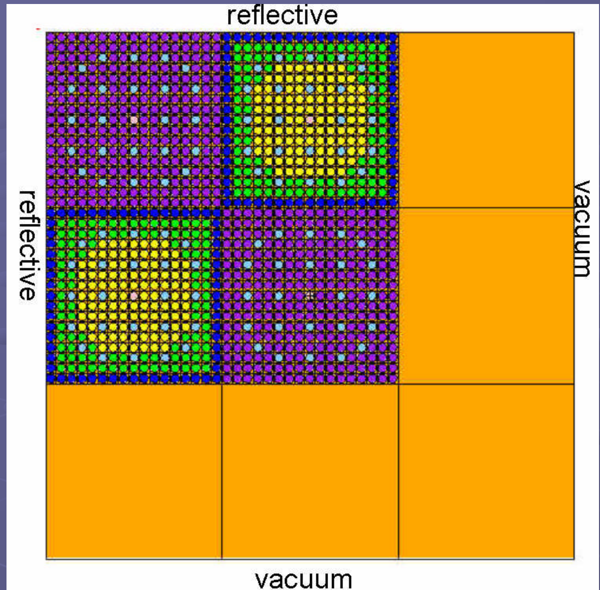
HEU Criticality Benchmark

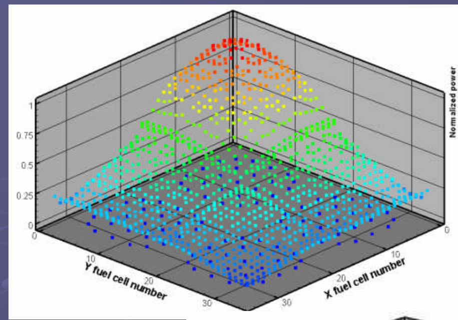


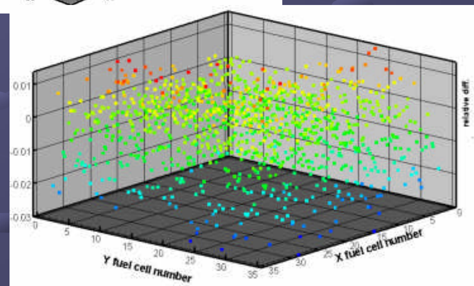


- HEU Annular Ring Criticality Benchmark
- Calculation yielding keff=0.994
- Exact agreement with MG-MCNP (+/-0.001)

OECD/NEA MOX 2-D, 3-D Benchmarks



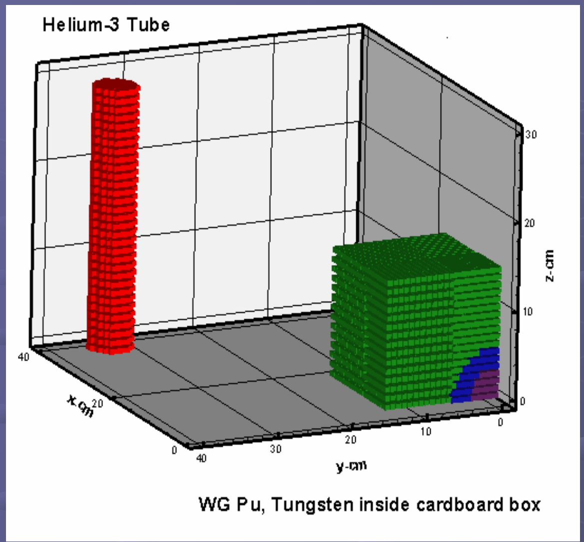


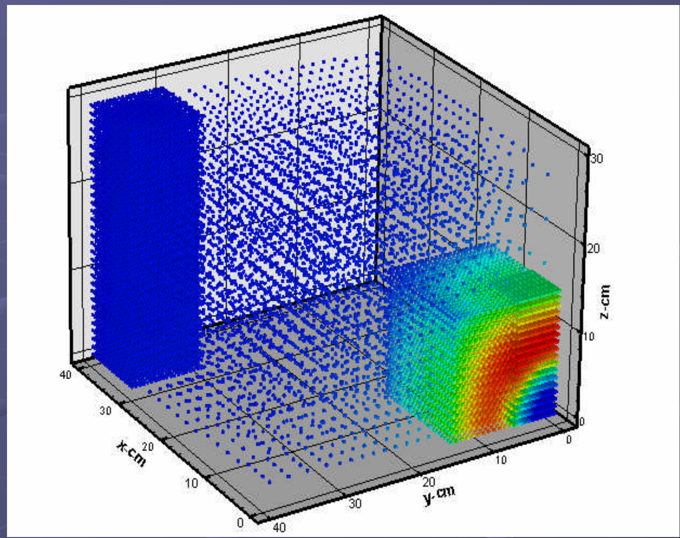


- OECD/NEA C5G7 MOX 2-D, 229,551 fine meshes, S16 (228 directions/cell), 7 energy groups (Left)
- PENTRAN keff=1.18760, <0.1% diff MCNP
- Rel power difference with MCNP (Bottom Right) avg diff 0.88%, stat err MCNP 0.4% to 1.24%.
- 3-D unrodded case, 946,080 spatial meshes keff=1.14323, within <0.09% of MCNP

(Yi and Haghighat, 2004)

Homeland Security Application





- “Pu-Ball in a Box” Problem
- 4 kg, 10-yr old alpha Pu surrounded by tungsten…
- $M_{\mathscr{L}} = 3.681$
- Neutron detection modeling and simulation applications

Other Parallel...

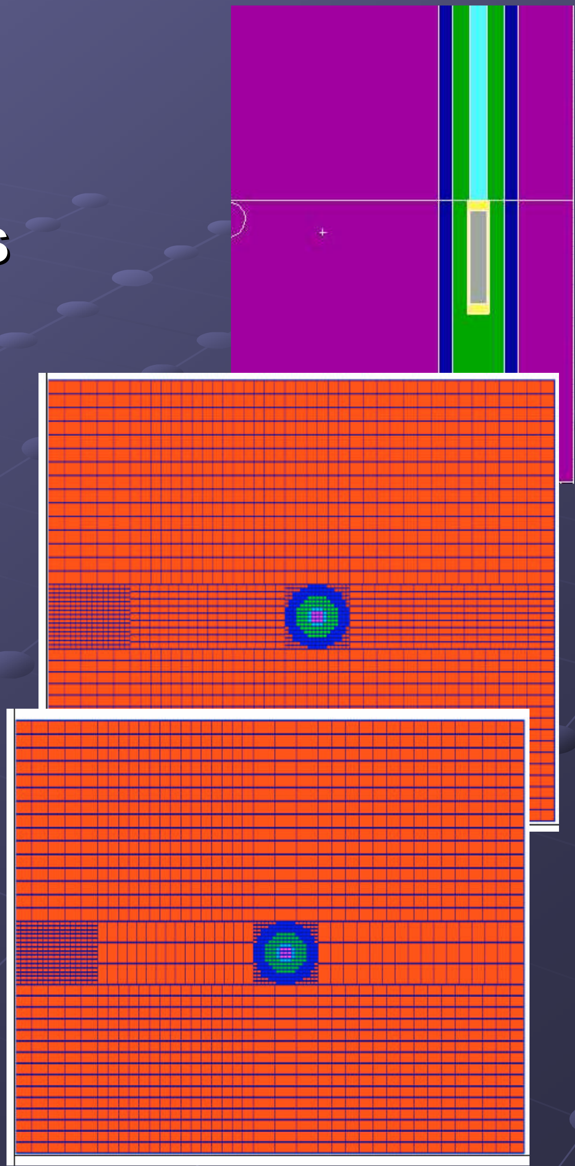
BWR Reactor Simulation, *PENTRAN* Scalability study				
Case	**No. of Directions**	**No. of Processors**	**Domain Decomposition (A/G/S)[1]**	**Wall-Clock time per iteration (s)**
1	24	6	1/1/6	30.12
2	48	12	1/1/12	33.28
3	80	24	4/1/6	29.52
4	169	48	8/1/6	36.12

[1](A/G/S) refers to the number of angular, group, and spatial subdomains

- PENTRAN has been applied to a number of problems, with demonstrated accuracy and efficiency
  - Experimental and/or Monte Carlo based benchmarks
  - Achieved excellent agreement
- Typically, PENTRAN results are within 5% (or less) of MC simulations

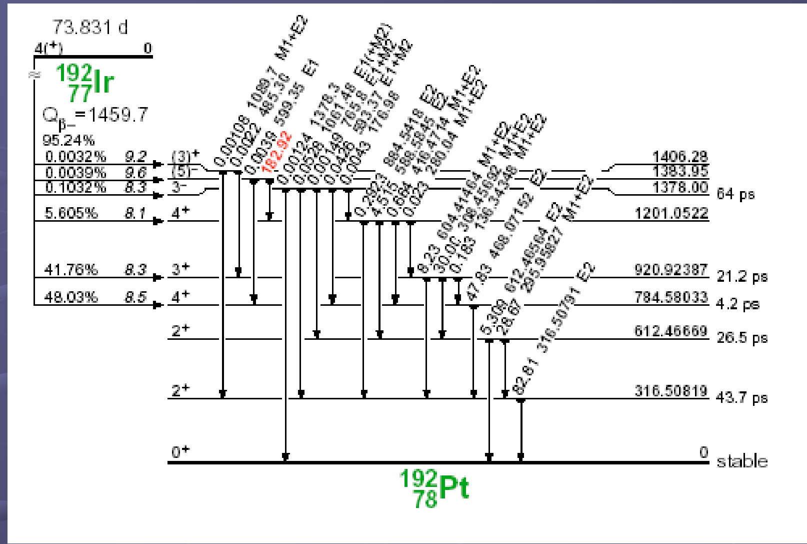
Brachytherapy Problem

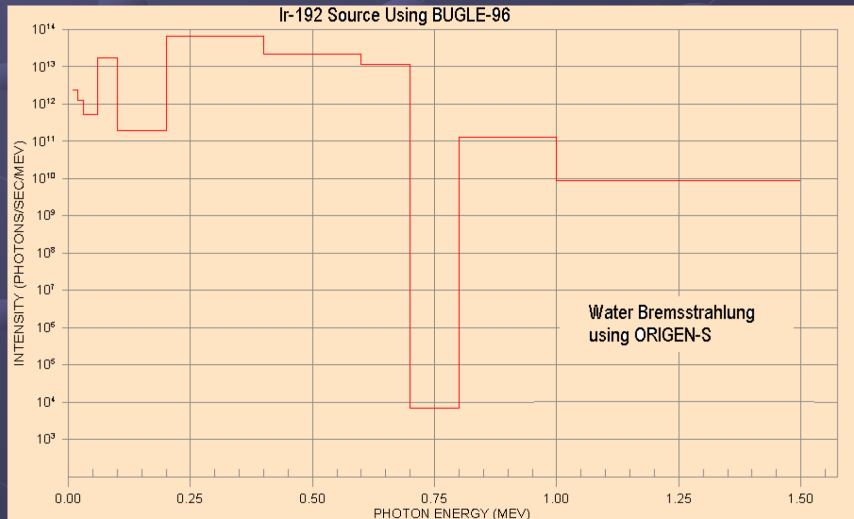
- QUADOS problems
  - **Several Medical Physics problems**
  - **Unique application opportunities for Deterministic modeling**
- Brachytherapy Problem
  - **Investigating Sn solutions to high dose rate problems (Ir-192)**
  - **Good Comparison to Monte Carlo**
  - **Ray effects must be treated...**



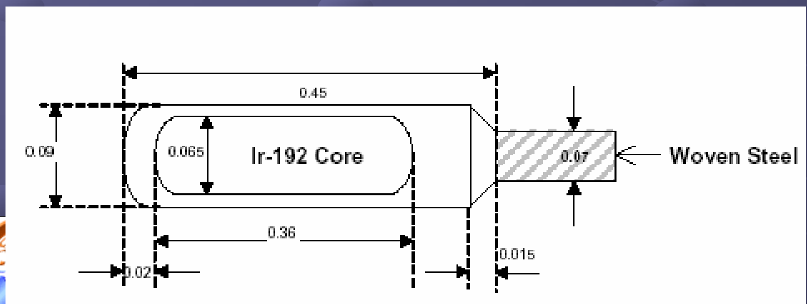
Brachytherapy Problem

- Ir-192 isotope contained SS source capsule
  - 0.45 cm long,
  - 26 mg Ir-192, ρ = 22.4 g/cc
  - T½ = 73.8 days β–γ emitter
    - 26 photons, 22 electrons, 5 betas





- Capsule attached to a woven steel cable



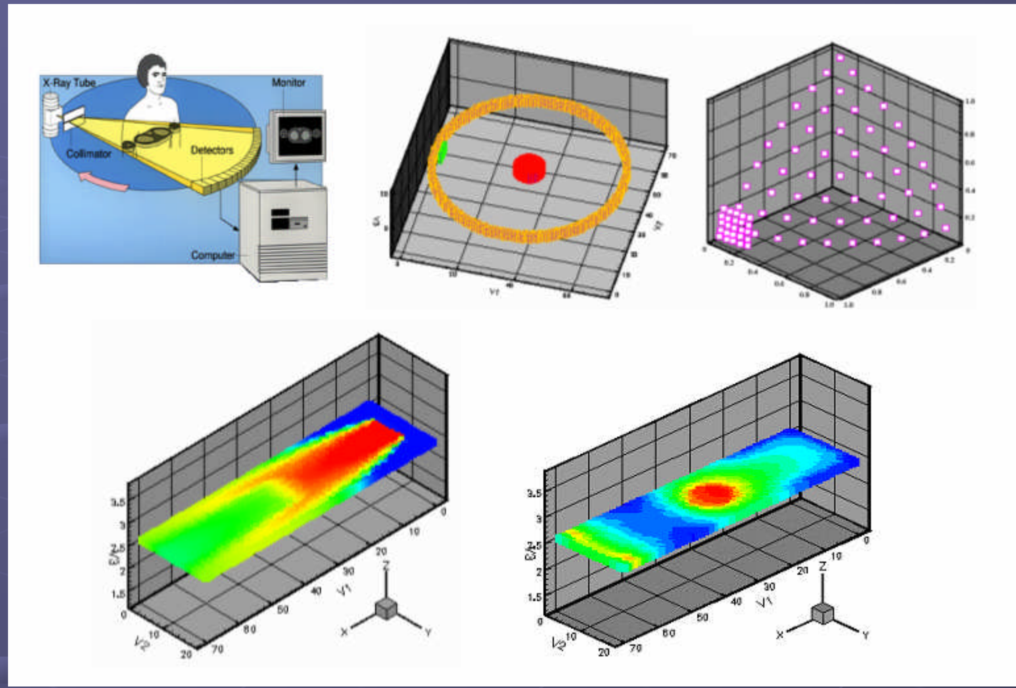
Brachytherapy Modeled Results

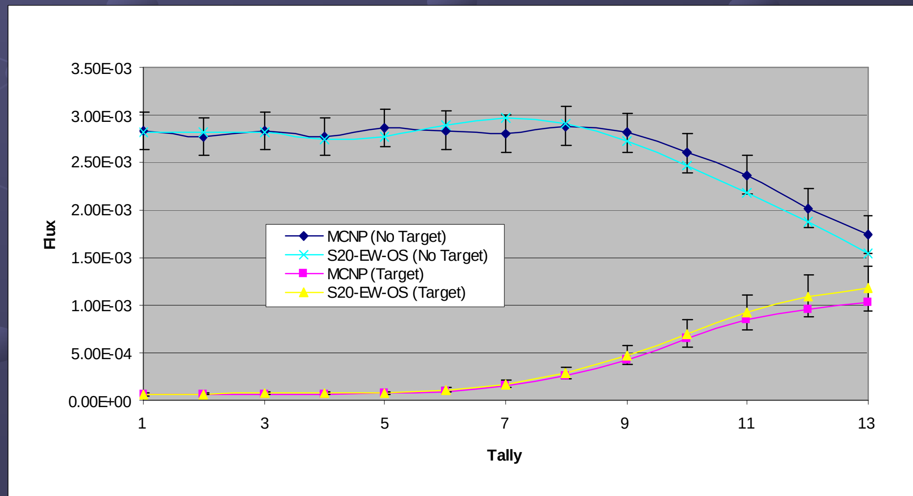
				Normalized Flux: Pentran/MCNP					
				Grid A			Grid B		
Photon Group	Upper Energy, MeV	MCNP Flux (ph/cm2/s)	R	S8	S14	S20	S8	S14	S20
1	1.5	3.04E+08	0.0036	0.09	0.44	0.75	0.49	0.92	1.02
2	1	1.76E+09	0.0021	0.09	0.44	0.75	0.49	0.92	1.03
3	0.8	3.54E+07	0.0407	0.56	0.70	0.84	0.88	1.20	1.29
4	0.7	7.24E+10	0.0014	0.09	0.44	0.75	0.49	0.92	1.03
5	0.6	2.94E+11	0.0019	0.09	0.42	0.75	0.48	0.92	1.02
6	0.4	8.14E+11	0.0019	0.13	0.37	0.66	0.52	0.90	1.02
7	0.2	1.32E+11	0.0059	0.75	0.82	0.90	0.90	0.97	1.03
8	0.1	2.03E+10	0.0074	0.55	0.60	0.66	0.72	0.85	0.90
9	0.06	2.29E+10	0.0110	0.03	0.03	0.03	0.03	0.04	0.04
10	0.03	6.84E+07	0.0898	0.01	0.01	0.01	0.01	0.01	0.01
11	0.02	1.14E+08	0.3304	0.00	0.00	0.00	0.00	0.00	0.00

- Sn-P3 Good agreement with MCNP for S20 in Groups 1-8
  - S8 (80 dir) inadequate due to ray effects; compare Grid A, B
  - S14 (224 dir) better (good results for Grid B)
  - S20 (440 dir) very good agreement (Grid B)

Ordinate ("Omega") Splitting (OS)

- OS First introduced by Haghighat and Brown as a method of eliminating ray effects in a CT-Scan simulation with PENTRAN
- OS implemented as an option in PENTRAN for any direction
- Yielded very good agreement with MCNP CT-Scan simulation





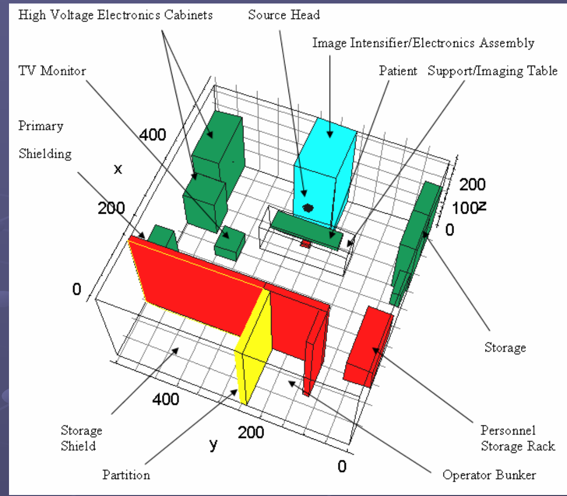
Ordinate ("Omega") Splitting

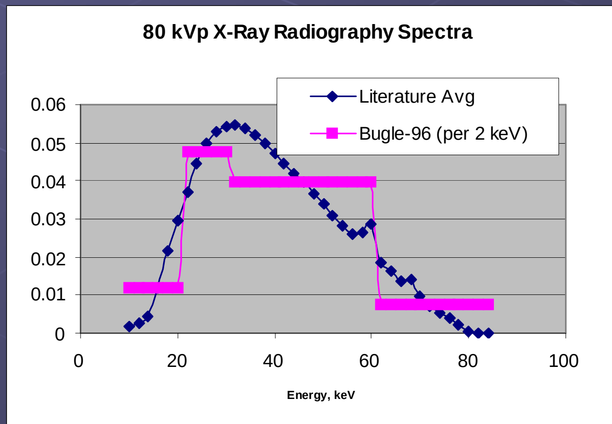
- Ordinate splitting feature allows for important directions to be covered
- Important in Medical Physics applications
- EXAMPLE: S8
  - normally 10 dir/octant
  - Split in 42 directions among octant ordinates 1, 5, 7 10
- Mitigates Ray Effects...
- Directly accessible in PENTRAN

```
Geometry: 3d

 S8 3D Level Symmetric Angular Quadrature
 Number of Omegas per Octant  :  42
 ABS Minimum Direction Cosine :  .129520460963249

Omega Sampling Order: Sn Angles

             S8                xi
         (+ + +) Octant        1
         m-Level Diagram     2   3
           (Sweep 2)       4   5   6
                         7   8   9  10
                       mu            eta

              Omega Splitting Segments:

                          x--x--x
             9:1          |  |  |
         Equal weight   x- 1--x  Ordinate:  1,  2 Segment(s)
          Splitting       |  |  |
                          x--x--x

                          x--x--x
             9:1          |  |  |
         Equal weight   x- 5--x  Ordinate:  5,  2 Segment(s)
          Splitting       |  |  |
                          x--x--x

                          x--x--x
             9:1          |  |  |
         Equal weight   x- 7--x  Ordinate:  7,  2 Segment(s)
          Splitting       |  |  |
                          x--x--x

                          x--x--x
             9:1          |  |  |
         Equal weight   x-10--x  Ordinate: 10,  2 Segment(s)
          Splitting       |  |  |
                          x--x--x
```

X-Ray Room Modeling ...

- 90 m³ room discretized into >110,000 3-D cells
- PENMSH™ code (8 "z-levels" floor to ceiling)
- BUGLE-96: last 4-group photon xsecs
- 80kV radiographic W-anode
  - 32 mAs x-ray burst
  - Rotating anode water cooled source
- Use PENTRAN's angular ordinate feature
  - Angular Dependent Surf Source on patient
  - Planar, only $-\Omega z$ directions





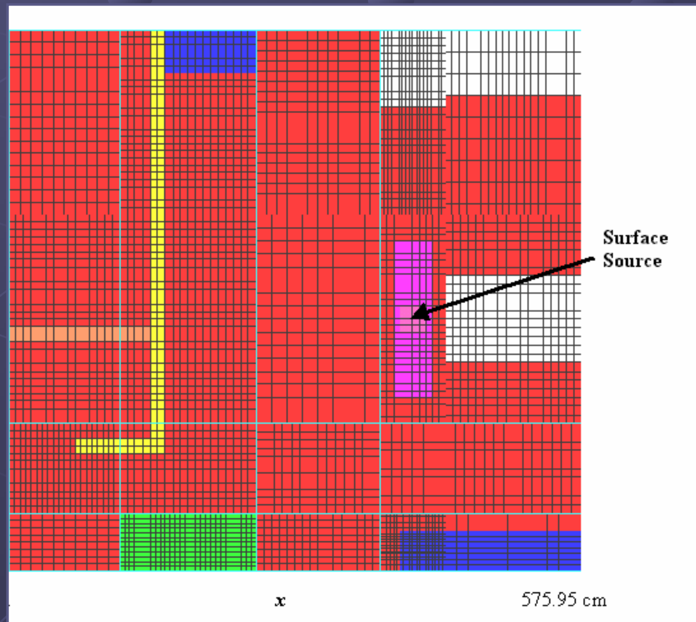
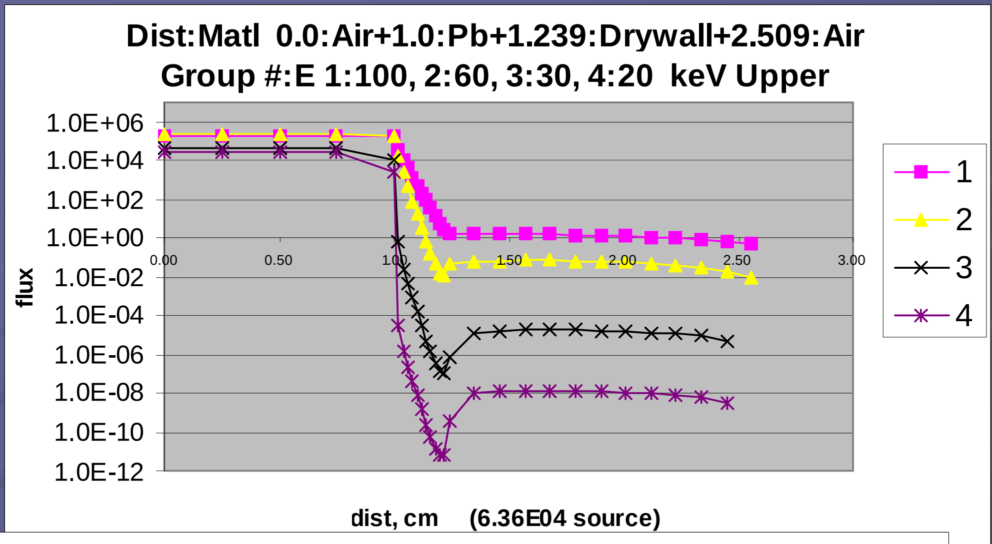
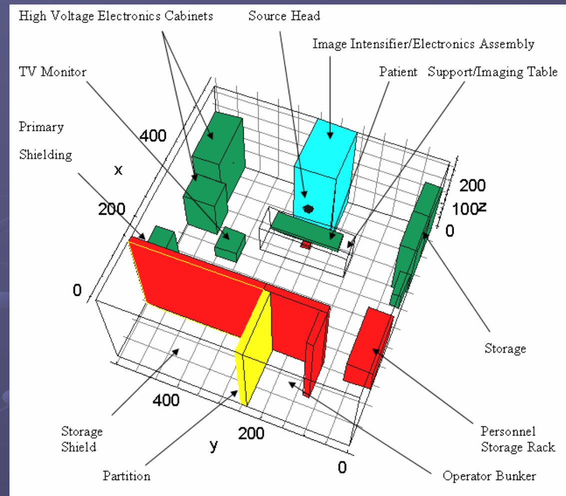


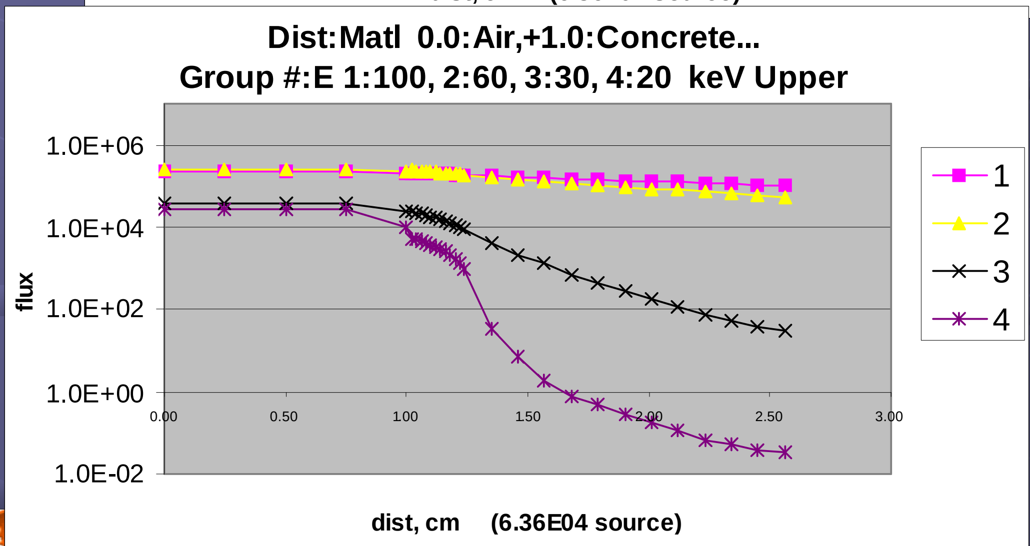
Figure 2. z-level 3: 86.6 cm to 100.44 cm along z-axis.

Nuclear and Radiological Engineering

X-Ray Room Model: B.C.'s

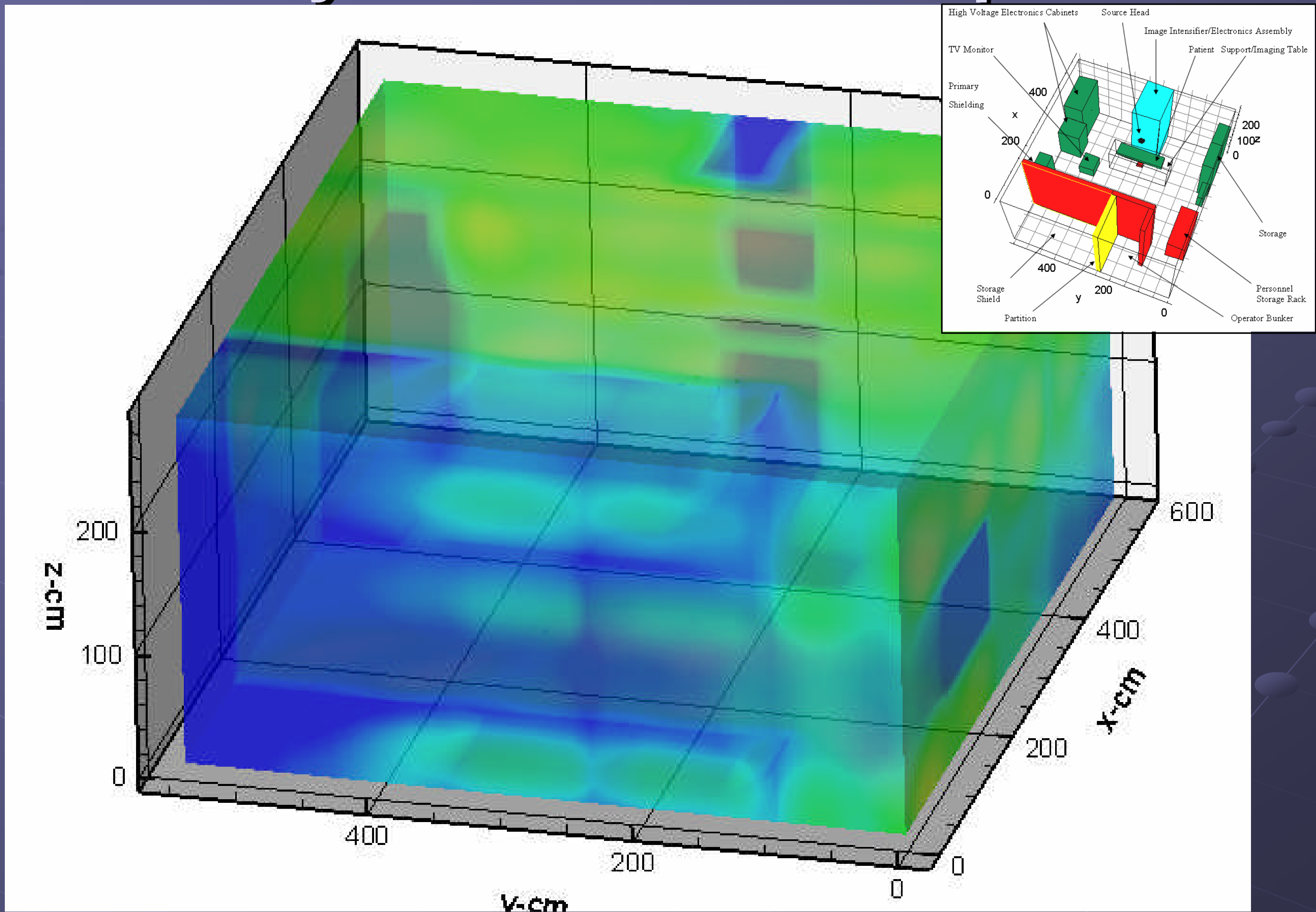






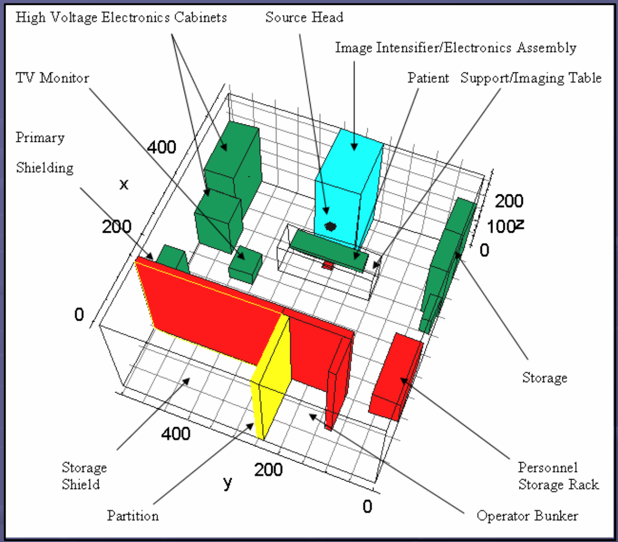
- In MP applications, we do not want to discretize walls and floor
  - Perform 3-D (1-D) albedo calculations (4 group)
  - Scatter through patient important to albedos
  - Obtain group dependent α's = J-/J+

X-Ray Room Model: Grp 1



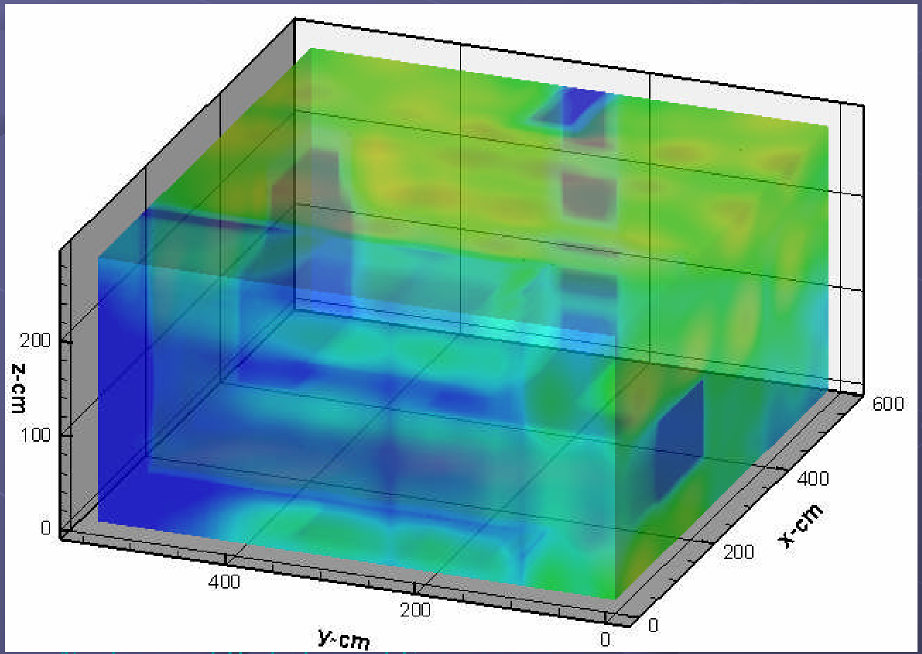
4 Grp S8 P1, 4 procs A/G/S=2/1/2, OS--42 Dir/oct, 2013s

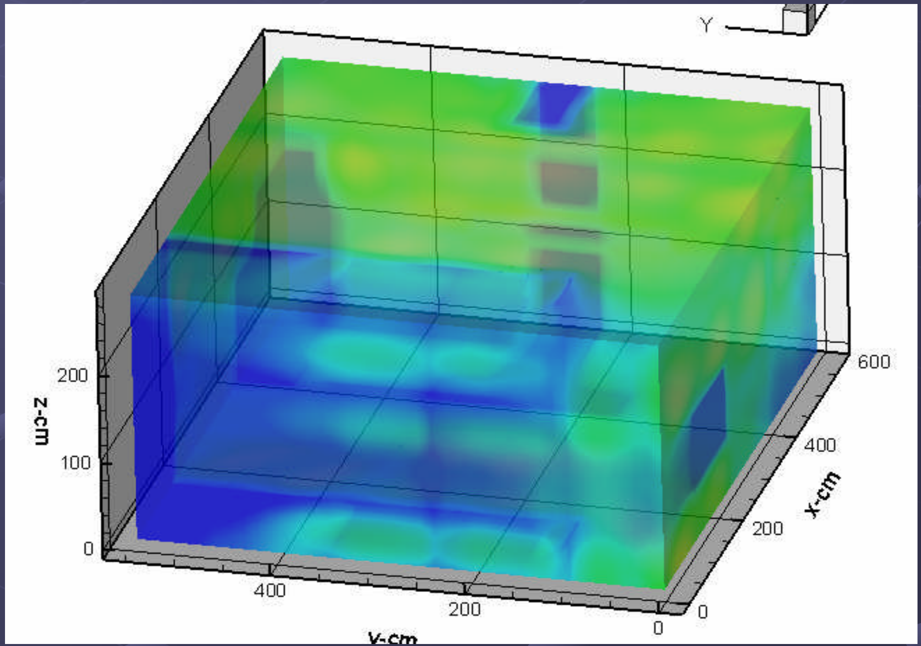
Ordinate Splitting Comparison, G1



- S8, A/G/S=2/1/2

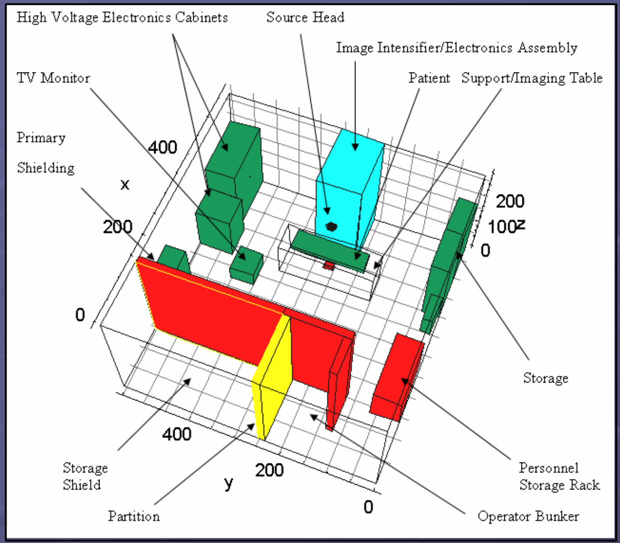
S8+OS A/G/S=2/1/2 (1,5,7,10)



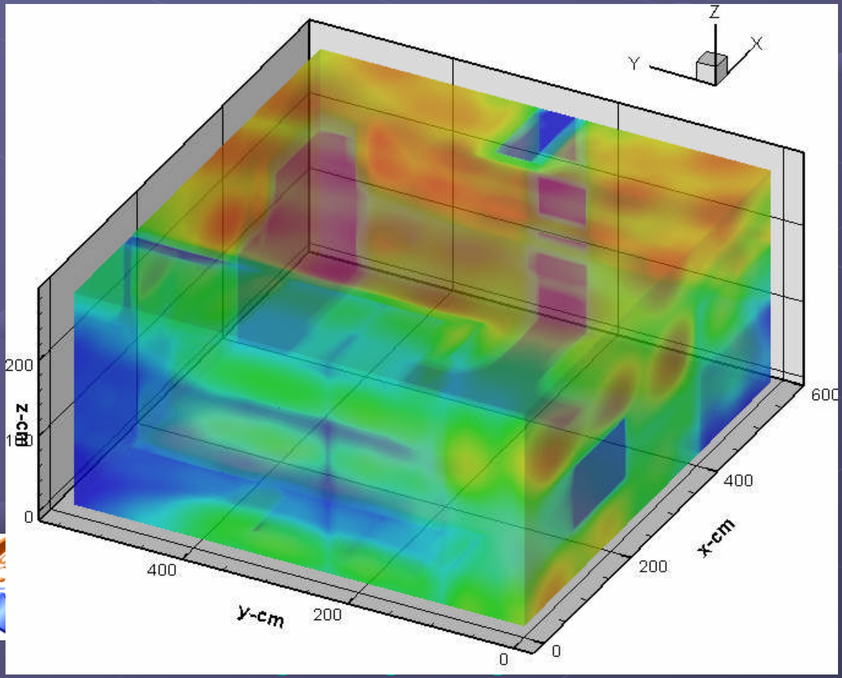


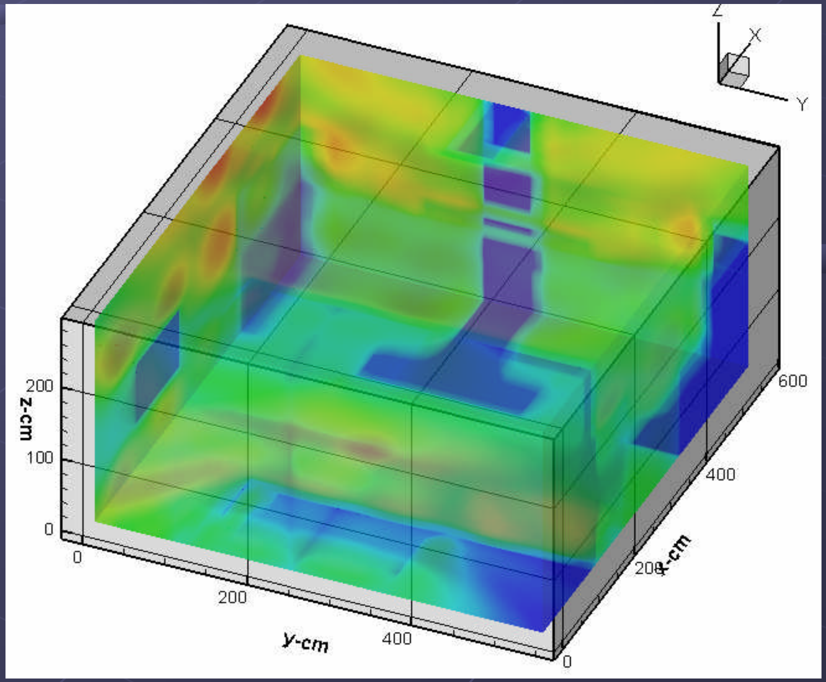
Ordinate Splitting Comparison, G2

- S8, A/G/S=2/1/2

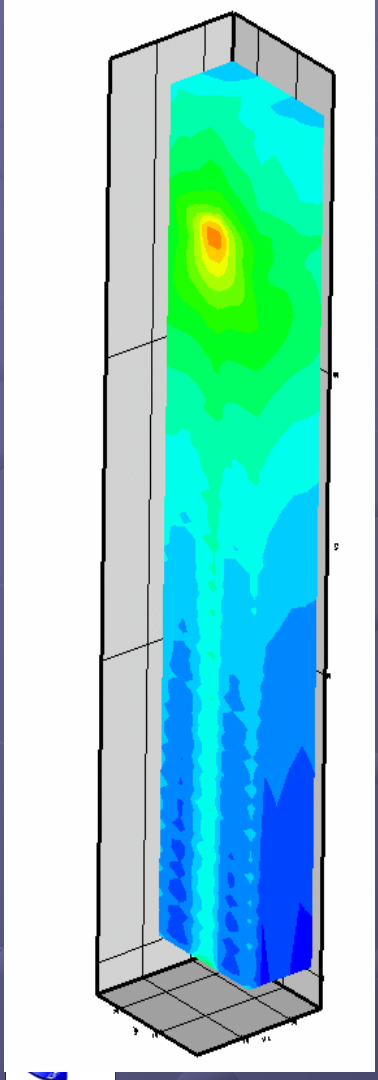


S8+OS A/G/S=2/1/2 (1,5,7,10)



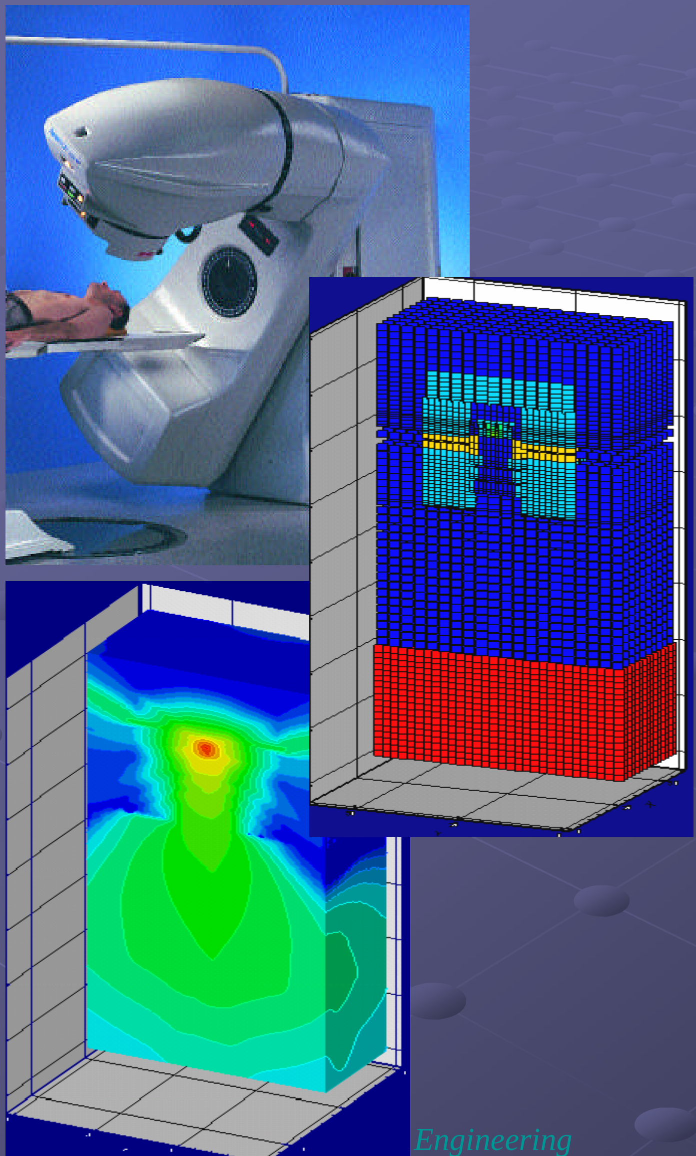


Deterministic Radiation Transport Simulations in γ-Ray IMRT Devices



- Medical Physics Modeling and Simulation Effort
  - *Ahmad Al-Basheer, PhD Grad Asst*
  - *Dr Sjoden (PI)*
  - Cooperative effort with Dr Haghighat, Dr Dempsey (Radiation Oncology),
    Monica Ghita, Benoit Dionne, PhD *Grad Assts*
  - Apply neutral particle transport methods
    - Total energy release/convolution methods to approximate neutral and charged particle dose effects in 3-D.
  - Focus on Parallel Sn methods, Benchmark with Monte Carlo Methods (PENTRAN and MCNP)
  - *Goal: minimize dose effects, extrapolate electron dose, accelerate data extraction and treatment planning; create PENTRAN-MP for Med Physics*

Photon Transport Calculations for Medical Physics Problems & Treatment Planning



- Research interests

  Hybrid Monte Carlo-Deterministic Methods for Simulating Radiation Interactions with Matter. Particle transport methods and numerical methods for solving medical physics problems, and high performance computing.

- This summer

  Al-Basheer, A., M. Ghita, G. Sjoden, B. Dionne, "Comparison of 3-D Deterministic and Monte Carlo Cross Sections for Medical Physics Problems," American Nuclear Society, Washington D.C. Meeting,

  American Nuclear Society, June 2005.

Engineering

"Comparison of 3-D Deterministic & Monte Carlo Cross Sections for Medical Physics"

- Al-Basheer, Ghita, Sjoden, and Dionne

- Snapshot of our efforts to compare and contrast parallel multigroup SN computations to Monte Carlo solutions
- Traditional deterministic radiation transport cross section libraries
  - Limited application in medical physics problems
  - Energy group structure issues
  - Broad group basis
- We compare the performance of 3 cross section libraries available from nuclear engineering, physics communities
- To compare these libraries, we computed 3-D flux distributions in a water phantom exposed to gamma-rays
- PENTRAN parallel SN compared to CE MCNP Monte Carlo
  - S42 angular quadrature (1848 directions/mesh/group)
  - P3 scattering anisotropy.
- Consider slices through various parts of the model.

Comparing xsecs for MP Applications

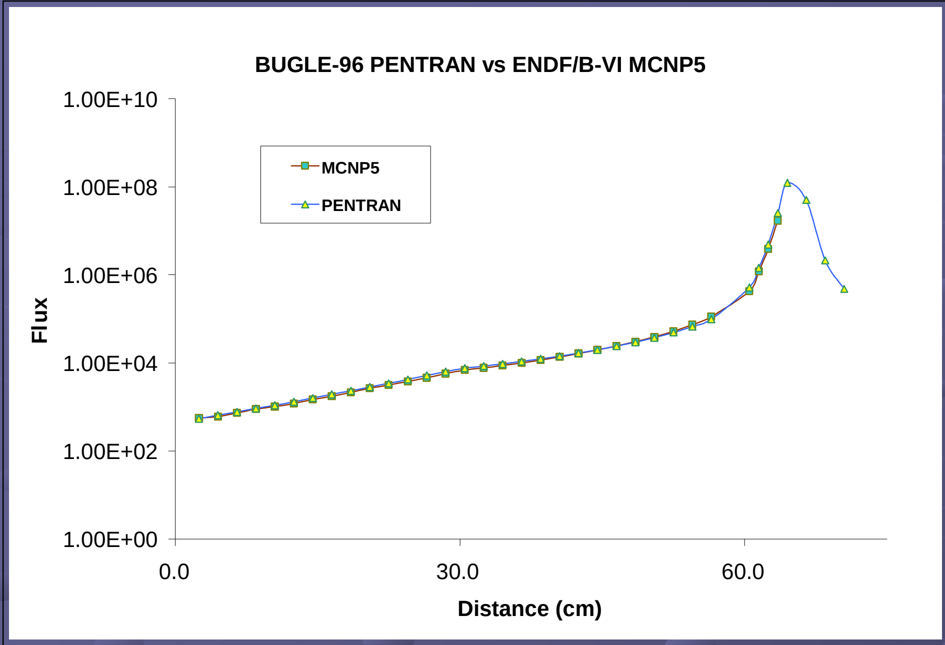


Figure 1

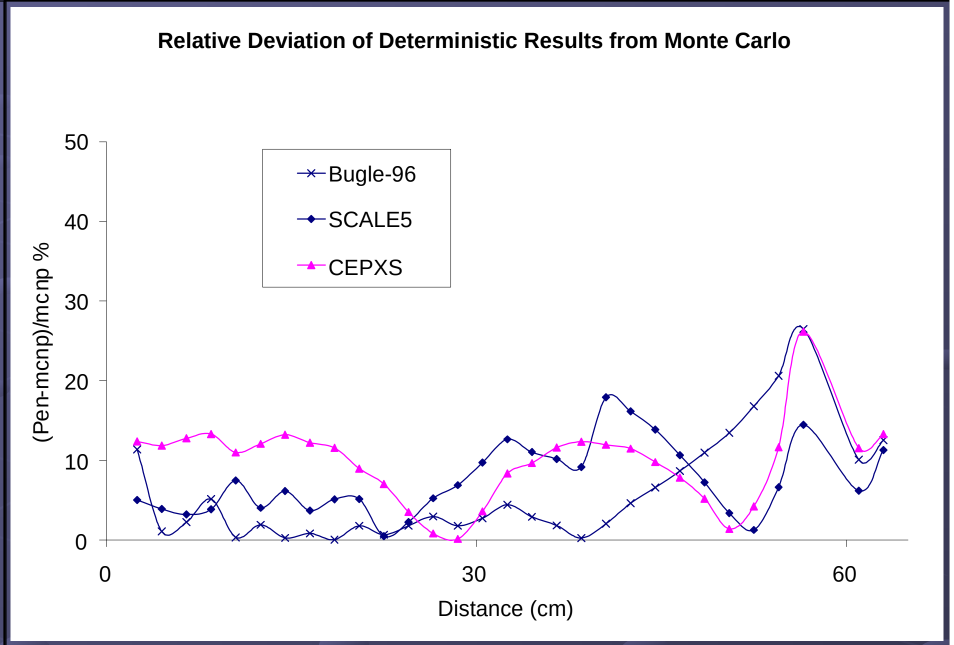


Figure 2

Fig 1: scalar flux distributions generated by PENTRAN for a single energy group of each library using the MCNP5 solution as reference

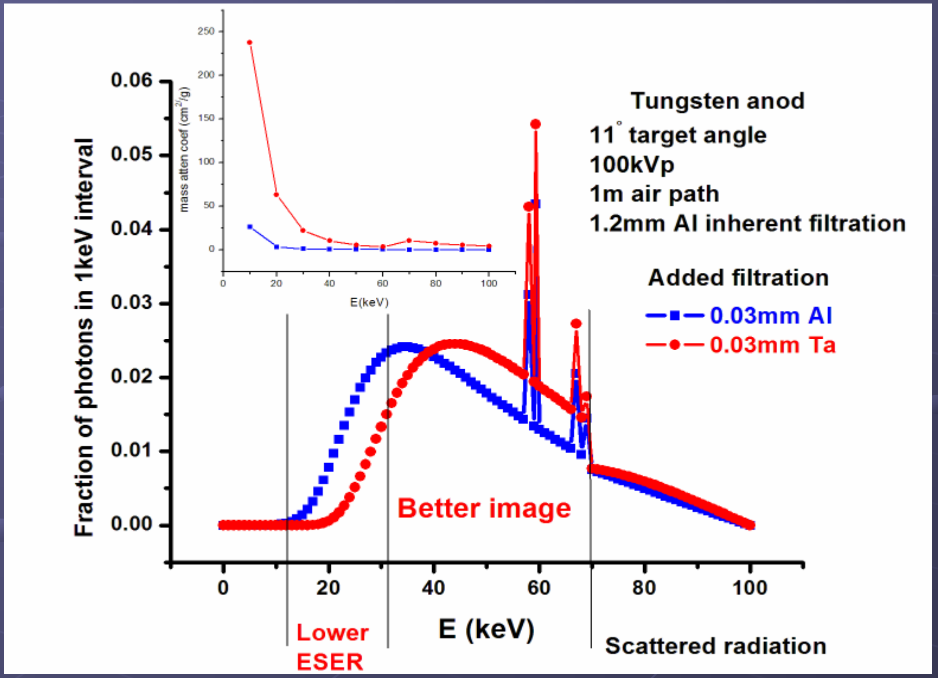
Fig 2: deterministic results using BUGLE-96 were overall best …in the water phantom, BUGLE-96 results were within the Monte Carlo statistical error

Simulation of Novel Beam Filtering in the Shands Hospital Toshiba X-Ray Facility

- Nuclear Engineering Modeling support for Medical Physics Simulation efforts
  - *Monica Ghita, PhD GA*
  - Cooperative effort with Dr Manuel Arreola, Dir of Clinical Radiological Physics, Carly Williams, Ph.D. student
  - Assess efficacy of new beam filtering procedures in Toshiba methodology using computational models (PENTRAN and MCNP), link with clinical data, trials
  - *Goal: Evaluate beam fidelity, dose effects, and facility performance to augment treatment planning*
    - Cooperative effort: NRE/Medical Physics Staff

Simulations of Novel Beam Filtering Methods in Shands Toshiba X-ray facility

- Source spectra, continuous and characteristic X-ray, corresponding to any operational parameters (kVp, target angle, filtration)
  -- computationally generated
  -- experimentally validated (stripped from the pulse height spectrum of the HPGe-detector)



- Deterministic transport calculations for improved prediction of dose
- Computational (stochastic-MCNP and deterministic-PENTRAN) assessment of the novel Ta filter: effects on the entrance skin dose and the image quality
- Development and testing of appropriate schemes for discrete ordinates spatial differencing

Closing Remarks

- PENTRAN used to solve a number of problems
  - Large problems demand parallel execution
  - Parallel speedup defined by slowest processor
- Medical physics applications...
  - Need robust angular treatment
  - Angular dependent source feature in PENTRAN permits ready simulation of photon beamlets
  - Now coupling CT voxel image data for different tissue
  - Analysis of accuracy with adaptive differencing needed
  - Decoupling of boundaries with group dependent albedos may be best with group-spatial decomposition

Simulations of Novel Beam Filtering Methods in Shands Toshiba X-ray facility