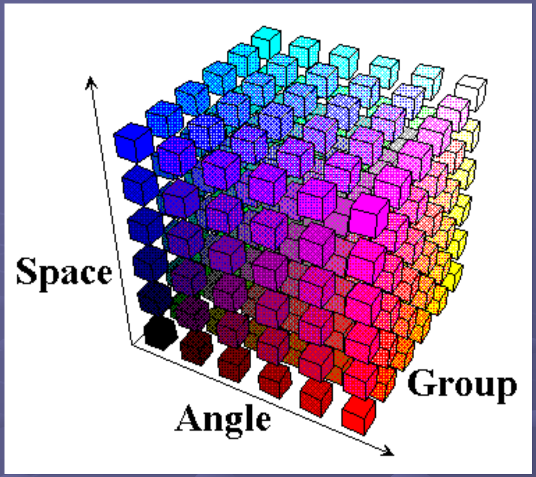
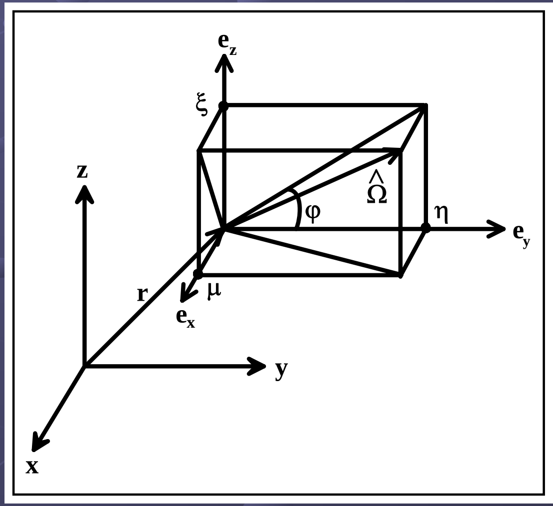


Parallel PENTRAN Applications

G. E. Sjoden and A. Haghighat
Nuclear and Radiological Engineering
University of Florida

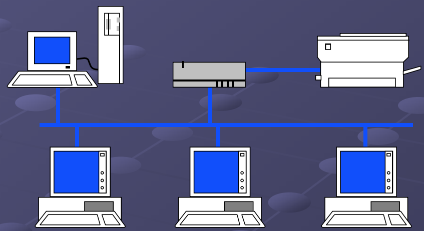
Overview

- Introduction
- Parallel Computing & MPI
- Boltzmann & Transport
- PENTRAN™ Code System
- Problem Solving Experience
- Discussion and Summary
- Questions



What is Parallel Computing?

- Computer with many processors
  - "Lumped" or *Network* "Distributed"
  - Divide problem up on processors



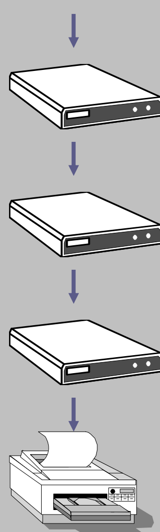
- Serial...

Task1

Task2

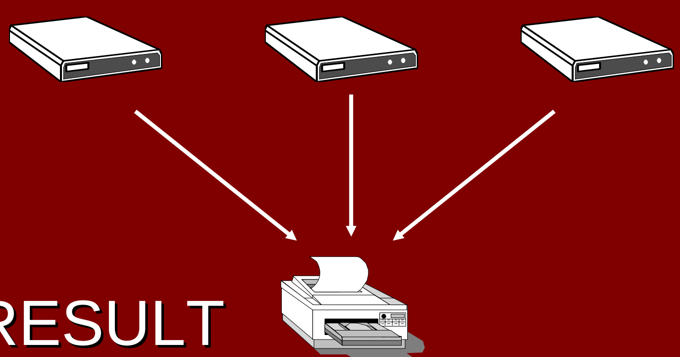
Task3

RESULT



- Parallel...

Task1 Task2 Task3



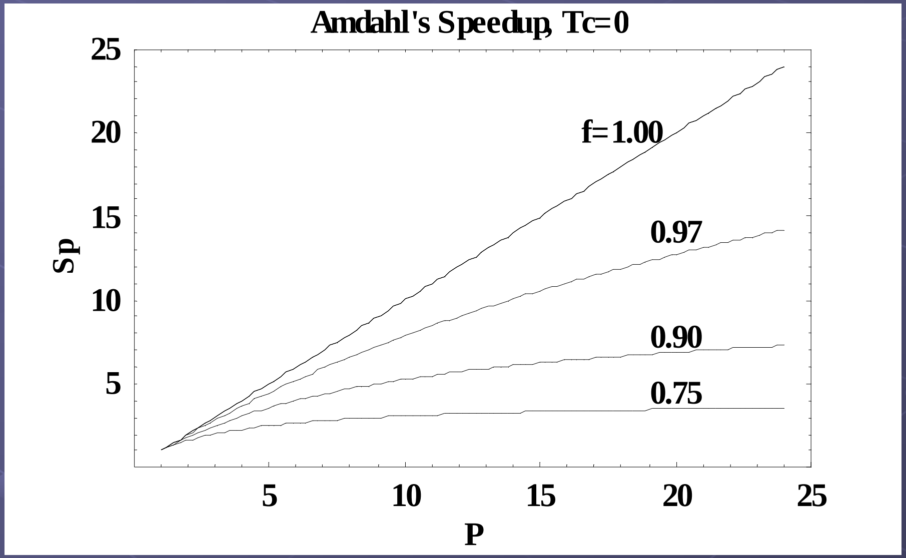
RESULT

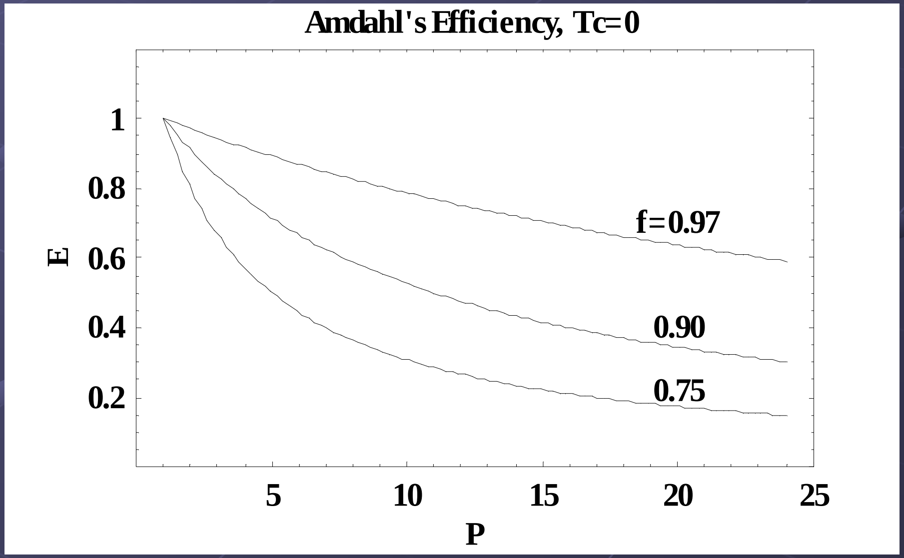
About MPI...

- MPI (Message Passing Interface) Library
  - Began with “MPI Vendor Forum” May 1994
    - Formalized in 1995
  - For distributed memory machines (FORTRAN, C, other language variants support)
- ANSI-like “standard” in message passing
  - Process com groups, parallel decomposition topologies
  - Port code directly to architectures running MPI
  - For any parallel architecture/cluster, SCANs

Amdahl's Law: Limited Speedup

- (Parallel Code Fraction = *f*)
- $S_p = ((1-f) + f/p + T_c/T_s)^{-1}$
- Speedup= $S_p = T_s / T_p$, Efficiency= $E = S_p / P$
- If f =0.8, then max S_p =5.0 as P->Infinity





Distributed Memory Programming

- Efficient message passing algorithms…
  - View message passing as a *last resort*
    - Minimize serialization, barriers
  - Use a partitioned memory storage of data
    - Only way to *solve larger problems*
    - *Process mapping arrays* to determine "who's where"
- Overall...
  - Use a coarse-grained code structure
  - Many flops performed before messages passed
  - Don't forget about *Amdahl's Law*

3-D Boltzmann Equation

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

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

$$\left. \left[\phi^k_{C\,g',l}(x,y,z)\cos(k\varphi) + \phi^k_{S\,g',l}(x,y,z)\sin(k\varphi) \right] \right\} + \frac{\chi_g}{k_0} \sum_{g'=1}^{G} \nu \sigma_{f g'}(x,y,z)\, \phi_{g',0}(x,y,z)$$

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

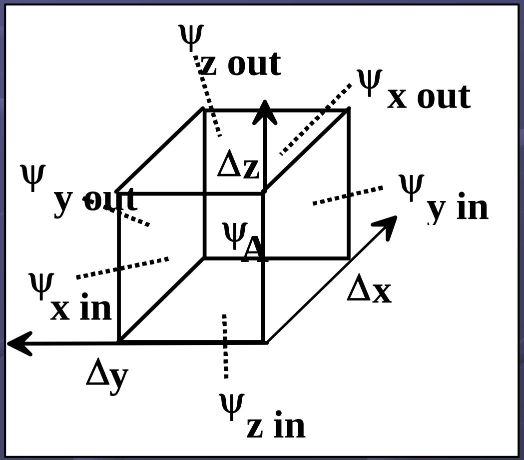
Transport Theory

- Boltzmann transport methods
  - Monte Carlo method
  - Discrete Ordinates (S_N) method
  - Each has specific …

    Advantages (+)

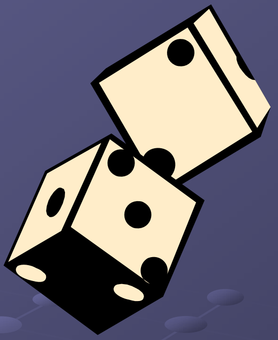
    Disadvantages (-)

    Issues



- Both methods can take advantage of parallel processing!

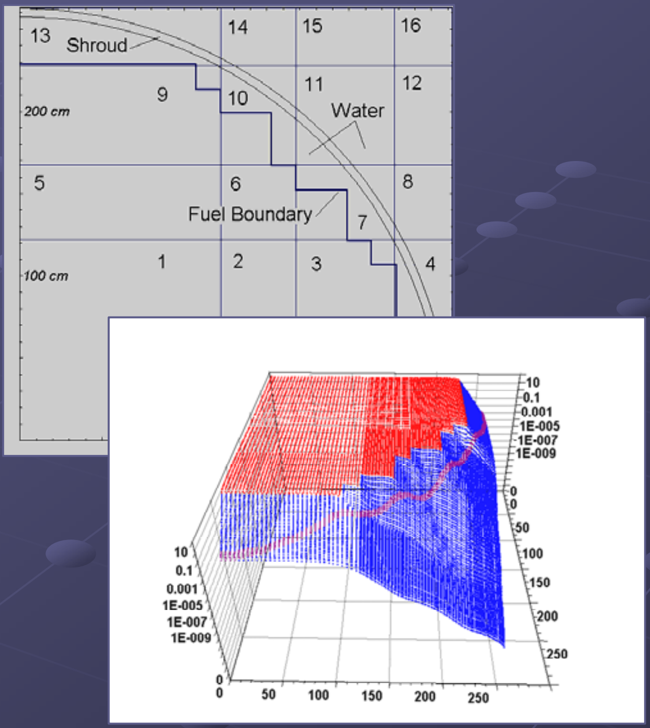
Monte Carlo



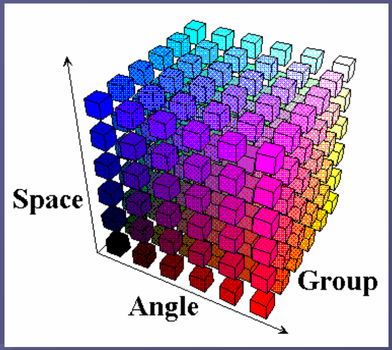
- Advantages
  - Traditional, straight forward
  - Geometrically precise
  - Robust particle physics--Continuous-Energy xsec
  - Parallelization obvious: particle histories
- Disadvantages:
  - Processing time, Non-analog variance reduction
  - Inevitable uncertainties and Central LT
  - “Global” solution difficult to obtain
  - Results can be limited in application

Discrete Ordinates

- Advantages
  - Model entire geometry
  - Fast and accurate
  - Global flux distribution
  - Directly allows for burnup, etc
- Disadvantages:
  - Proper multi-group cross sections
  - Geometry discretized
  - Memory, storage, differencing scheme issues
  - Parallelization--coupling in *angle, energy, space*

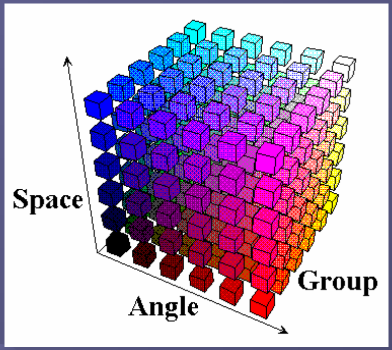


PENTRAN™ (1)



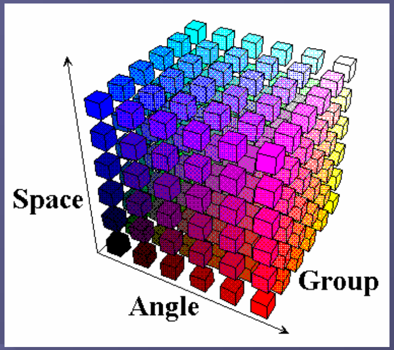
- *P*arallel *E*nvironment *N*eutral-particle *TRAN*sport
  - Introduced in 1996, under continuous development that began in 1995 by Sjoden and Haghighat
  - Parallel S_N in *angle*, *energy*, and *space* & *I/O*
  - ANSI FORTRAN over 38,000 lines
  - Industry standard FIDO input
  - Solves 3-D Cartesian, multigroup, anisotropic transport problems
  - Forward and adjoint mode, Fixed source, criticality eigenvalue problems

PENTRAN™ (2)



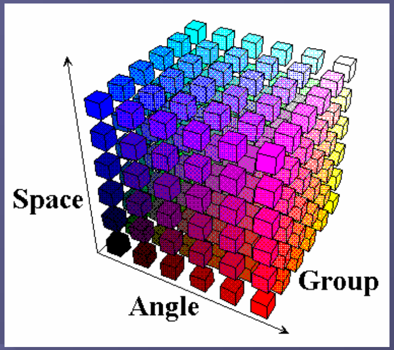
- Uses MPI Message Passing Interface library
  - Standard for MIMD systems
- Performs all I/O in parallel by each processor
- Uses a local, partitioned memory for memory intensive arrays (angular fluxes, etc)
- Auto-tuning feature for optimum memory allocation
- Builds processor communicators
  - minimized message traffic
  - communication across decomposition "planes" of processors

PENTRAN™ (3)



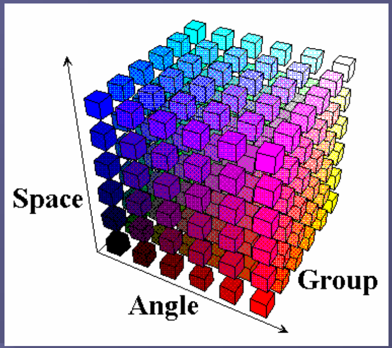
- Performs automatic scheduling based on a user-specified decomposition weighting vector
- Allows for adaptive differencing among coarse mesh zones using problem physics
- Adaptive Differencing Strategy...
  - Diamond Zero (DZ)
  - Directional Theta-Weighted differencing (DTW)
  - Exponential-Directional Weighted (EDW)
  - Exponential-Directional Iterative (EDI) (see Feb07 NSE)

PENTRAN™ (4)



- Allows for a fully discontinuous variable meshing between coarse meshes
- Uses a novel higher order mesh coupling scheme: Taylor Projection Mesh Coupling (TPMC)
- Accelerations…
  - Two-grid 3-D TPMC-coupled "/" multi-grid transport acceleration
  - PCR with a zoned rebalance acceleration
- Multigroup & One-level SI schemes

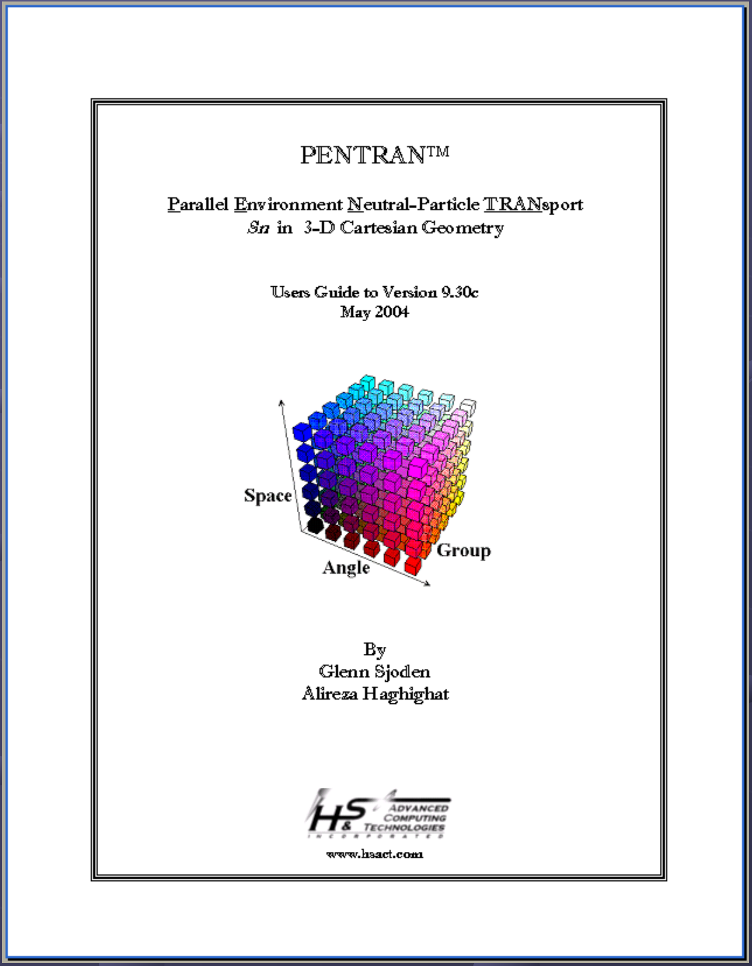
PENTRAN™ (5)



- Allows for automatic Red-Black or Block-Jacobi
- Automatic load balancing
- Anisotropic scattering via Legendre Pn moments to arbitrary order
- 3-D angular quadratures level symmetric through S20, Legendre-Chebychev (Pn-Tn) to arbitrary order
- Vacuum, reflective, group-albedo boundaries
- Volumetric sources & plane surface fluxes
- PENDATA, PENMSH-XP utilities

PENTRAN

- Demonstrated 97% to 98% parallel fraction
  - Performance depends on problem, decomposition
  - Development focus on high accuracy & parallel efficiency
  - *Numerous applications over the past 12 years*
- Speedups of ~50 readily achievable
  - Demonstrated scalability
  - *www.hswtech.com*


PENTRAN™

Parallel Environment Neutral-Particle TRANsport
Sn in 3-D Cartesian Geometry

Users Guide to Version 9.30c
May 2004

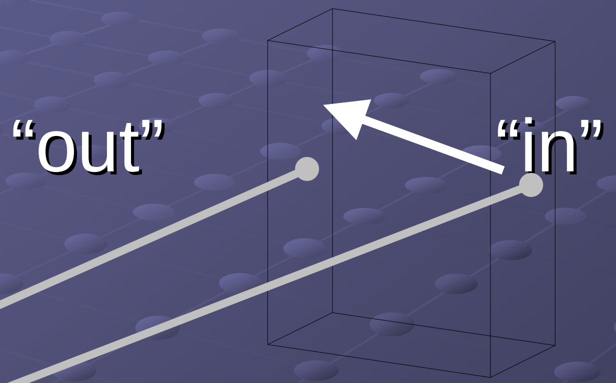
Space
Angle
Group

By
Glenn Sjoden
Alireza Haghighat

HSW Advanced Computing Technologies Incorporated
www.hsact.com

3-D Discrete Ordinates

- Balance Equation…

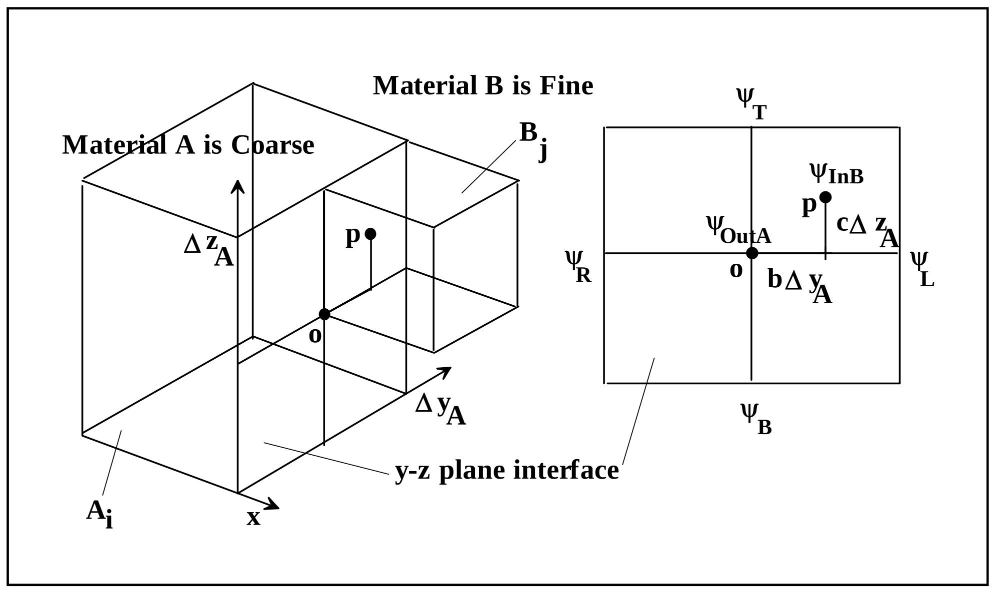


$$\frac{|\mu_m|}{\Delta x}(\psi_{\text{out}\,x}-\psi_{\text{in}\,x})+\frac{|\eta_m|}{\Delta y}(\psi_{\text{out}\,y}-\psi_{\text{in}\,y})+\frac{|\xi_m|}{\Delta z}(\psi_{\text{out}\,z}-\psi_{\text{in}\,z})+\sigma\psi_A=q_A$$

$$\psi_{\text{out}\,x}=\frac{1}{\Delta y\Delta z}\int_0^{\Delta y}\int_0^{\Delta z}\psi_m(\Delta x,y,z)\,P_0(y)\,P_0(z)\,dy\,dz$$

Taylor Projection Mesh Coupling

- Discontinuous grid densities
  - Allow high definition in ROIs, parallel load balance
- First Order Taylor projection of angular fluxes at interface between discontinuous grid surfaces
  - Flow Step
  - Particle Balance Step
  - Important for “Coarse to Fine”

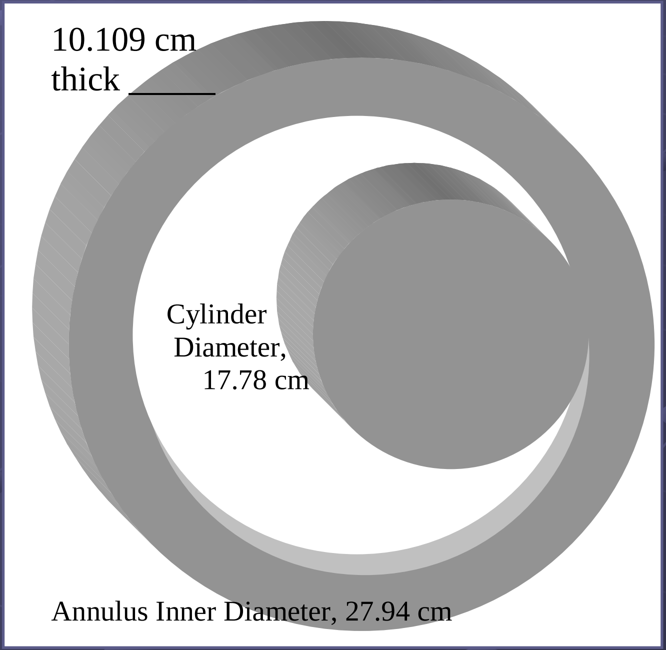


$$\psi_{\text{inB}} = \psi_{\text{outA}} + b\,\Delta y_A \frac{\partial \psi}{\partial y}\Big|_A + c\Delta z_A \frac{\partial \psi}{\partial z}\Big|_A + O(\Delta^2)$$

A "Demo" Problem

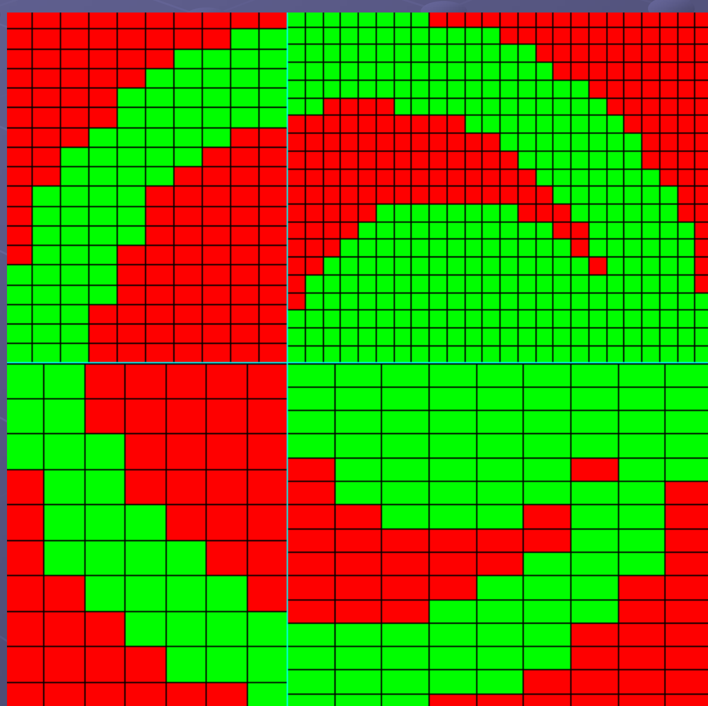
- Annular region (38.1 cm OD) encompassing cylinder in x-y-z
  - k=1.00*, fast metal systems, 93.263% U-235 (tare U-238)
  - Placed in vacuum, non-metal regions are void
- 16-G Hansen-Roach MG xsecs
  - Zero pot dilute absorber O(MeV)n
  - <0.4% n groups 7 to 16 (< 17 keV)
  - Uncertainties lead to ~1%

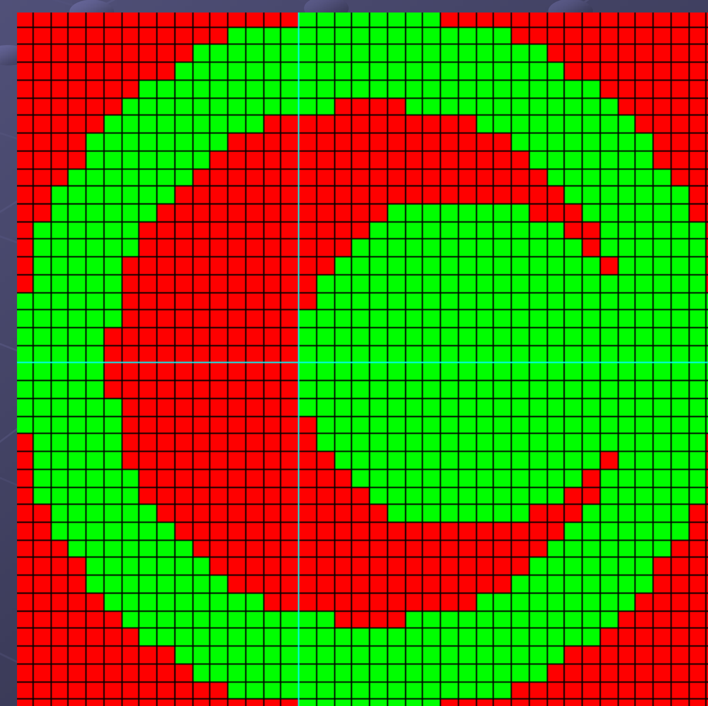
*(KENO results from Wagner et al, 1992)



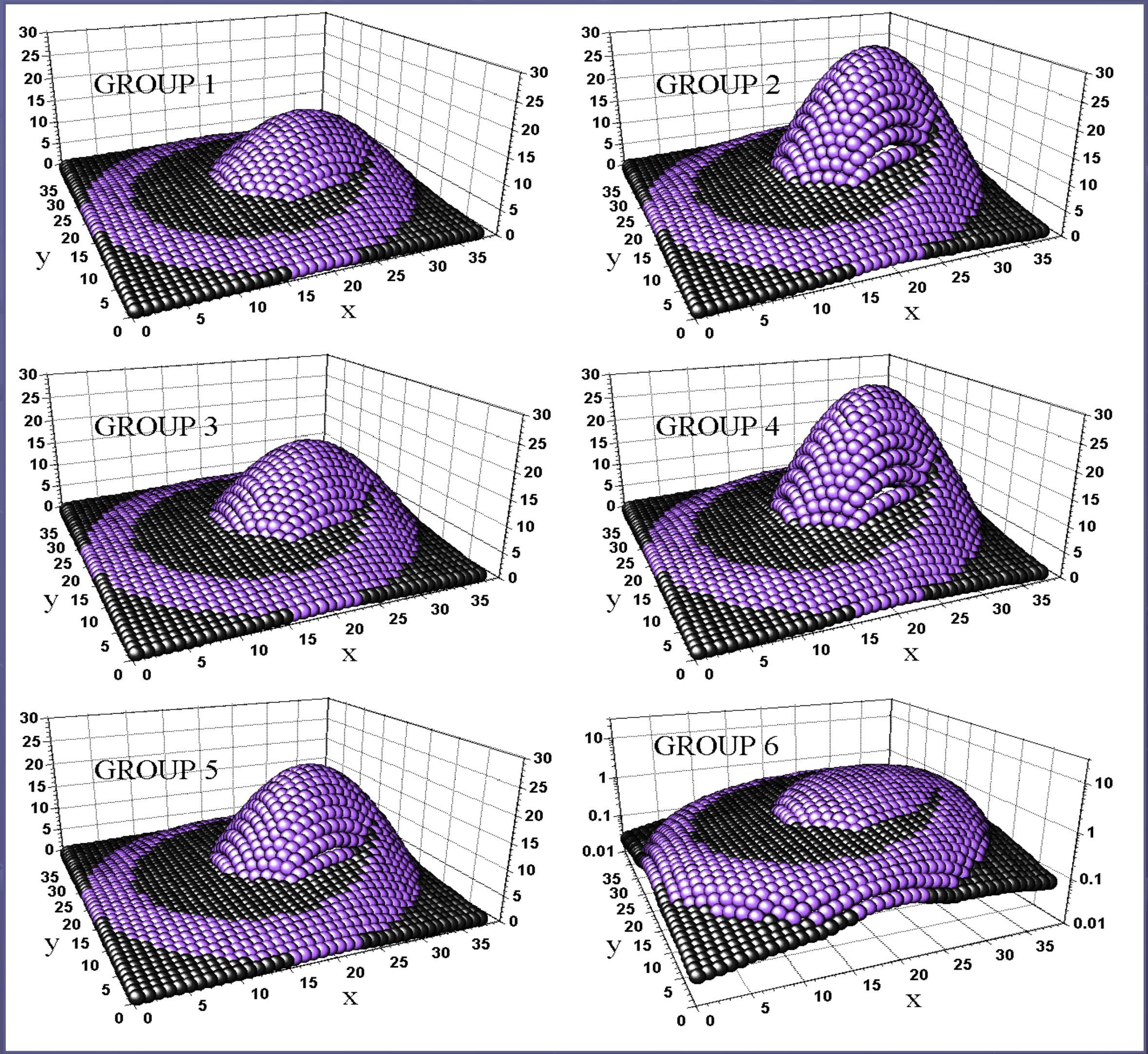
Geometric Model Setup

- PENMESH-XP- automatically sets up problem
  - You define shapes, 3-D intervals, it does the rest…
- Example: Ring Problem, 4 coarse meshes:

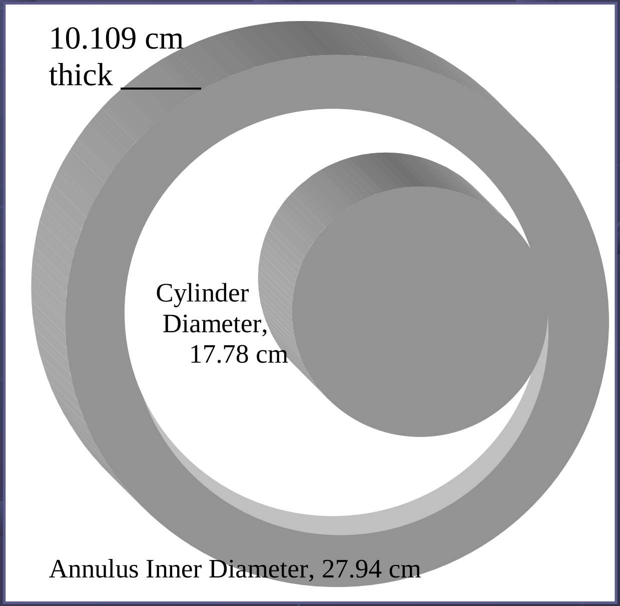




Results: Ring Problem



k=0.994
PENTRAN &
MCNP-MG



Venus-3 Shielding Problem

- Owned/operated by SCK-CEN in Mol, Belgium
- Practical model of a PWR
  - 16 "15x15" sub- assemblies, 1.26 cm pitch
- Types of fuel:
  - 4% enriched uranium, 3.3% enriched uranium
  - partial length 3.3% fuel upper/ stainless steel lower
- Other unique features
  - Water hole, SS baffle, Pyrex rods among 4% rods
- OECD Source, G1-26 of BUGLE-96, P3-S8
  - PENTRAN Runs for 4, 8, 16, 32 SP2 Processors

Venus-3 Shielding Problem

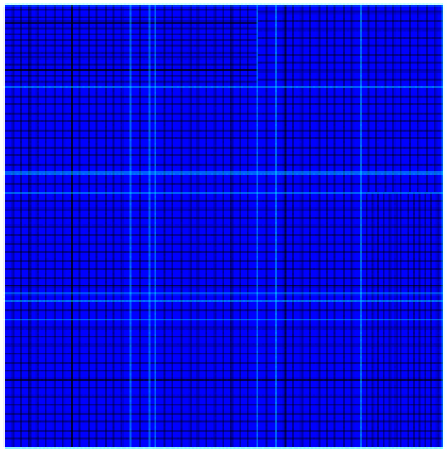


Figure 1a: Z-Level 1

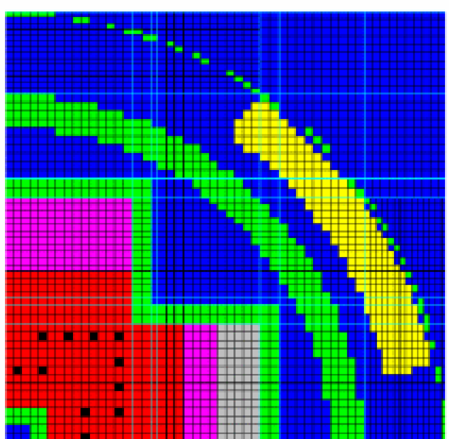


Figure 1b: Z-Level 2

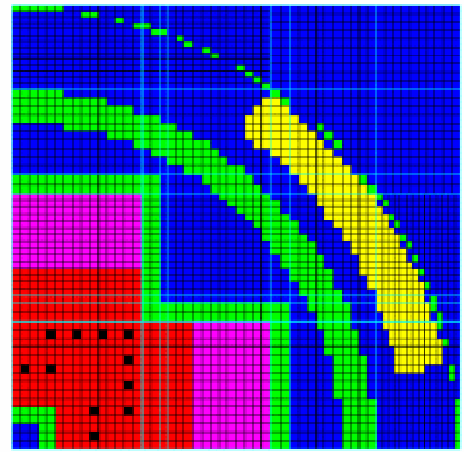


Figure 1c: Z-Level 3

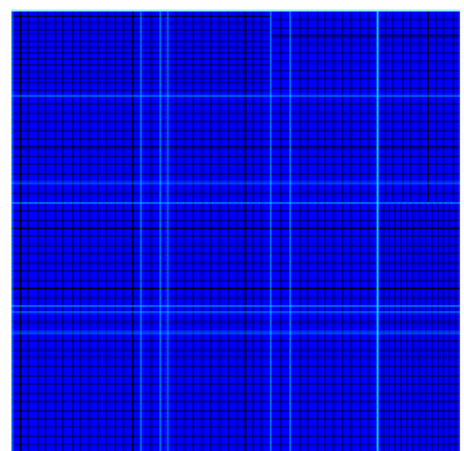


Figure 1d: Z-Level 4

Venus-3

- PENMSH-XP code used to generate 3-D Cartesian Grid
- ~85,000 cells
- 26 Groups
- P3-S8 Discrete Ordinates

- Group 1 Flux Solution:

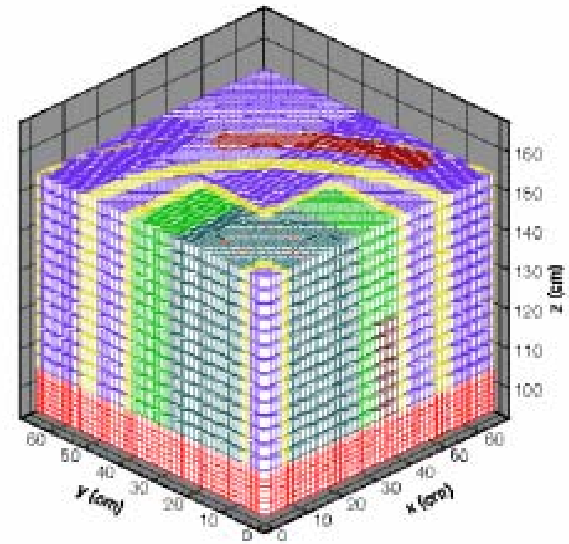


Figure 2: 3-D Mesh and Material distribution of PENTRAN Venus-3 Model (upper reflector not shown)

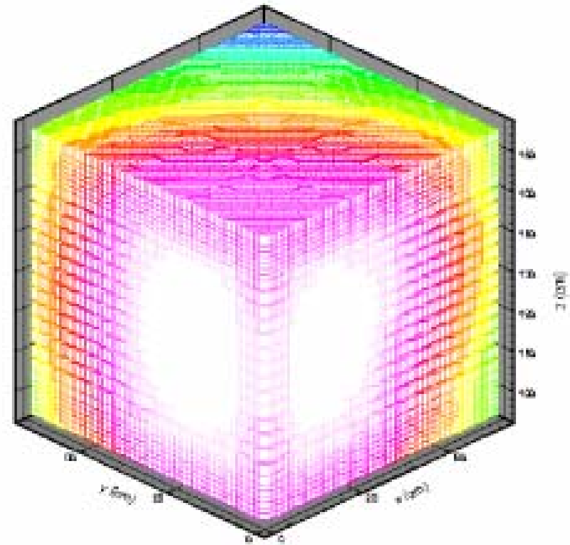
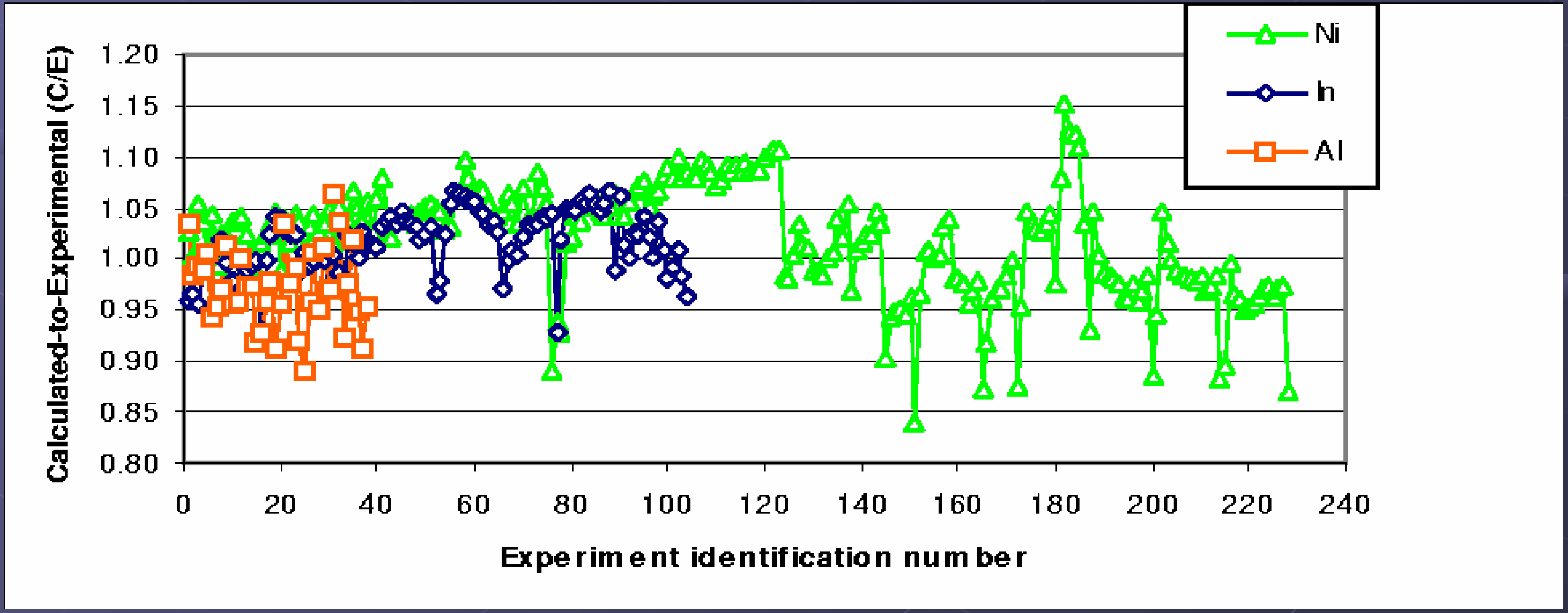


Figure 3: Group 1 Flux Distribution for PENTRAN Venus-3 Model

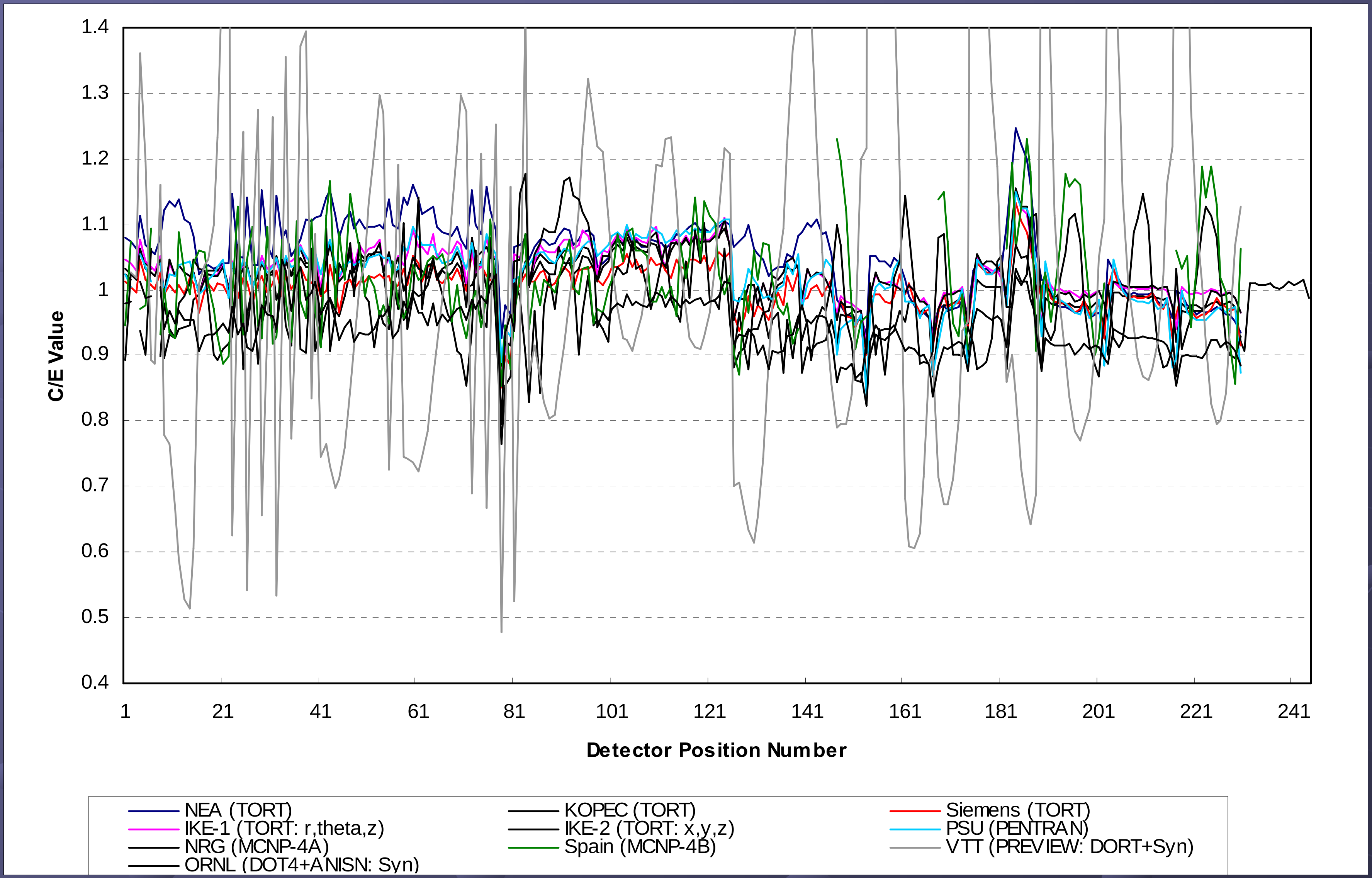
Venus-3 Results

- Compared 370 Measured Rxn Rates (Ni, In, Al dosimeters)
- vs Integral Rxn Rates computed from PENTRAN P3-S8 26 group-dependent fluxes.
- 95% C/E values +/-10%; 5% within +/-15% (near P/L rods).



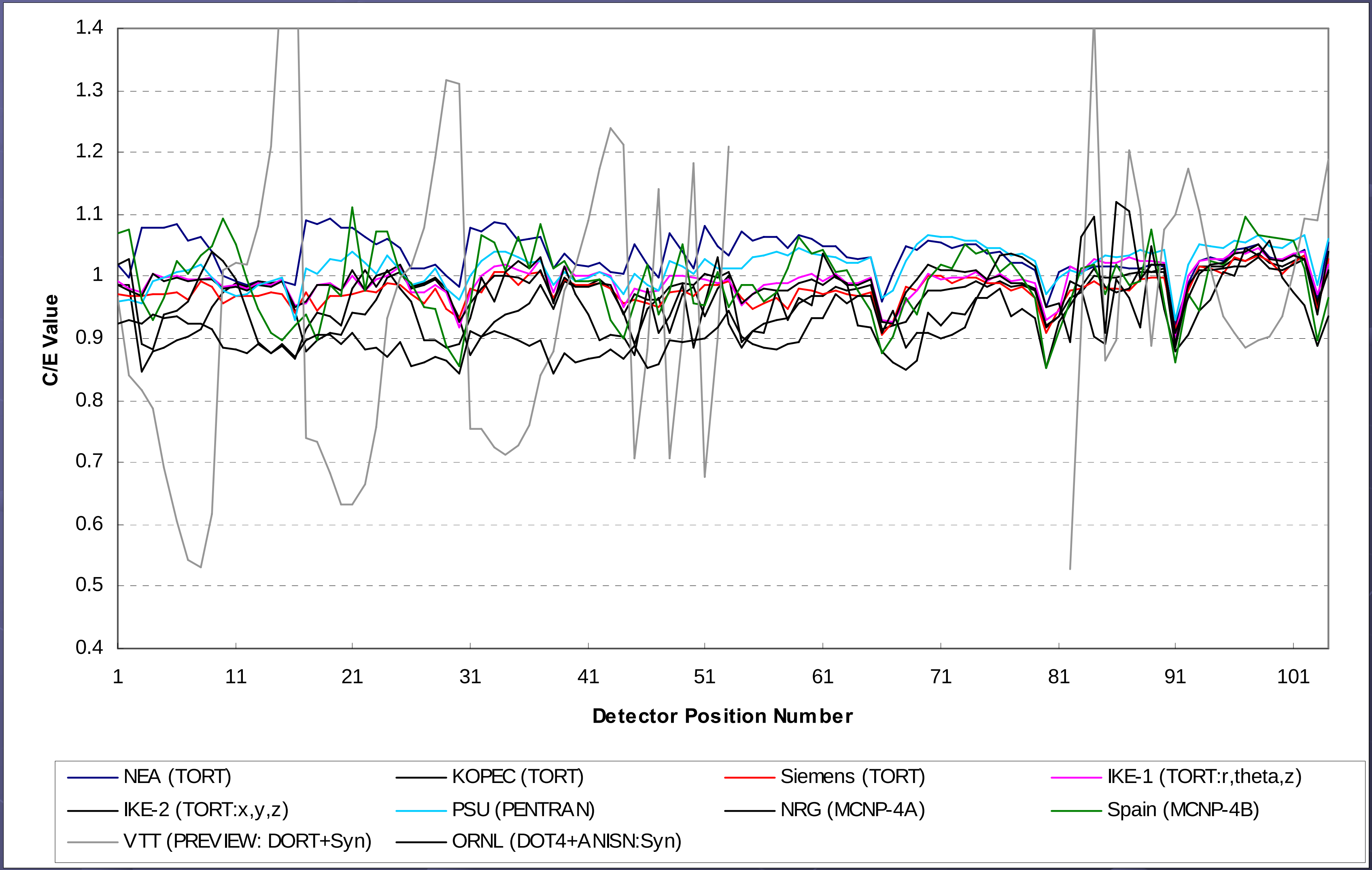
Comparison with others

C/E Equivalent Fission Flux for the $^{58}Ni(n,p)$ reaction



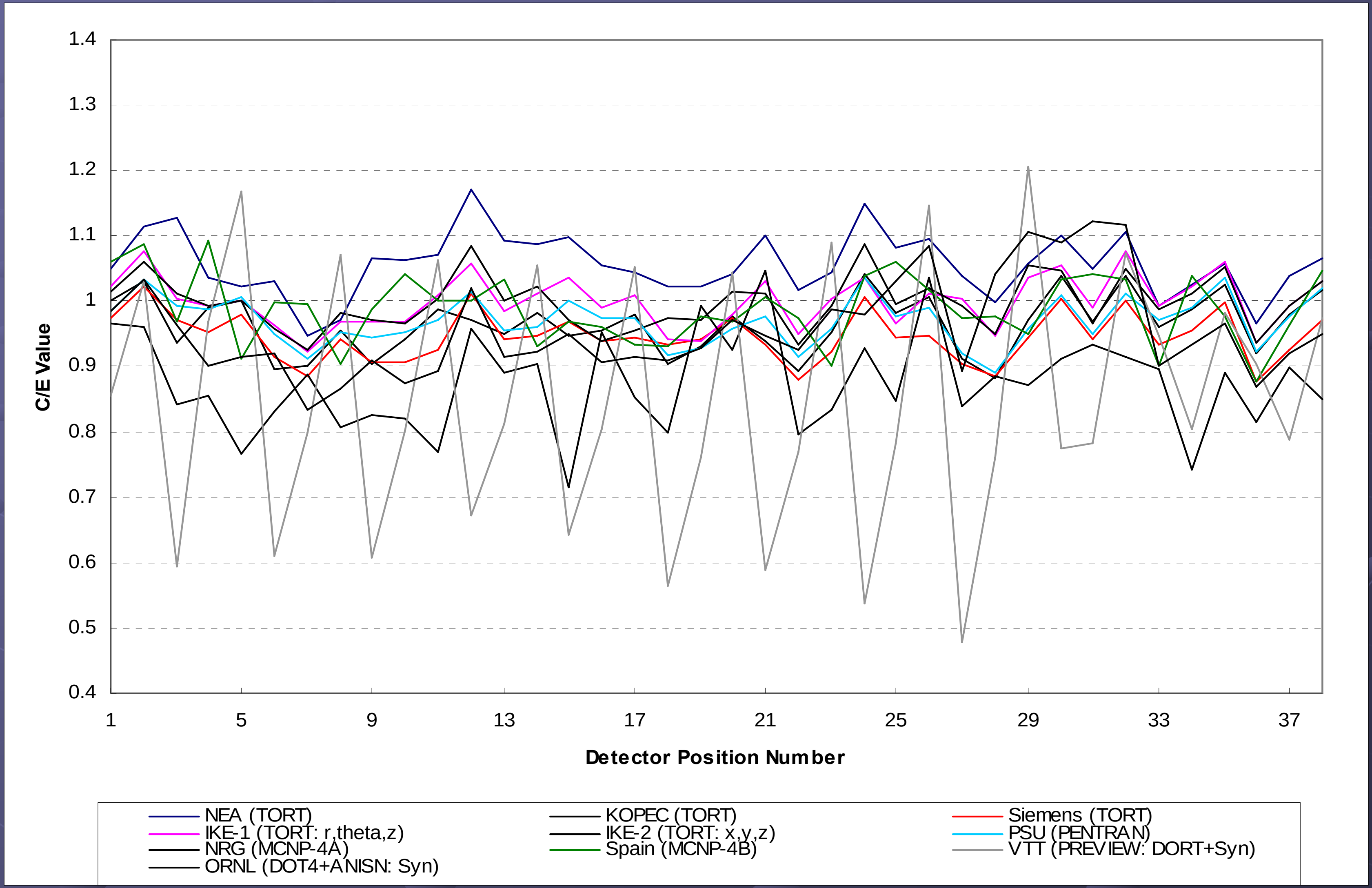
Comparison with others

C/E Equivalent Fission Flux for the ^{115}In(n,n') reaction

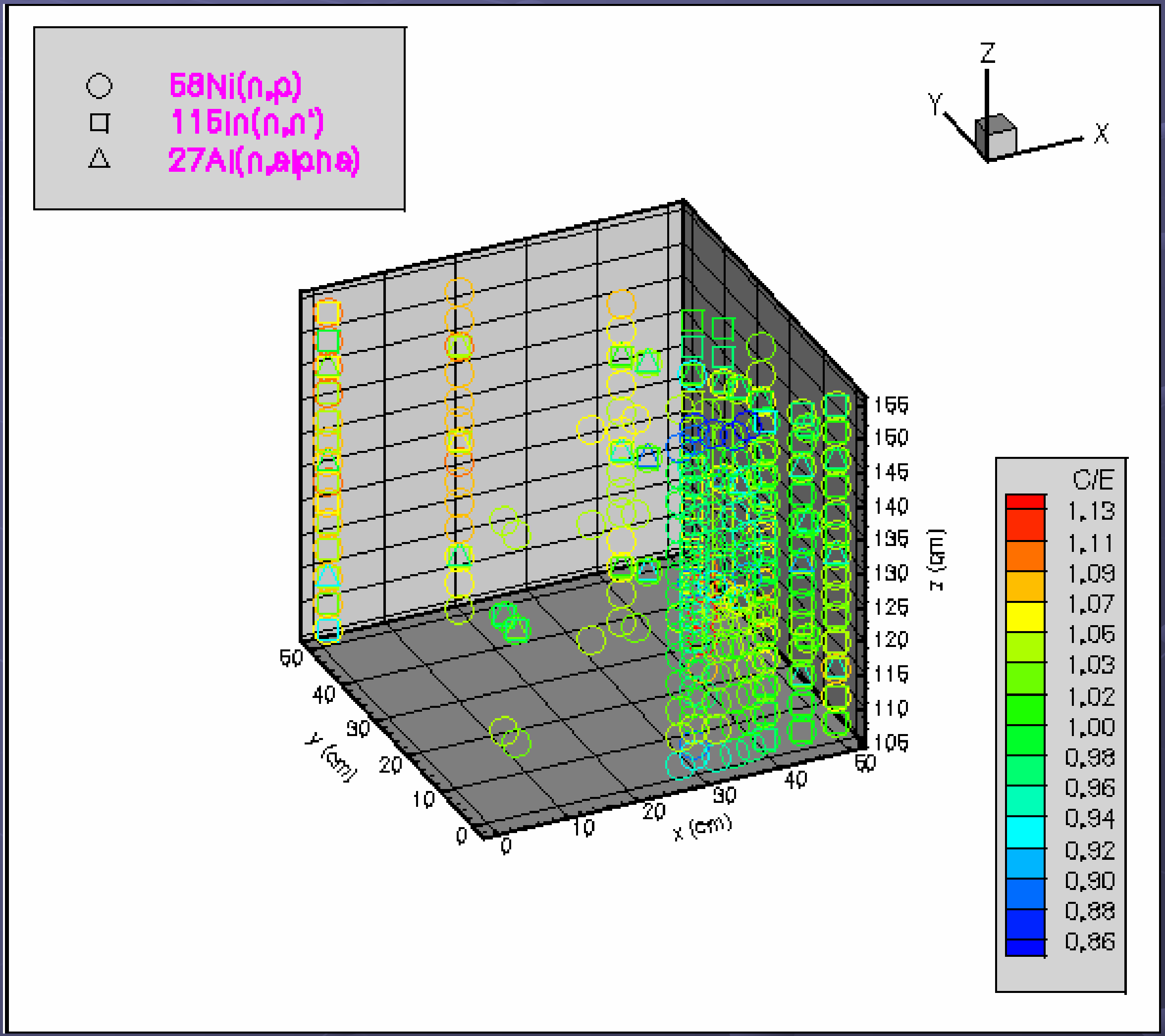


Comparison with others

C/E Equivalent Fission Flux for the $^{27}Al(n,\alpha)$ reaction



PENTRAN results are very close to experimental results; more than 95% of the Calculated-to-experimental (C/E) values are within ±10%, and only 5% of values within ±10% and ±15%.



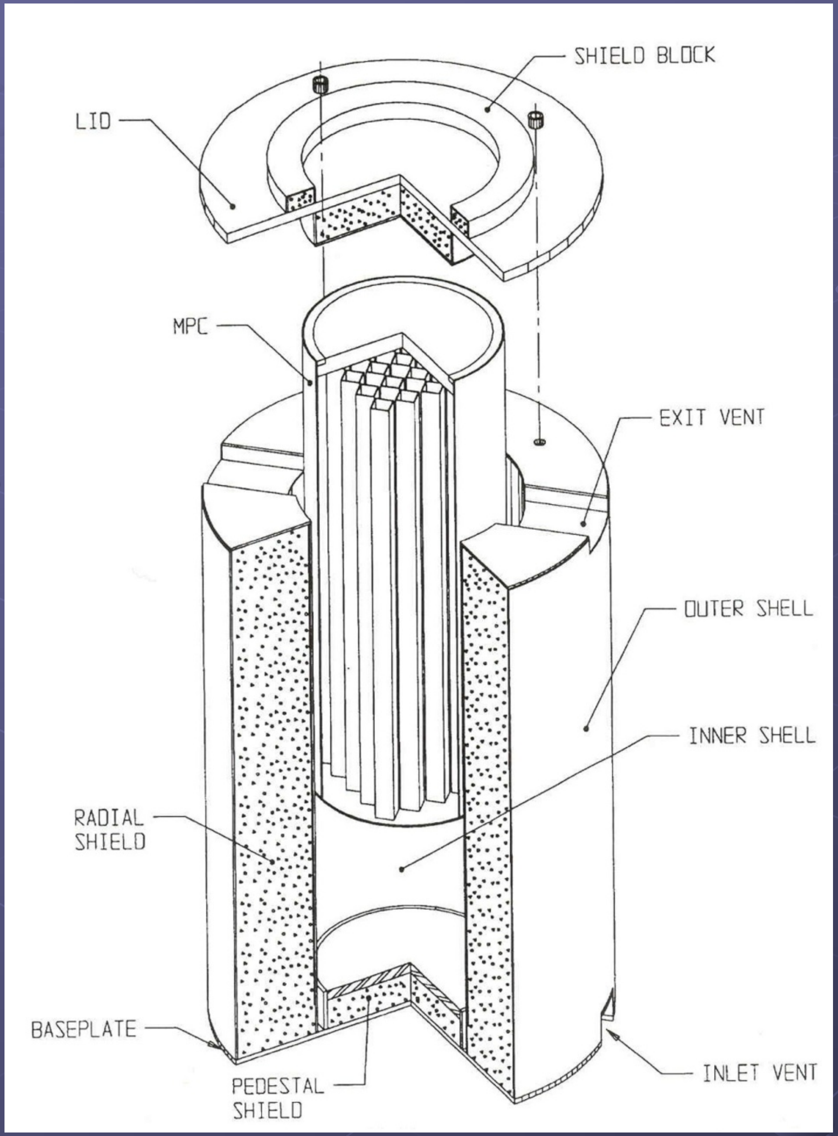
Venus-3 Parallel Performance

Table II: Dosimeter Number Locations in Regions of Venus-3

Case	Processors	A/G/S Decomposition	Wall-clock Time, min	Speed-Up (4-node base)	Efficiency
1	4 (1-set)	4/1/1	551.8	1.00	–
2	8 (2-sets)	8/1/1	311.9	1.77	88
3	16 (4-sets)	8/1/2	153.3	3.60	90
4	32 (8-sets)	8/1/4	84.3	6.54	82

Haghighat, A., H. Ait Abderrahim, and G. Sjoden, "Accuracy and Parallel Performance of PENTRAN Using the VENUS-3 Benchmark Experiment," **ASTM STP 1398 on Reactor Dosimetry at the 10th International Symposium on Reactor Dosimetry**, Osaka, Japan, 1999.

HI-STORM Cask Simulation

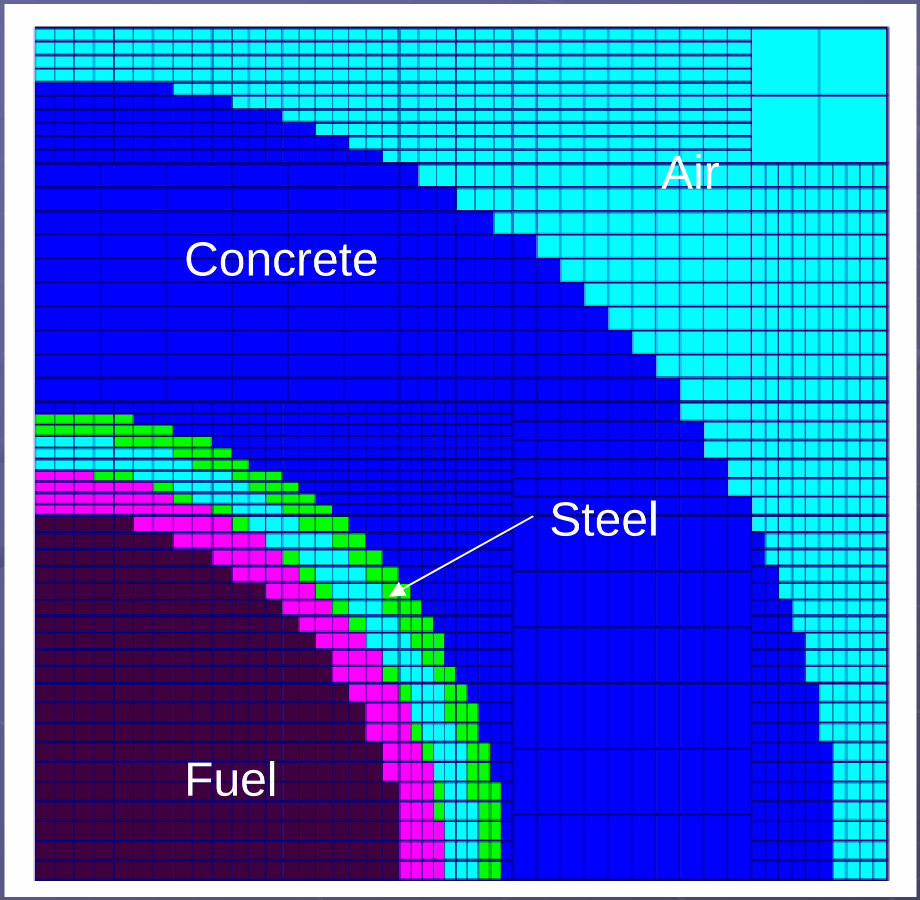


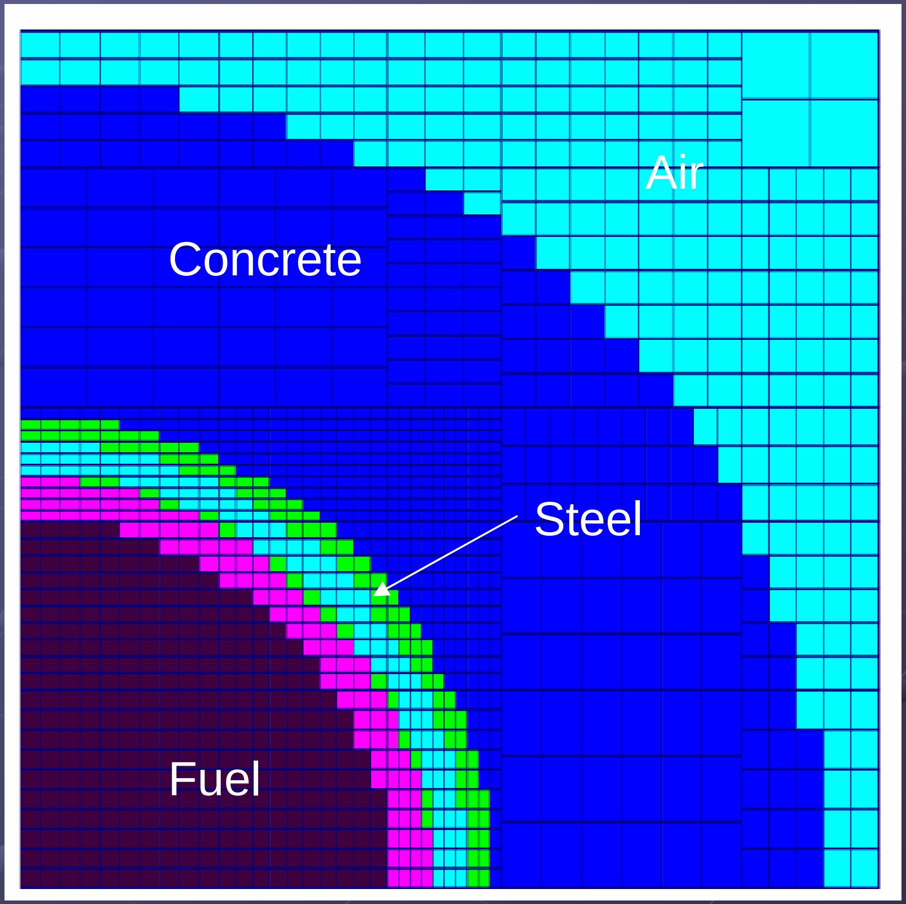
- 24 PWR Assemblies
- 68 BWR Assemblies
- 1 Multi-purpose Canister (MPC)
- 6.7 cm for air flow gap

Spent Fuel Storage Cask Modeling

- Height ~ 610 cm
- Shell O.D. ~340 cm
- Shell I.D. ~187 cm
- Empty Weight 269,000 lbs (55.3 MT)
- Max. Loaded Weight 358,000 lbs (162.4 MT)

‘Large’ and ‘Small’ S_N Cask Models

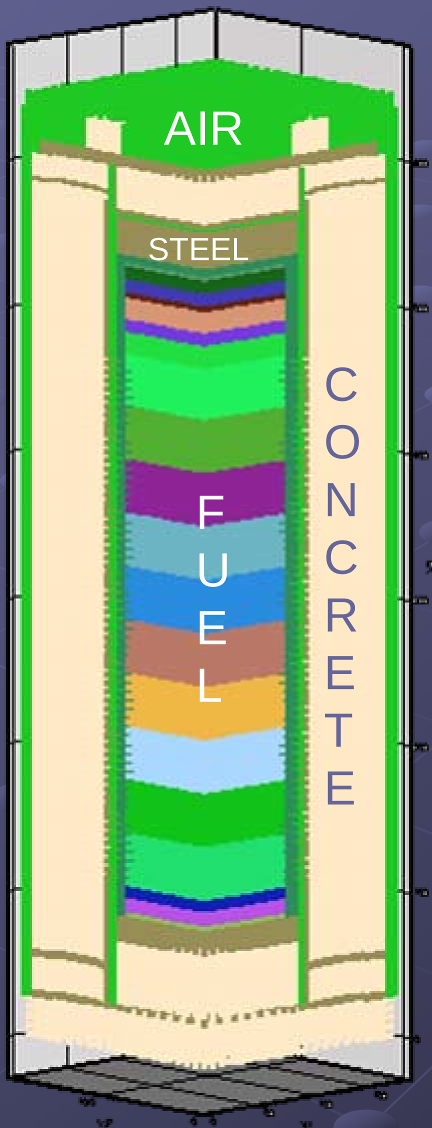




‘Large’ model has more meshes in the concrete and air.

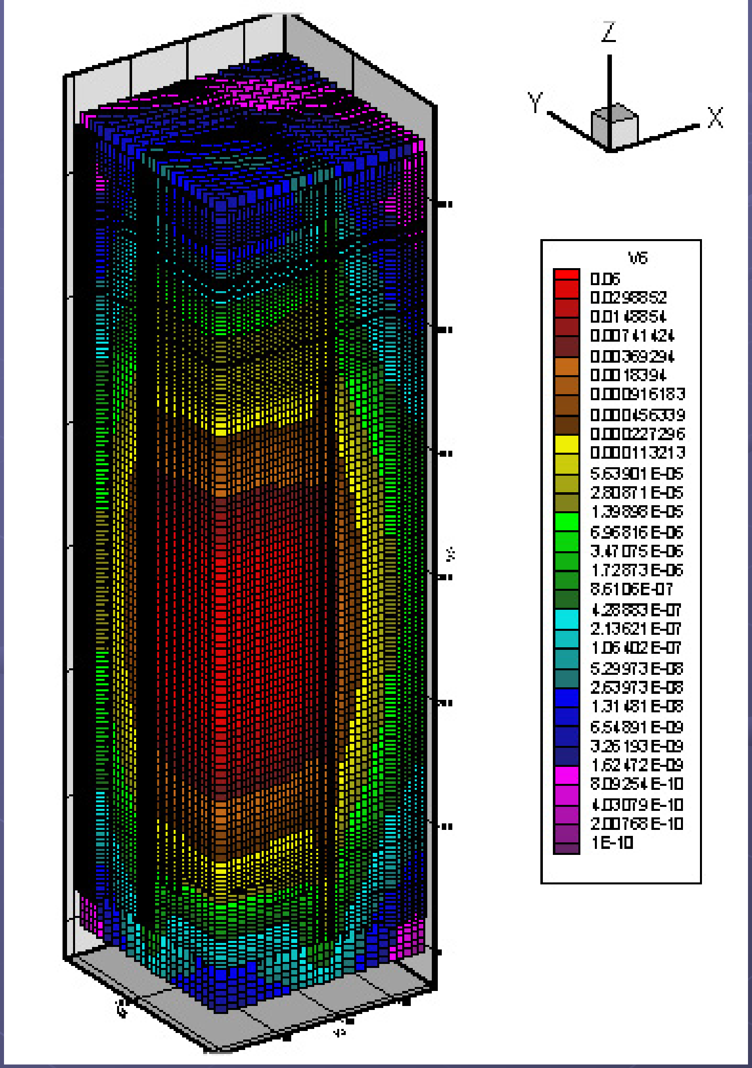
Cask S_N Models Summary

- **'Large' Model**
- CASK library (22n, 18g)
- 17 Materials
- 318,426 fine meshes (1000 coarse meshes) (40 z-levels)
- P_3, S_{12} (168 directions)
- 1.48 GB per processor 8 processors (~12 GB Total)

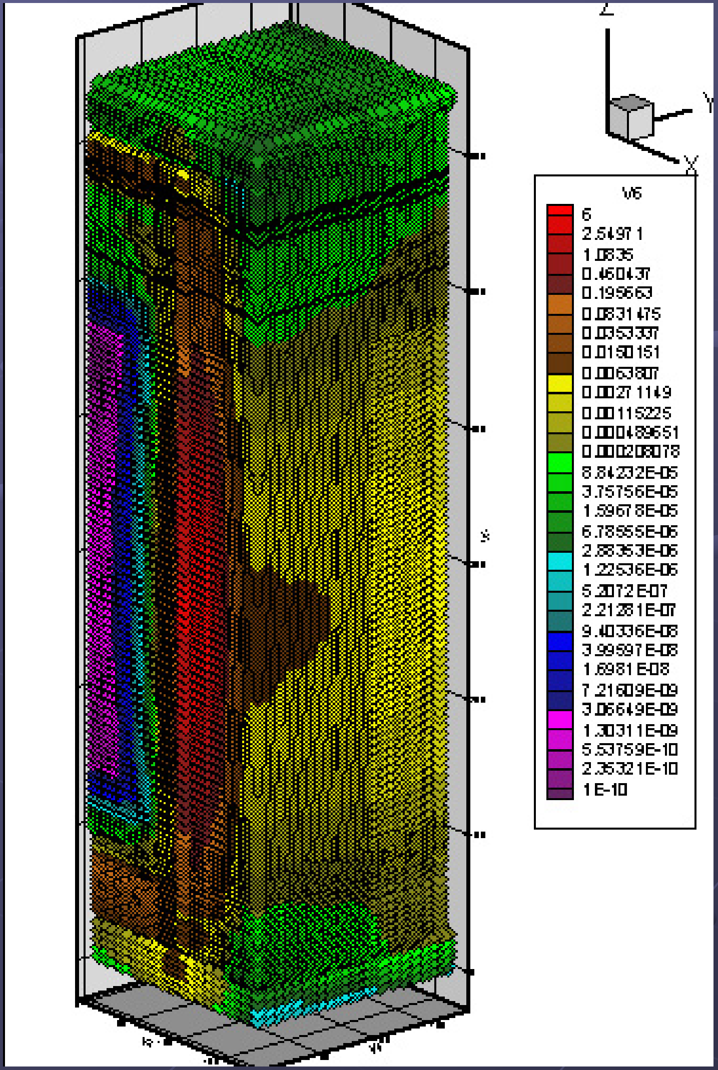


- **'Small' Model**
- CASK library (22n, 18g)
- 17 Materials
- 195,144 fine meshes (1000 coarse meshes) (40 z-levels)
- P_3, S_{12} (168 directions)
- 1.15 GB per processor 8 processors (~9.2 GB Total)

Cask 3-D Flux Distribution

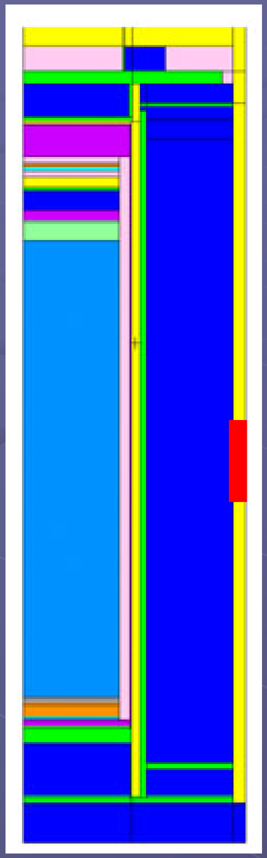


Group 1



Group 22

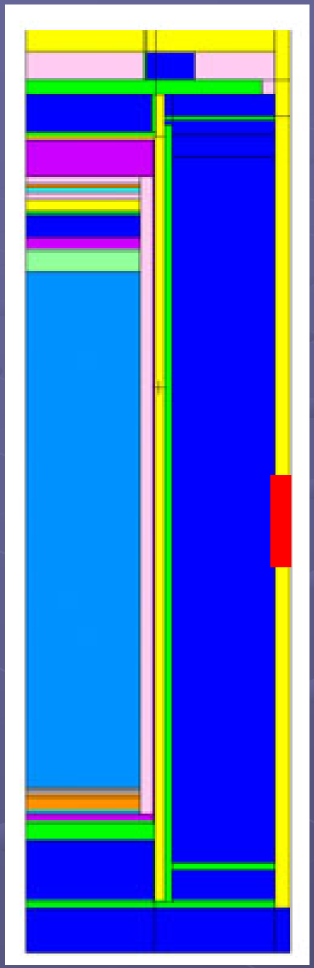
Cask Comparison Four Annular Segments Near Source Centerline (300 cm), 'Large' Model



Monte Carlo Results			PENTRAN/MC	
A^3MCNP Cont. Energy [(mRem/hr)/ n/cm^2/s]	MCNP Cont. Energy [(mRem/hr)/ n/cm^2/s]	MCNP Multigroup [(mRem/hr)/ n/cm^2/s]	Multi-group	Cont. Energy
1.75E-04 (0.91%)	1.78E-04 (1.25%)	1.25E-04 (1.30%)	1.04	0.74
2.12E-04 (0.83%)	2.13E-04 (1.14%)	1.50E-04 (1.18%)	1.04	0.74
1.98E-04 (0.95%)	1.97E-04 (1.19%)	1.39E-04 (1.23%)	1.04	0.73
1.43E-04 (1.09%)	1.42E-04 (1.41%)	1.00E-04 (1.46%)	1.04	0.73

- 'Small' Model (PENTRAN/MC)
  - Multigroup PENTRAN/MC average: 1.05
  - Continuous PENTRAN/MC energy average: 0.74 (due to CASK MG library)

Cask Model Timing Results



MC is an average in four annular tally segments
(Axial Mid-plane)
(1σ Relative Error = 1%)

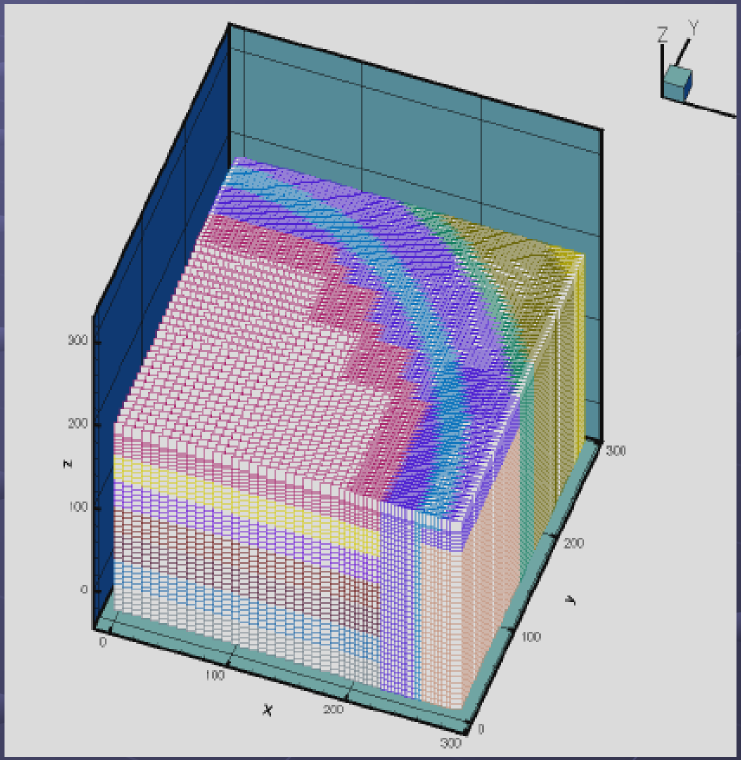
Model	# CPU	Dose Ratio to Reference	FOM	Run Time (hrs)	Speedup
A3MCNP Cont. Energy	1	1.00	109	1.5	140
Unbiased Cont. Energy	8	0.99	0.78	214	1.0
Unbiased Multigroup	8	0.70	0.46	362	0.6
PENTRAN ‘Large’ Model	8	0.74		165	1.3
PENTRAN ‘Small’ Model	8	0.74		123	1.7

Cask Performance Comparison: S_N and MC

Model	# CPU	Run Time (hrs)	Values/Hour
A^3MCNP Cont. Energy	1	2.5	1,856
Unbiased Cont. Energy	8	140	30
Unbiased Multigroup	8	220	19
PENTRAN ‘Large’ Model	8	165	42,100
PENTRAN ‘Small’ Model	8	123	35,000

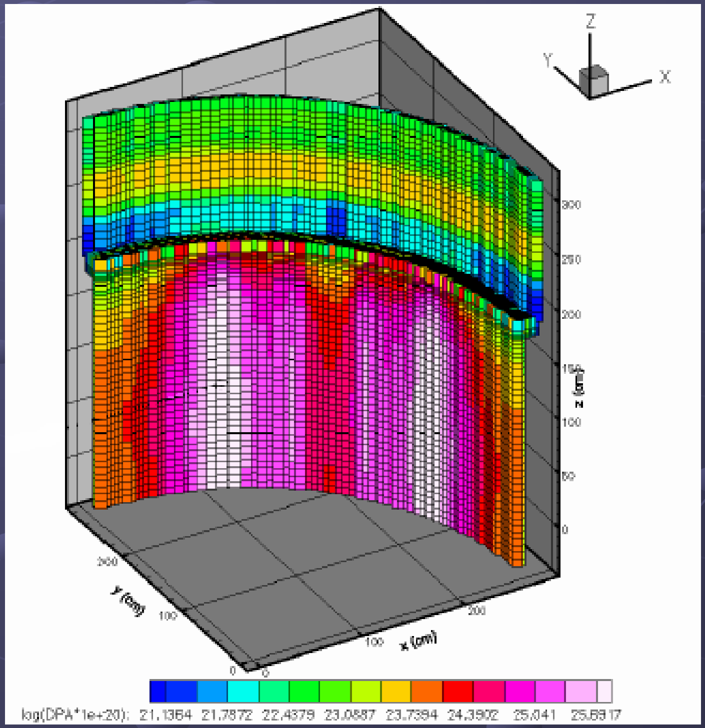
BWR Core Shroud Problem

- BWR reactor and Core Shroud Assembly…
- …with baffles, jet pumps, steam voids, etc.
- (Top) 67 Group P3-S8 coupled neutron-gamma calculation
- 265,264 fine mesh cells
- Solved in 12 hours on 48 IBM-SP2 processors, 8 processors angular, 6 processors spatial decomposition.



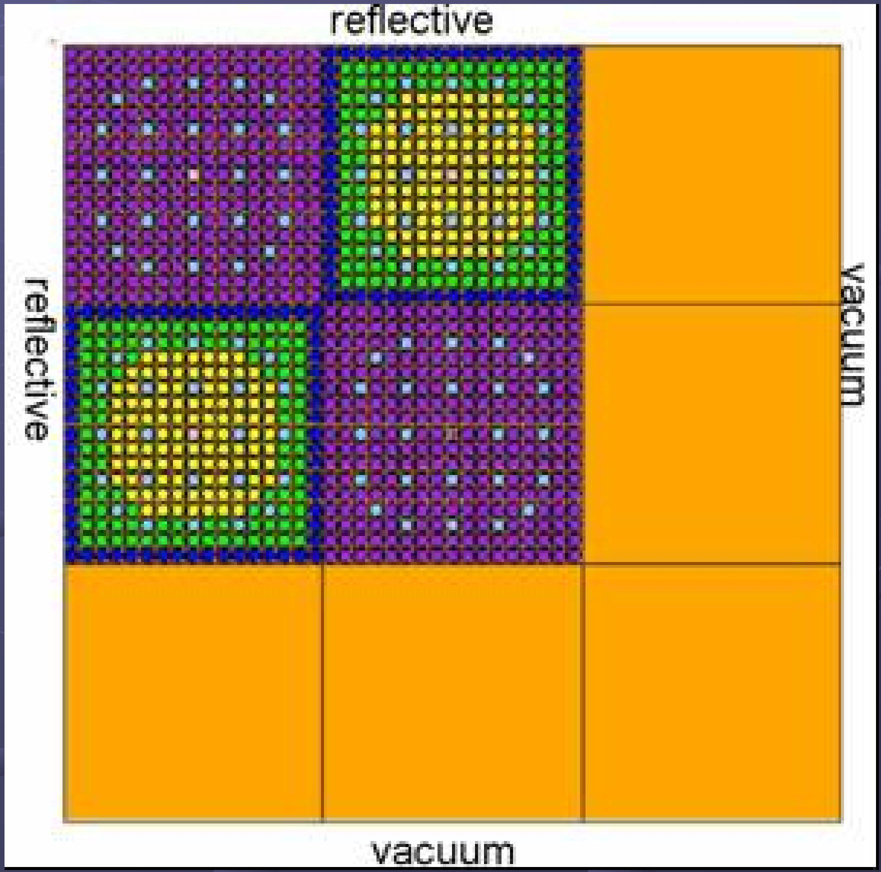
BWR Core Shroud Results

- Displacement per Atom (DPA) in the core shroud shows intense radiation damage where fuel is close to the shroud.
- Results were verified independently by Monte Carlo computations
- Multigroup PENTRAN (using BUGLE-96) values were within 5-15% of continuous energy MCNP values.
- (Kucukboyaci, et. al, 2000).



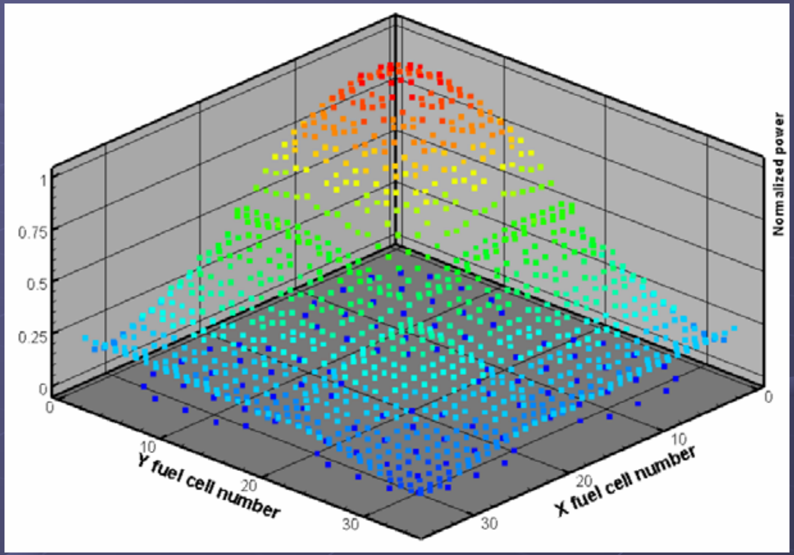
C5G7 MOX Benchmark

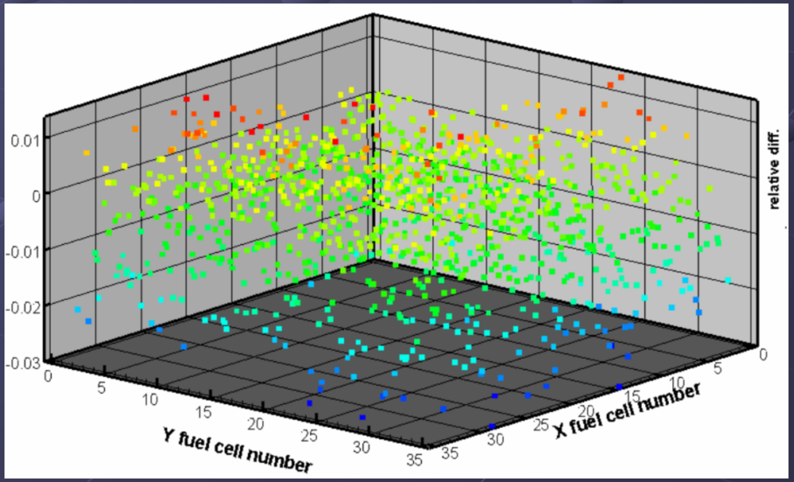
- *OECD/NEA C5G7 MOX 2-D Benchmark Problem*
- *PENTRAN Mesh distribution*
- *Specific pins represented among 229,551 spatial meshes*
- *S16 quadrature (228 directions)*
- *7 groups*



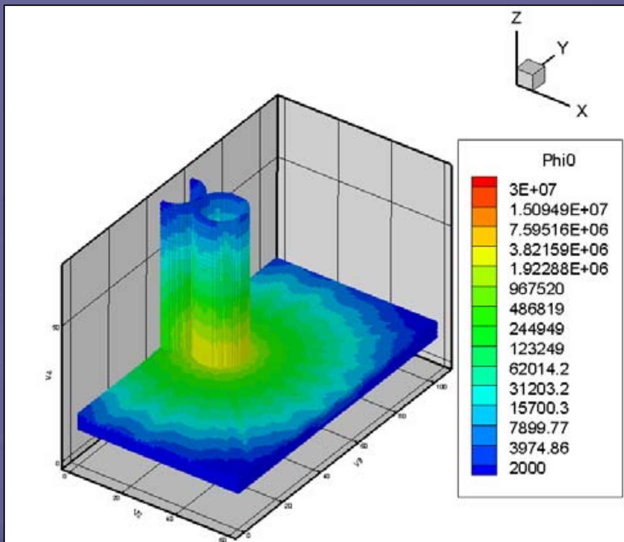
C5G7 MOX Benchmark Results

- *PENTRAN power distribution*
  - *keff=1.18760*
  - *within <0.1% of MCNP*
- *Relative power difference from MCNP avg difference is 0.88%*
- *Compared to a statistical MC error 0.4% to 1.24%.*
- *3-D unrodded case*
  - *modeled with 946,080 spatial mesh cells*
  - *keff=1.14323, +/-<0.09% of MCNP*
  - *(Yi and Haghighat, 2004).*

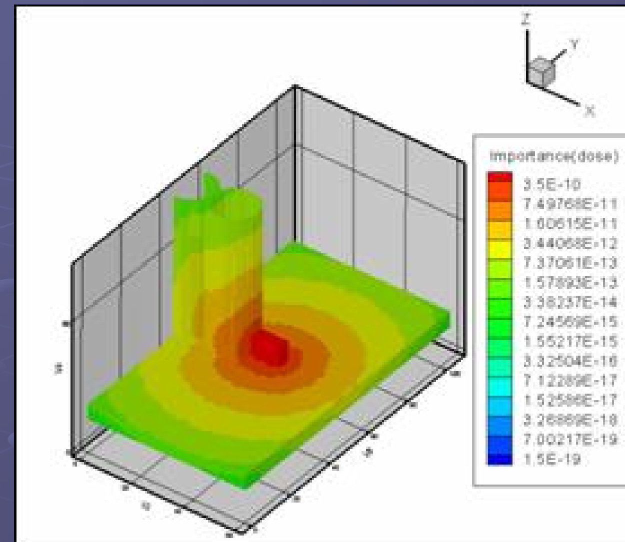




Recent Work for Industry

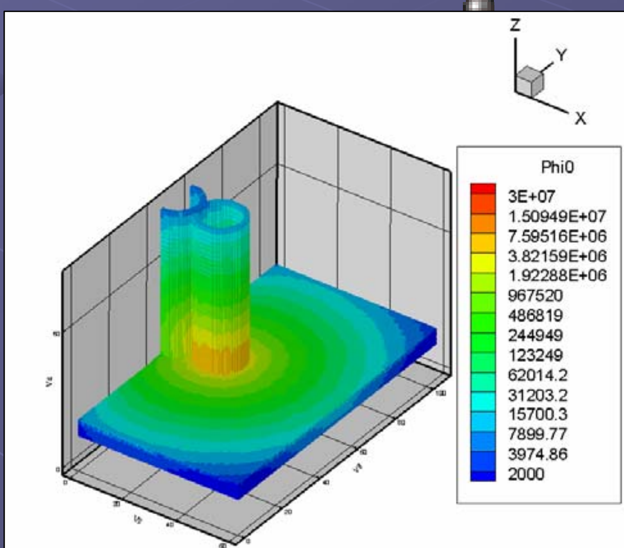


0.5 MeV
forward

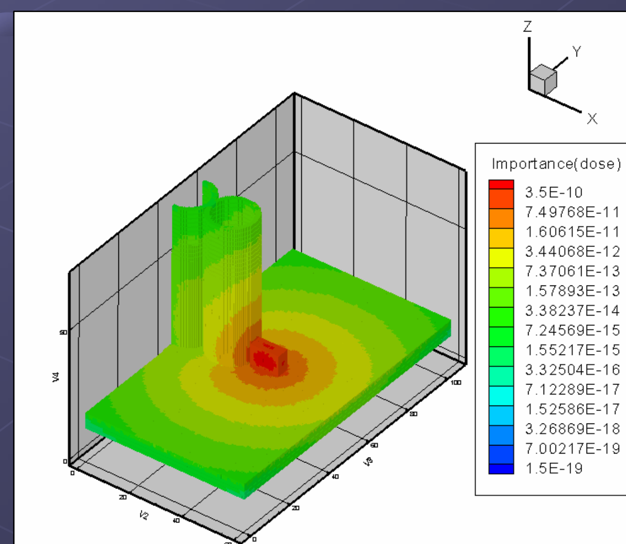


0.5 MeV
adjoint

relative to detector response



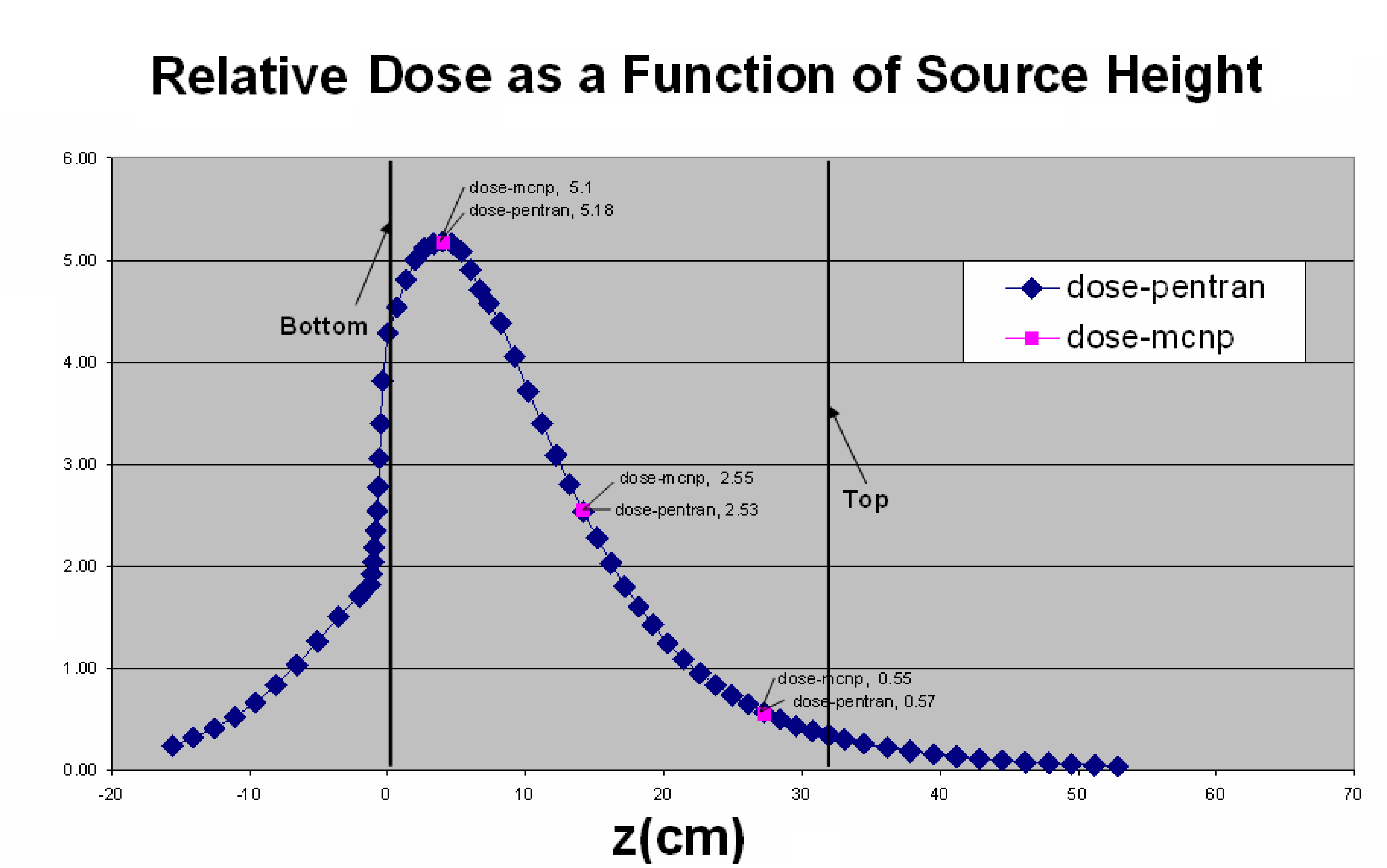
0.15 MeV
forward



0.15 MeV
adjoint

- Gamma transport problem/assessment

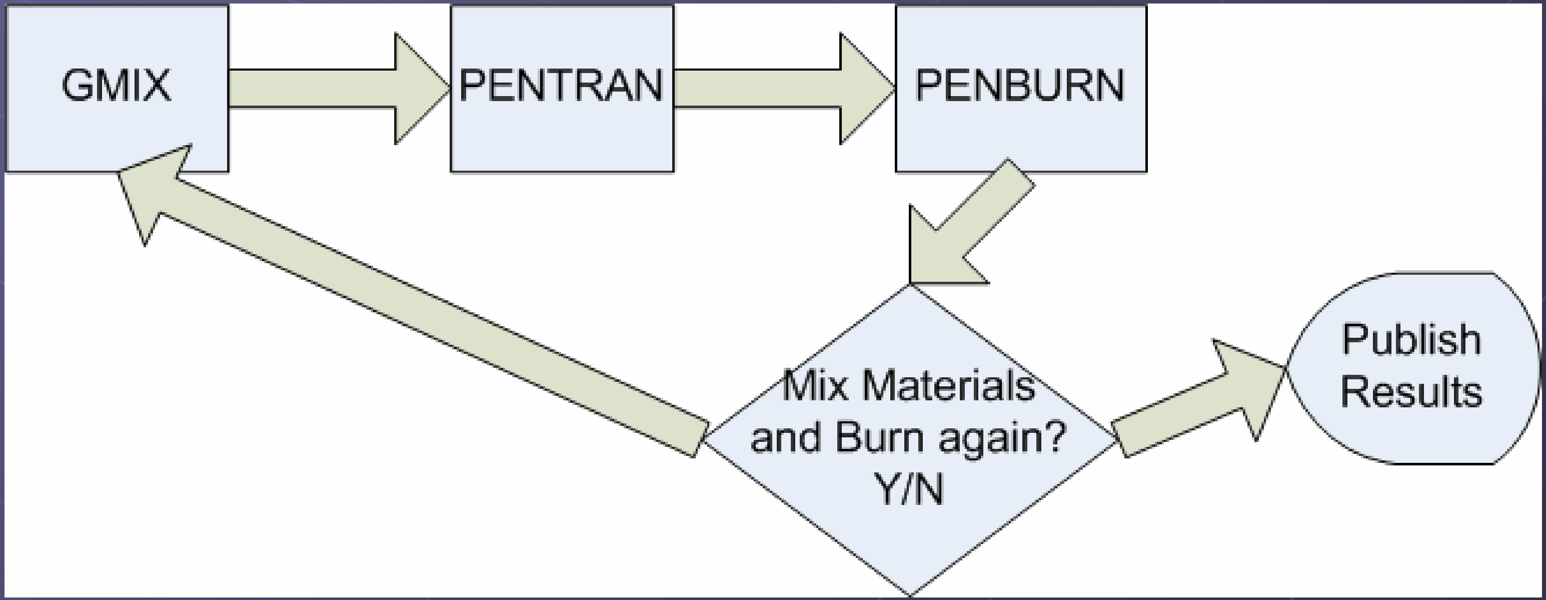
Recent Work for Industry (2)



- Gamma transport problem/assessment

PENBURN 3-D Burnup Module

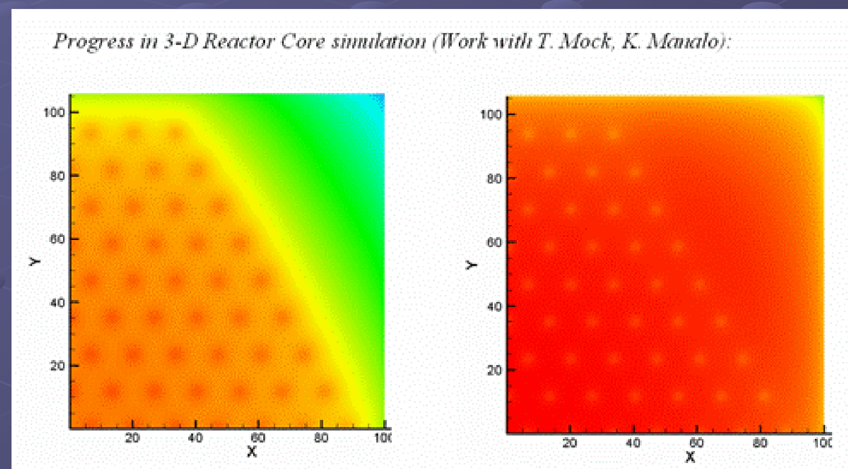
- Sponsored by the US Air Force
- Goal: Construct a 3-D zoned fuel burnup solver compatible with multiprocessing
- Solution of nuclide chains is obtained via quasi-static burnup steps
  - Explicit Bateman solver
- Distribute chains across processors

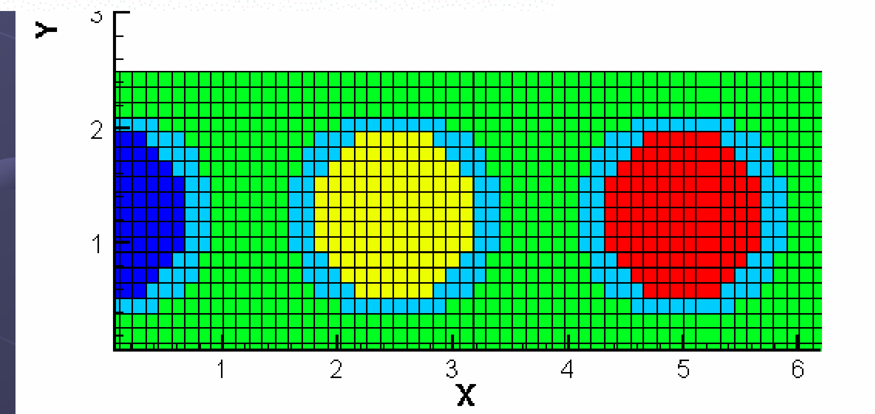


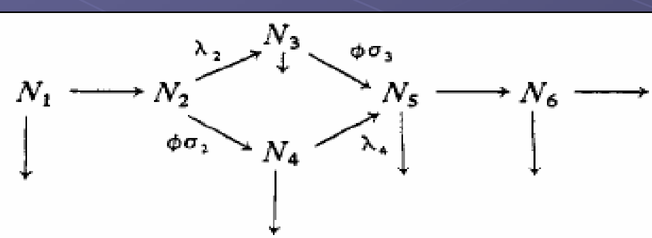
PENBURN 3-D Burnup Module (2)

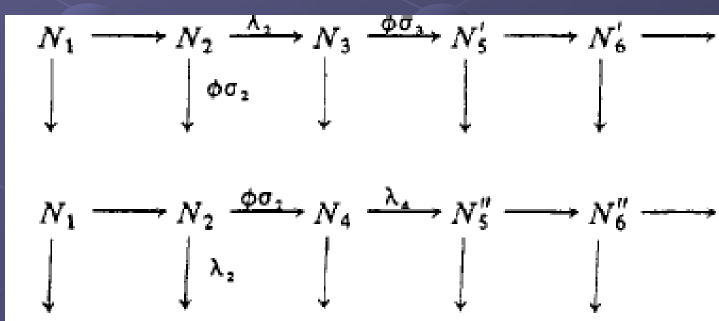
Bateman's equations are stored using "path matrices" with "chain-linking precursors"

$$N_i = \sum_{l=1}^{i-1} \left[N_l^0 \xi_l \xi_{l+1} \cdots \xi_{i-1} \sum_{j=l}^{i} \frac{e^{-\mu_j t}}{\prod_{\substack{k=l \\ k \neq j}}^{i} (\mu_k - \mu_j)} \right] + N_i^0 e^{-\mu_i t}$$



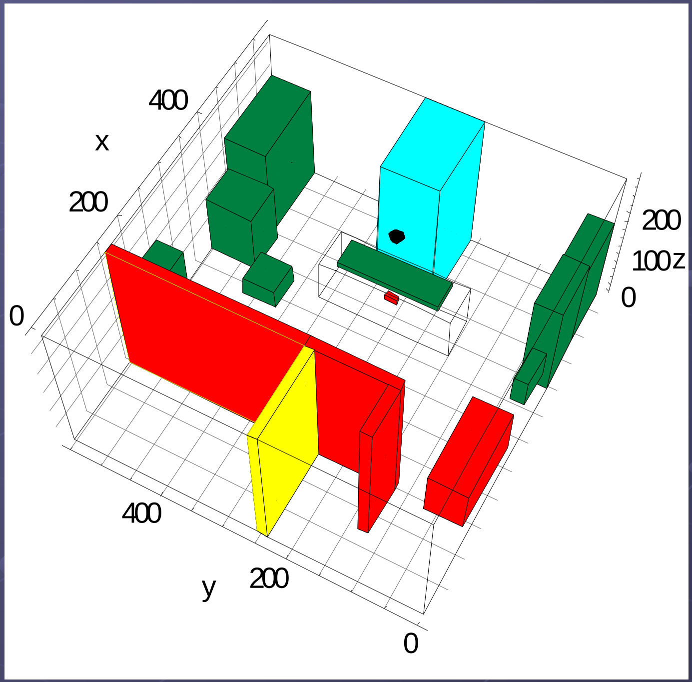


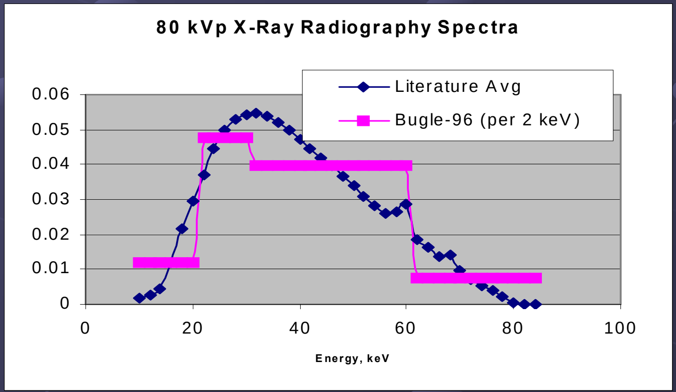




X-Ray Modeling ...

- 90 m^3 room discretized into ~131,000 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
- Hybrid X-ray Spectrum
  - Characteristic X-rays
  - Bremsstrahlung continuum





X-Ray Modeling … "z-level 3"

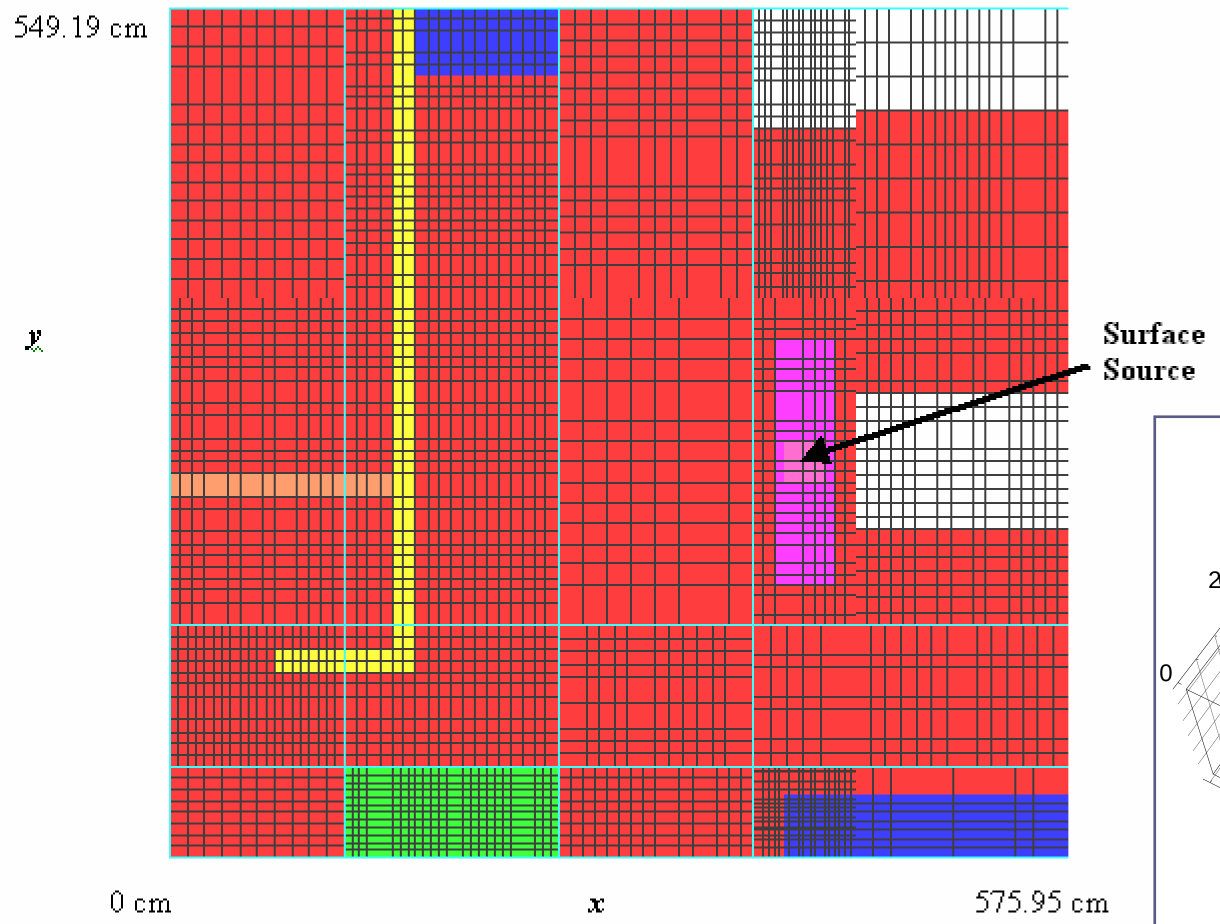
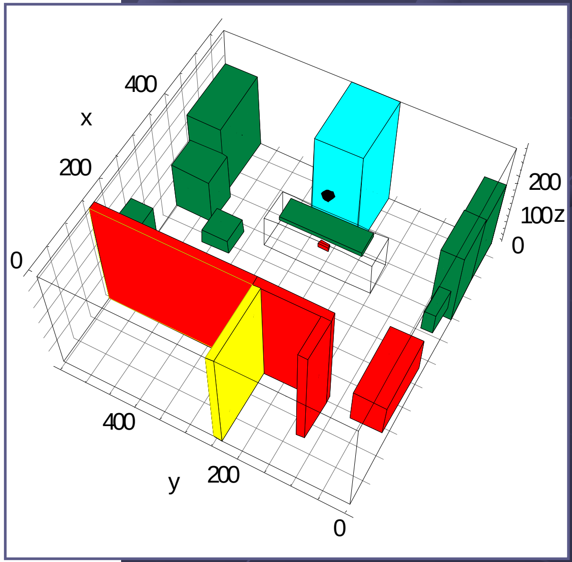
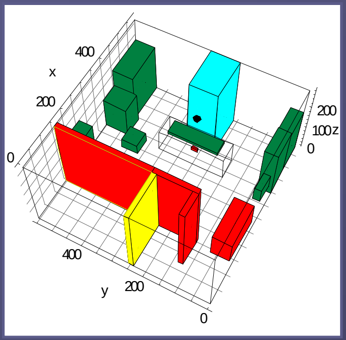
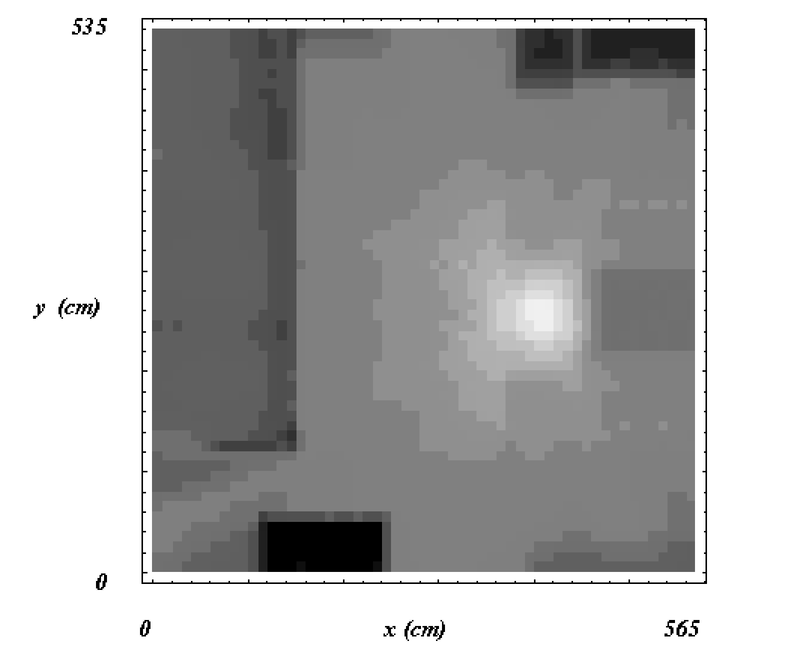


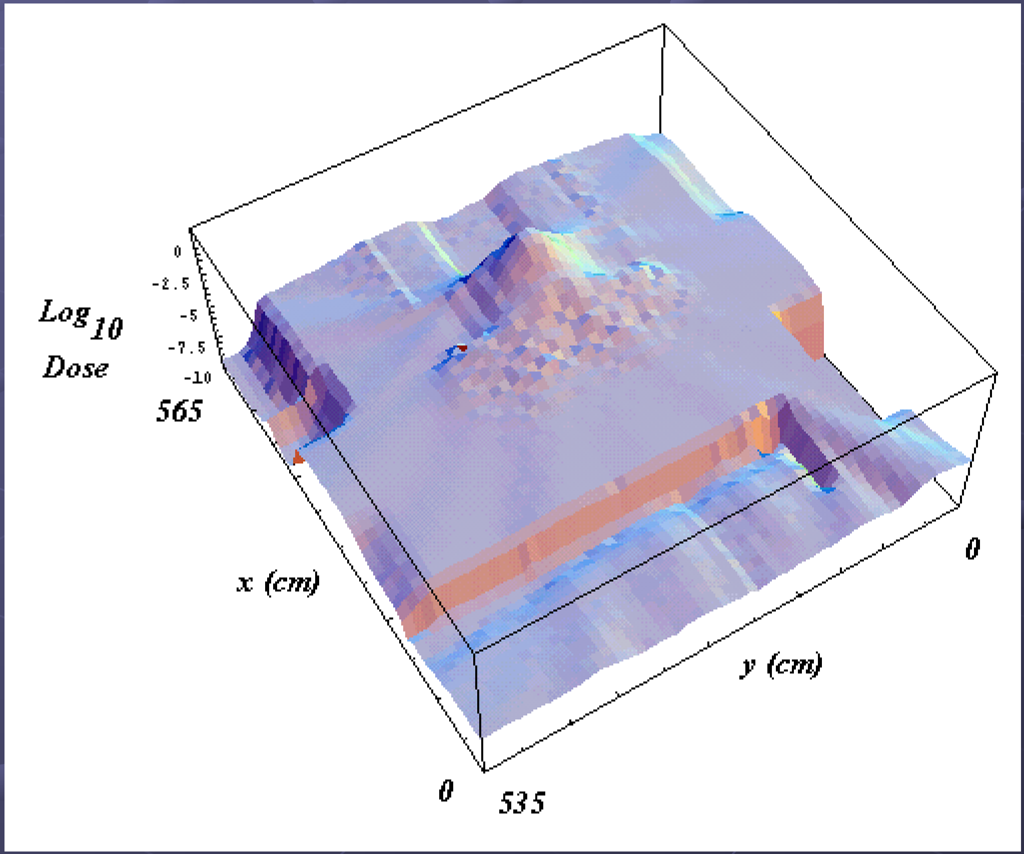
Figure 2. z-level 3: 86.6 cm to 100.44 cm along z-axis.



X-Ray Dose, z=100 cm







Conclusions

- Parallel Computing
  - Deterministic Transport: PENTRAN™ Code System
  - Wide Variety of Problems
  - Automatic Mesh generation, adaptive numerical differencing, grid projections
  - Acceleration schemes
- In 2007, emphasis on Whole Core 3-D Transport Modeling
- Questions?