

8th International Training Course/ Workshop

**Methodologies for Particle Transport Simulation
and Their Application to Nuclear Systems**

June 25-29, 2001

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Day 1 (Monday, June 25)

Opening remarks (A. Haghghat)

Penn State Transport Theory Group (PSTTG) and its activities (A. Haghghat)

Invited speaker, Dr. Hamilton Hunter, Director of RSICC, ORNL

Overview of calculational procedures for reactor dosimetry/shielding applications (A. Haghghat)

Specific issues related to different applications (A. Haghghat)

Introduction to the computer lab (V. Kucukboyaci)

Introduction to MCNP input preparation (A. Haghghat)

Introduction to TORT and PENTRAN input preparation; Introduction to PENTRAN (V. Kucukboyaci and A. Haghghat)

Day 2 (Tuesday, June 26)

Transport theory (transport equation, S_N method, adjoint transport, Monte Carlo method, CADIS methodology) (A. Haghghat)

Multigroup cross sections (Methodology, Preparation) (A. Haghghat)

An advanced multigroup cross section generation at Penn State (A. Alpan)

Multigroup cross section preparation for transport codes (V. Kucukboyaci)

Introduction to DORT/TORT input preparation : A simple example (V. Kucukboyaci)

3-D S_n Calculations for reactor applications - shielding problems (problem definition, 3-D mesh, source, and material generation with PENMSH, input preparation for DORT/TORT) (A. Haghghat and V. Kucukboyaci)

Day 3 (Wednesday, June 27)

Major issues in numerical solutions and computer codes (S_N method, Monte Carlo biasing, A^3 MCNP, adjoint versus forward, serial versus parallel processing, production codes, PENTRAN)(A. Haghghat)

3-D S_n calculations for a typical shielding problem (source preparation, calculation of reaction rates/activities, interpretation of results) (A. Haghghat & V. Kucukboyaci)

Adjoint S_N calculations with DORT/TORT (V. Kucukboyaci)

Monte Carlo calculations for reactor applications (A. Haghghat, A. Patchimpattapong)

Table of Contents (continued)

Day 4 (Thursday, June 28)

Sensitivity analysis and uncertainty estimation (linear perturbation theory, LEPRICON, PSU's approach) (A. Haghightat)

Methods to reduce uncertainty and/or improve efficiency (developed at Penn state)(A. Haghightat)

- Directional T-Weighted (DTW) differencing Scheme
- S Adjoint-weighted bi-linear method for multigroup cross-section generation
- S PENTRAN - A 3-D parallel Sn code and its pre- and post-processing codes
- Automatic Adjoint Accelerated MCNP (A³MCNP)

Monte Carlo shielding calculations using A³MCNP (A. Haghightat, A. Patchimpattapong & V. Kucukboyaci)

Day 5 (Friday, June 29)

3-D Sn calculations using PENTRAN code system, with computer exercises (A. Haghightat & V. Kucukboyaci)

- i) PENMSH
- ii) PENINP
- iii) PENTRAN (Parallel Environment Neutral-particle TRANsport)
- iv) PENDATA
- v) PENPRL

Benchmarking, Verification, and validation of 3-D Sn calculations (A. Haghightat)

Sn and Monte Carlo methods (advantages/disadvantages) (A. Haghightat)

Opening Remarks

by

**A. Haghghat
Monday Morning**

? **Organizing/Advising Committee**

Prof. Alireza (Ali) Haghghat, Chair
Mr. Vefa Kucucboyaci, Co-Chair
Dr. Bojan Petrovic, Westinghouse
Mrs. Bernadette Kirk, ORNL
Dr. Douglas Muir, IAEA
Dr. Enrico Sartori, OECD/NEA

? **Assistants**

Miss Arzu Alpan, PSU
Mr. James Brown, PSU
Mr. Shane Gardner, PSU
Mr. Aarash Haghghat
Mr. Gianluca Longoni, PSU
Ms. Holly Muir, PSU
Mr. Apisit Patchimpattapong, PSU
Mr. Dan Shedlock, PSU
Ms. Kim Sterndale, PSU
Mr. Mike Wenner, PSU

? **Workshop Co-Sponsors**

Nuclear Engineering Program
Mechanical and Nuclear Engineering Department
RSICC, ORNL
OECD/NEA Data Bank
In co-operation with the IAEA

Increasing need for particle transport simulations

Why?

- ? Radiation induced material damage in nuclear Aging nuclear systems; Possibility of plant life extension
- ? Improved core design (economy and safety)
- ? Oil well-logging
- ? Criticality safety
- ? Shipping cask/storage
- ? Identification/assaying of nuclear waste/nuclear materials
- ? Radiation therapy and medical diagnostics
- ? Decommissioning of nuclear systems

What is needed?

- ? It is necessary to estimate (accurately/efficiently) the energy-dependent neutron and gamma flux/fluence throughout a large and complex physical model

Goals of this training course

? **To learn the state-of-the-art methodologies for particle transport simulation in real-life nuclear systems**

To become familiar with the transport theory methods and their limitations and associated uncertainties

To become familiar with techniques for estimating uncertainties in transport theory calculations

To become familiar with ongoing research on advanced transport theory techniques and codes developed by the PSTTG group

To acquire sufficient knowledge for decision making (developing in-house capabilities, performing calculations), or identifying critical issues related to particle transport simulations

**Penn State Transport Theory Group (PSTTG) and
Its Activities**

by

**A. Haghghat
Monday Morning**

Penn State Transport Theory Group

Group Members

Director: Prof. A. Haghighat

Assistant

Director: Dr. Vefa Kucukboyaci

Associates: Colonel G.E. Sjoden (USAF), Dr. Bojan Petrovic (Westinghouse), Dr. J.C. Wagner (ORNL), Prof. Arthur Motta (Nuclear Materials, PSU), Dr. A. Dulloo & Dr. T. Congedo (Westinghouse), Dr. Hamid Aït Abderrahim (SCK•CEN), Prof. R.E. Mattis (U. Pitt.), Dr. I.K. Abu-Shumays (Bettis), Lt. H.L. Hanshaw (US Navy), Dr. M. Mahgerefteh (GPU), Dr. S. Sitaraman (GE), Dr. T. Sutton (KAPL), Dr. Yousry Azmy (ORNL), Dr. Enrico Sartori (OECD), Dr. Doug Muir (IAEA), Mrs. Bernadette Kirk (RSICC), Dr. Luiz Leal (ORNL)

Former graduate students:

John DeMarco (B.S. with honors, 1991), Ronald Mattis (PhD, 1991)
Basil Nanayakkara (M.S., 1992), Asam Khan (M.S., 1993)
Chris Pozsgai (M.S., 1994), Lt. Heath Hanshaw (M.S., 1995)
Capt. Young-Su Kim (MS, 1995), Bojan Petrovic (PhD, 1995)
Melissa Hunter (MS, 1991; PhD, 1996), Wilford Stevenson (M.S., 1996)
Major Glenn Sjoden (PhD, 1997), John Wagner (PhD, 1997)
Hikaru Hiruta (MS, 1999), Vefa Kucukboyaci (PhD, 2001)

Present graduate students:

Arzu Alpan (PhD Candidate)
James Brown (MS)
Shane Gardner (MS)
Gianluca Longoni (PhD Candidate)
Apisit Patchimpattapong (PhD Candidate)
Dan Shedlock (MS)
Michael Wenner (MS)

Visiting Scholars:

Farida Mohd. Idris, MINT, Malaysia (Spring 1995)
Marion Dubuisson, INSTN, France (Spring 1997)
Veronique Souvignet, INSTN, France (Spring 1997)
Attiya Abou-Zaid, Egypt (Fall & Spring, 1999)

Penn State Transport Theory Group

Research:

Development of efficient and accurate methods for solving the transport equation.

Application of these methods for simulation of large/complex systems (reactor physics and shielding, radiation facilities, waste assaying devices, medical applications, etc.)

Teaching:

Courses on transport theory methods and high performance computing (HPC), and their application to reactor physics and shielding.

[Advanced Reactor Theory, Neutron Transport Theory methods, Monte Carlo Methods, Parallel/Vector Algorithms for Scientific Applications]

PSTTG's Distributed Computing & Visualization Lab

PCTRAN cluster, HP visualization workstations & NETComputing

Institute for HPC Applications (IHPCA):

Advisory board

A graduate minor in HPC

Distance Education:

Taught *Neutron Transport Theory* and *Monte carlo Methods* (with lecture notes on WWW) remotely (through CVI) to students from Westinghouse.

National & International Activities:

- International workshops on "Methodologies for Particle Transport Simulation and Their Application to Nuclear Systems", June 19-23, 1995, June 2-7, 1996, May 19-23, 1997, at Penn State; June 19-23, 1997 at the University of Stuttgart, Germany; May 25-29, 1998 at Sck.CEN, Mol, Belgium; May 17-21, 1999, and June 26-30, 2000 at Penn State.
- Chairing an ANS standards subcommittee on transport theory calculations for "Reactor Cavity Dosimetry"
- Member of an international committee on "Adaptation of Computer Codes in Nuclear Applications to Parallel Architectures"
- Member of an international task force on "Computing Radiation Dose and Modeling of Nuclear Radiation-Induced Degradation of Reactor Components"
- Benchmarking of transport theory methods for real-life problems
- Training international scholars

Penn State Transport Theory Group

Funding sources:

- NSF (Computer time, parallel course development)
- GPU Nuclear Corporation
- Penn State FERMI Project (Nuclear Engineering Dept. Affiliates Program : GPU, PP&L, PECO, PSE&G, Westinghouse, and Duquesne Light Company)
- PP&L
- IBM
- Harris Semiconductors
- Penn State Breazeale Reactor (PSBR)
- Westinghouse
- S DOE

Seeking international collaborations and funding:

- European trip (Finland (VTT), Germany (Rossendorf), NRI and Skoda (Czech Republic), Belgium (SCK/CEN), France (Saclay, OECD)); To form an international group on "Particle Transport Simulation (PTS)" for providing research and training services, 1996.
- Mexico (IIE) (IAEA expert, BWR project, graduate students), 1996.
- Austria (IAEA) (training courses, sponsorship, etc.), 1996-present.
- France (INSTN) (training students, graduate students), 1997.
- S Sabbatical leave at SCK.CEN, Mol, Belgium; training of the Fuel Research Unit on transport theory methods and codes, Spring and Summer, 1998.
- S Collaboration with the SCK.CEN personnel, 1999-present.

Penn State Transport Theory Group

Projects

Shielding and dosimetry

Developed improved methodologies for calculation of pressure vessel neutron fluence and associated uncertainties

Defined a benchmark problem for PWR cavity dosimetry

Developed methodologies for estimation of neutron and gamma flux and DPA throughout a BWR core shroud (using PENTRAN and A³MCNP)

Developing advanced methodologies for generation of multigroup cross sections based on the adjoint-weighting approach (FERMI)

Evaluation of neutron and gamma dose for a shipping cask/storage (A³MCNP)

Novel investigation of Fe cross-section using an iron shell shield and time-of-flight measurements and particle transport calculation (with NIST and U. of Ohio) (DOE/NERI) (using PENTRAN and A³MCNP)

Research Reactor

Monte Carlo modeling of the Penn State Breazeale Reactor (PSBR) Core

Monte Carlo modeling and optimization of the D₂O tank at the PSBR

Monte carlo modeling for the design of the Fast Neutron Irradiator (FNI)

Special devices

Optimization of the Westinghouse PGNAA device for assaying waste (Using MCNP and PENTRAN) (Westinghouse/DOE)

Simulation of CT scanning device (Medical Imaging, using PENTRAN and A³MCNP)

Advanced methods, formulations and codes

- Parallel algorithms, differencing schemes, acceleration methods, automatic variance reduction techniques, multigroup cross section generations
- PENTRAN™ code system (PENMSH/PENINP, PENTRAN, PENDATA/PENPRL)
- Advanced Algorithms and Automation Tools for Discrete Ordinates Methods in Parallel Environments (DOE/NEER)
- A³MCNP™ (Automated Adjoint Accelerated MCNP)

Benchmarking activities

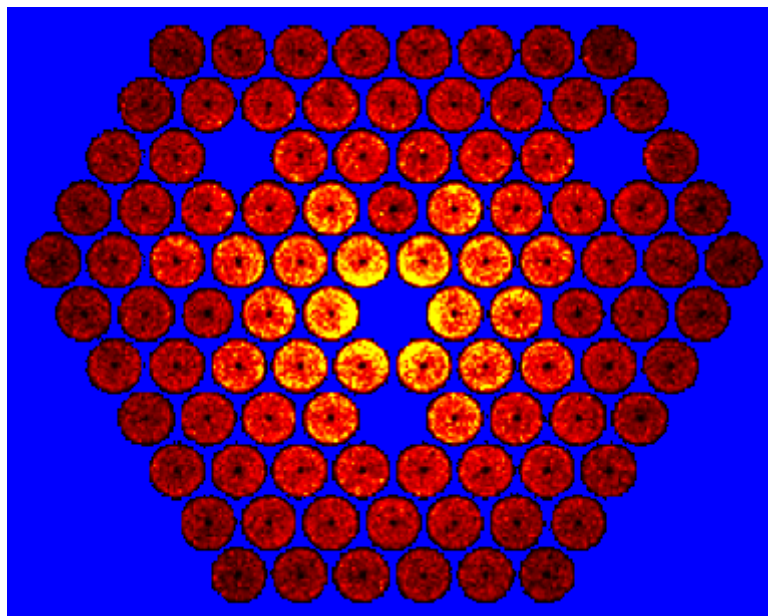
Simulation of the VENUS-3 experimental facility located at SCK•CEN, Mol, Belgium (organized by OECD)

Simulation of the 3-D Kobayashi benchmark problems (organized by OECD)

Modeling of the Penn State Breazeale Reactor (PSBR)

- Developed a 3-D MCNP model for the PSBR core
- Prepared a database of core loading and burnup between 1966-1995
- Performed criticality calculation to determine k , flux, power, and control rod worth
- Performed analysis on core loading for improving reactor safety margin

PSBR fission density distribution

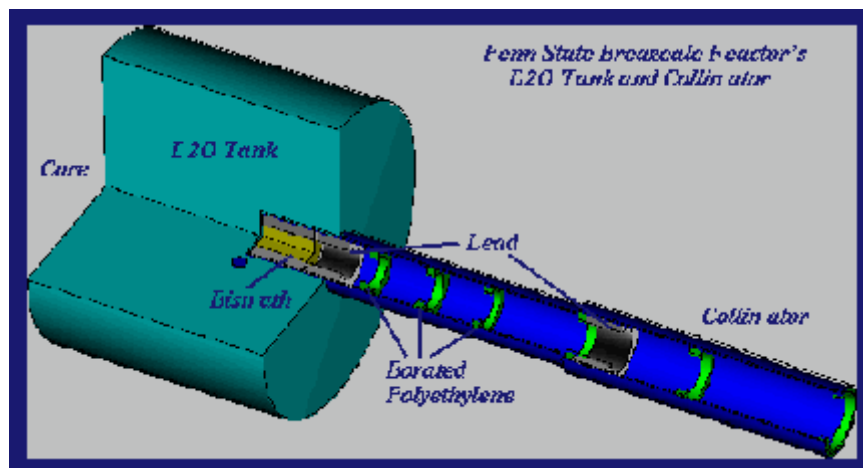


Modeling and optimization of the D₂O tank at the PSBR

This tank is used for generation of thermal neutrons for neutron radiography.

Using MCNP, analyzed the original D₂O tank, and developed a new design (size, shape, and orientation) by maximizing the thermal-neutron-to-gamma ratio

3-D MCNP model for the original D₂O Tank and collimator



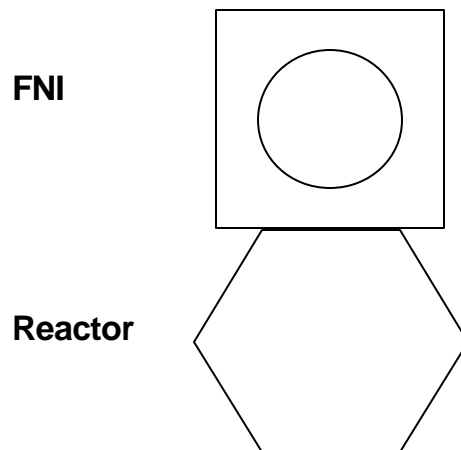
Design of the Fast Neutron Irradiator (FNI) facility

This facility is being used for irradiating semi-conductors.

Developed a 3-D MCNP model for the FNI for irradiation of 8" wafers

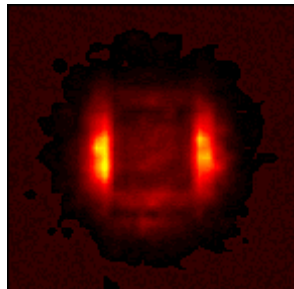
In this design, maximized the fast neutron, while minimizing the thermal neutron and gamma fluxes.

The MCNP model for the FNI design

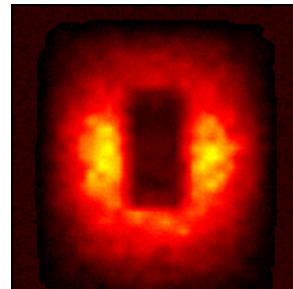


At the interface of the FNI and reactor

Thermal neutron



Gamma



PWR Pressure Vessel (PV) Fluence Estimation

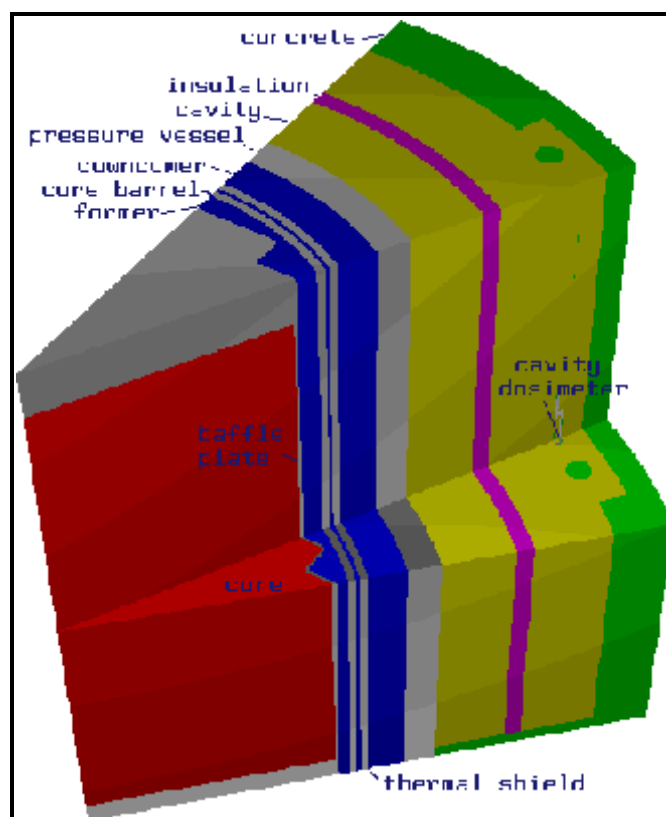
Numerous studies performed to estimate the neutron fluence at the reactor pressure vessel, and its dosimeters.

Besides the fluence, detailed sensitivity studies performed to estimate the uncertainties associated with the estimated fluence.

3-D fluence were obtained via a 3-D synthesis approach using the DORT code, and also the 3-D MCNP code for benchmarking.

Our sensitivity studies led to the development of more accurate and efficient methods and techniques for performing large deep penetration calculations.

Our studies have contributed to an ANS standard and also and OECD working group on reactor cavity dosimetry and PV fluence estimation.

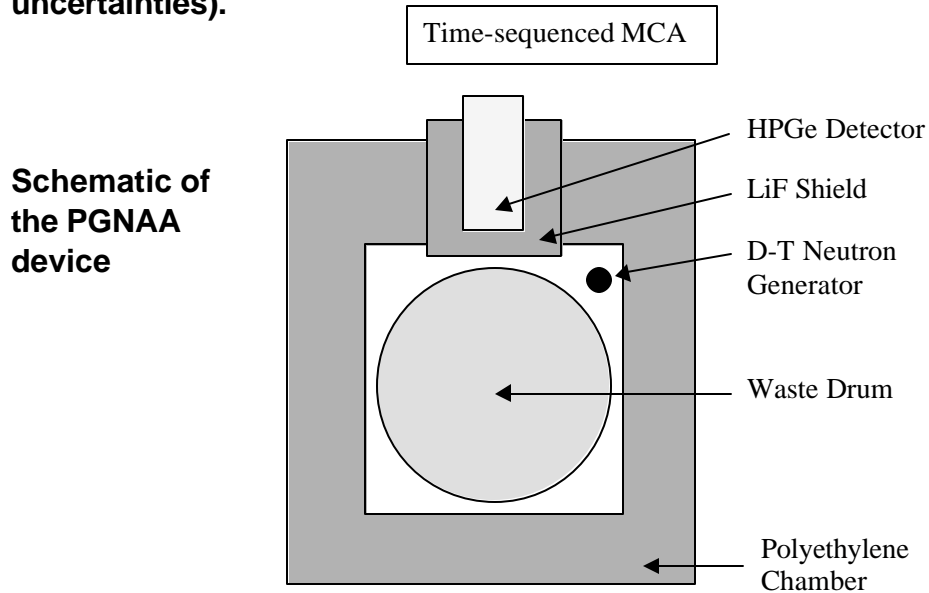


Optimization of the PGNAA device

Determined the thermal neutron flux distribution throughout the waste using a time-dependent MCNP model

Determined the gamma flux at the face of a gamma detector using an “importance function” obtained from a 3-D PENTRAN calculation.

Achieved excellent agreement with the experimental results (within the experimental uncertainties).



Mesh

Contribution to the detector

response

“Importance”
function

Simulation of the VENUS-3 experimental facility

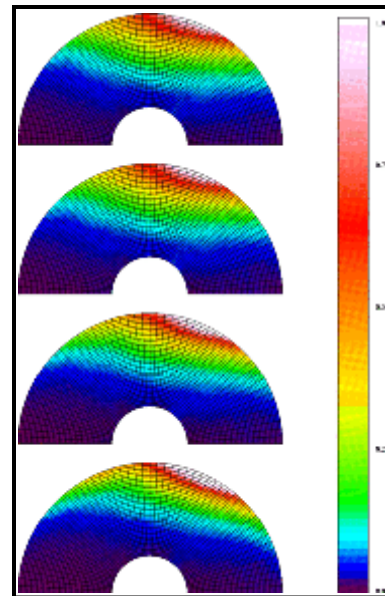
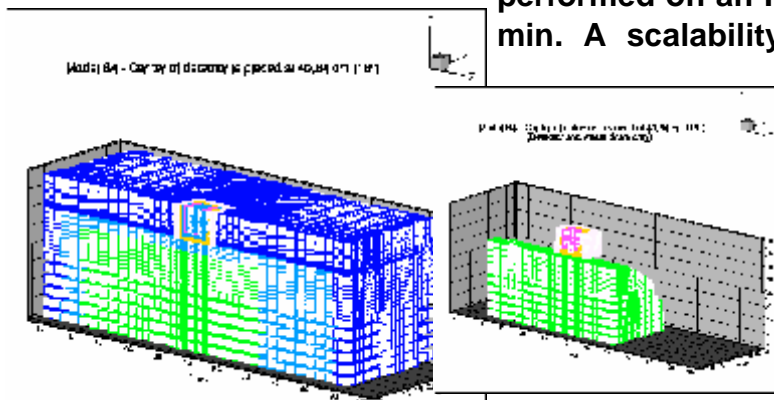
The VENUS-3 is the mock-up of a PWR with partial length assemblies (SCK•CEN, Belgium)

This facility has been used for an OECD activity on benchmarking computer codes used for shielding calculations.

Over 300 experimental values are available throughout the reactor.

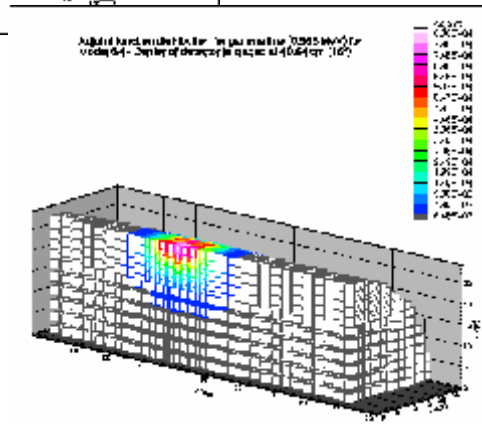
The PENTRAN 3-D parallel Sn code has been benchmarked based on this 3-D facility.

PENTRAN model includes 84748 meshes and 26 energy groups. The calculation is performed on an IBM SP2 parallel computer in ~80 min. A scalability of ~90% is achieved for this



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C/E (calculation-
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values are in a range of ±(5-10)%,

and only 16 values are in a range of $\pm(10-15)\%$.

PENTRAN simulation of the VENUS-3 facility
Mesh distribution C/E

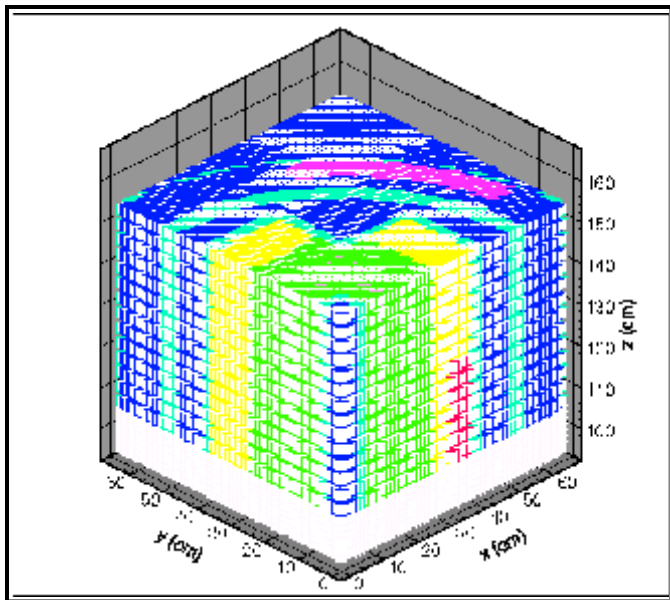
Kobayashi 3-D calculation benchmark

Kobayashi contributed three 3-D void duct problems to an OECD activity on benchmarking 3-D Sn codes.

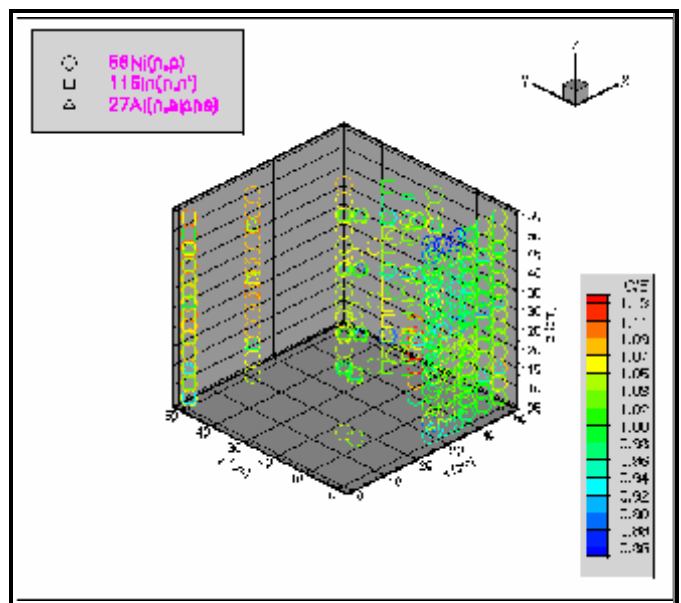
PENTRAN has been used successfully to simulate these problems. Here, we only present the results for the dog-leg void duct problem with a pure absorber. Excellent agreement has been achieved even at positions more than several mfp's from the neutron source.

We have demonstrated that PENTRAN's unique features including adaptive differencing, variable meshing, and TPMC projection scheme are essential for obtaining this close agreement.

Problem 3 with pure absorber

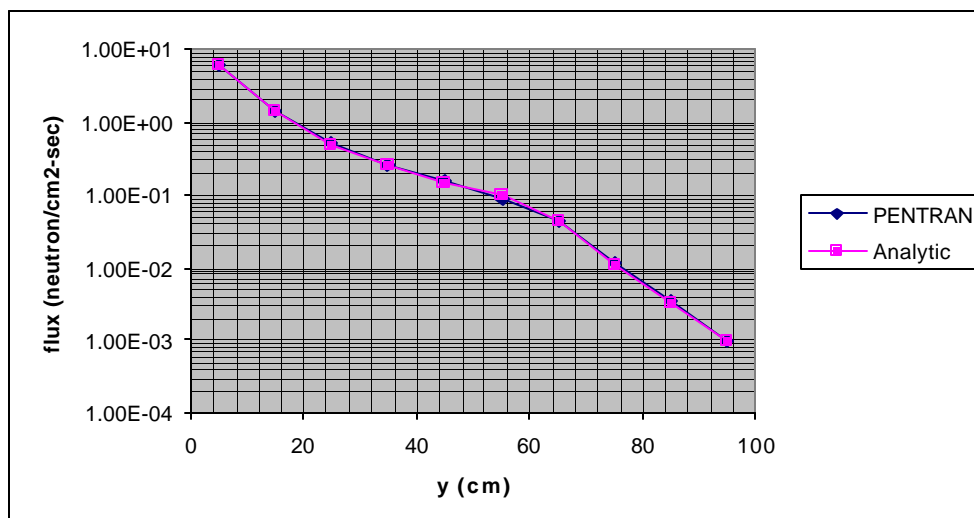
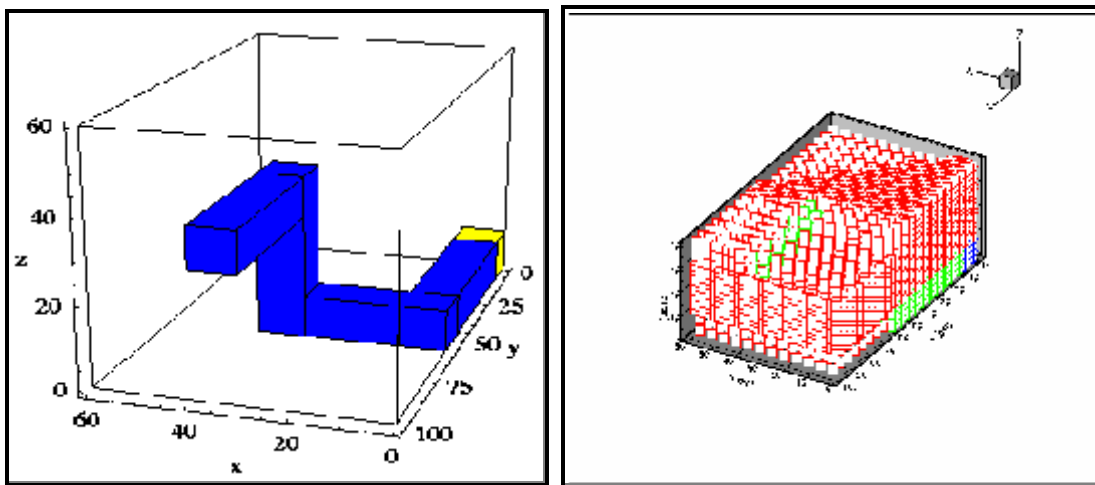


Model



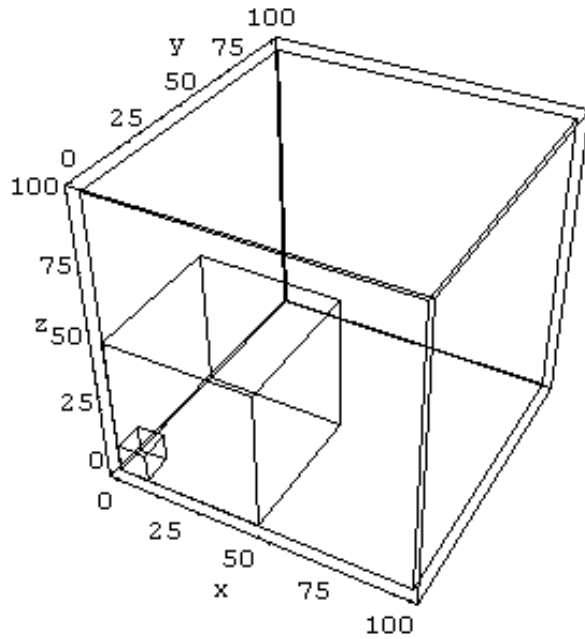
Mesh

Comparison of PENTRAN and Analytical fluxes along y at z=5 cm, x=5 cm



Kobayashi 3-D calculation benchmark (using A³MCNP)

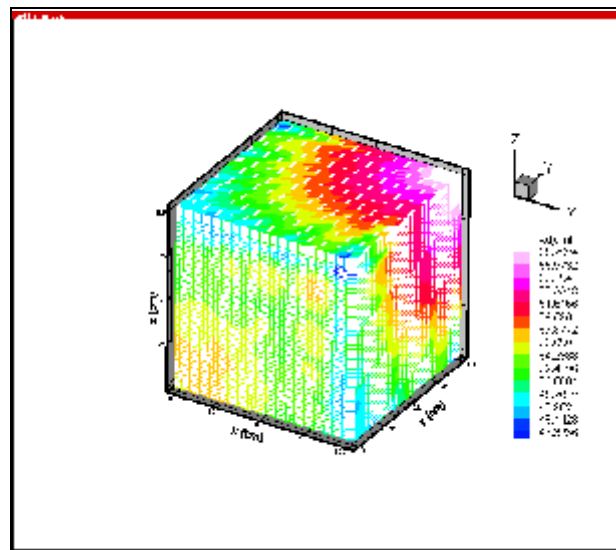
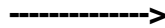
Kobayashi contributed three 3-D void duct problems to an OECD activity on benchmarking 3-D Sn codes. Problem 1 is simulated using the A³MCNP code.



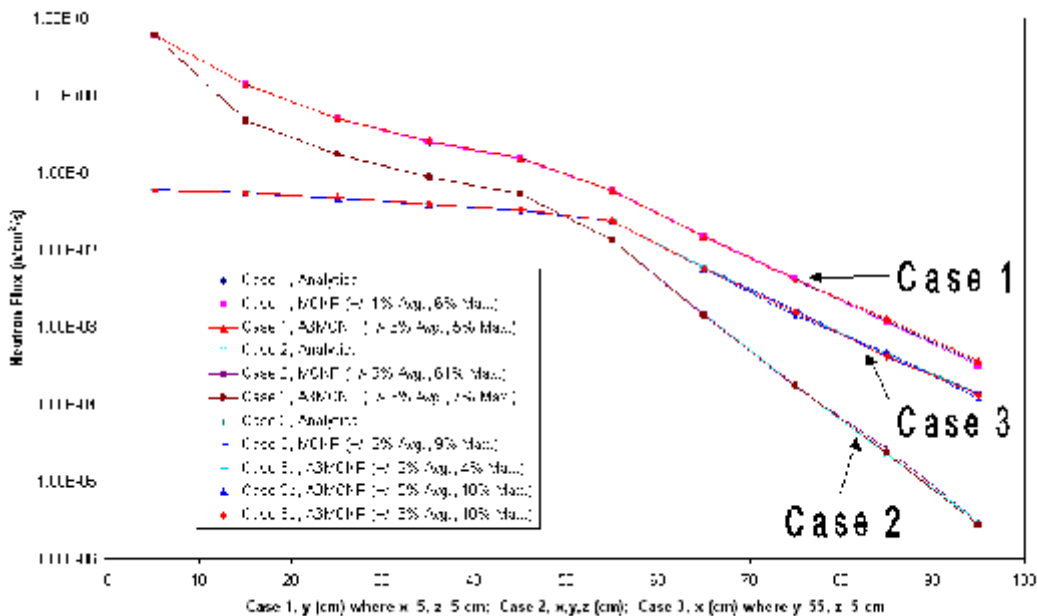
With this problem, we are examining the impact of the “ray-effects” on the performance of A³MCNP. It is demonstrated that even in such an extreme case, A³MCNP leads to a speedup of 40 over MCNP.

← Schematic of problem 1

Adjoint (“Importance”) function distribution, when our objective is obtain flux tallies along the main diagonal.



Comparison of A³MCNP tallies with



analytical results

BWR Core Shroud Modeling

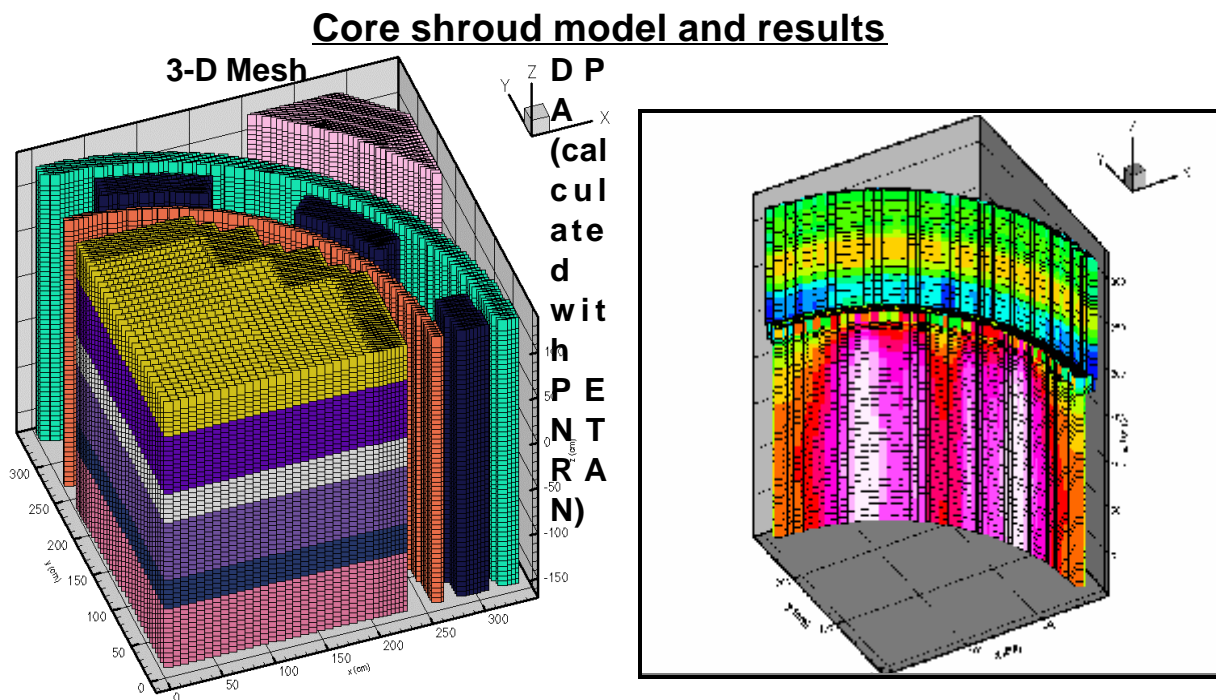
Neutron and gamma flux distributions are determined throughout a BWR core shroud.

Using the “importance function” obtained from 1-D and 2-D S_n calculations, we developed an effective control volume for simulating H4, H3, and H2 welds.

For this calculation, we have used the PENTRAN and A^3 MCNP codes. PENTRAN and A^3 MCNP results agree within the Monte Carlo statistical uncertainties.

PENTRAN calculation was performed on 48 processors of the San Diego Supercomputing Center in 12 hours; similar calculation with TORT required over 100 hrs and partitioning of the model into two segments.

A scalability of ~90% was obtained for this problem.



Comparison of DPA 's (PENTRAN vs. A3MCNP) at H3 weld

Gamma and Neutron dose determination for a Shipping/Storage Cask

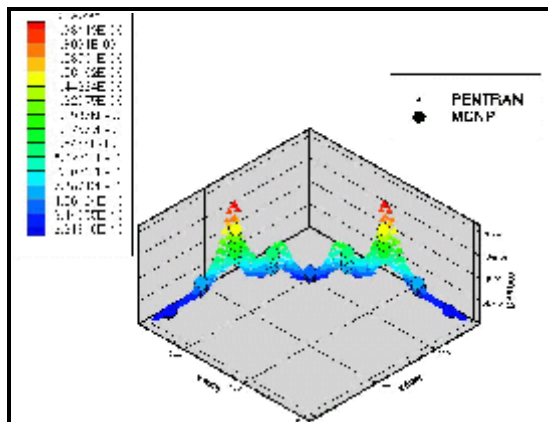
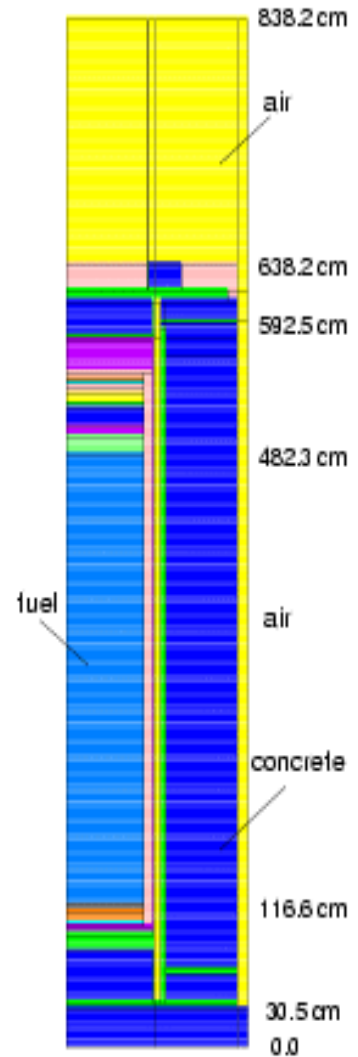
Using the A³MCNP code, neutron and gamma dose is calculated over the surface of a shipping cask.

The physical model is very large, 180 cm x 180 cm x 840 cm, so the particles have to travel several mean-free-paths. Hence a Monte Carlo simulation requires the use of variance reduction methods.

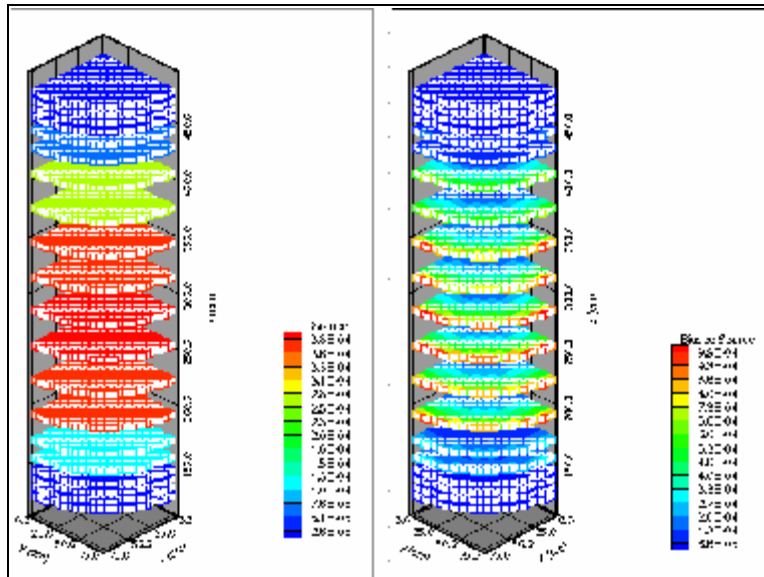
Figures below shows the unbiased and biased source for the situation that an estimate of gamma dose is needed only over the whole surface of the cask.

Unbiased Source

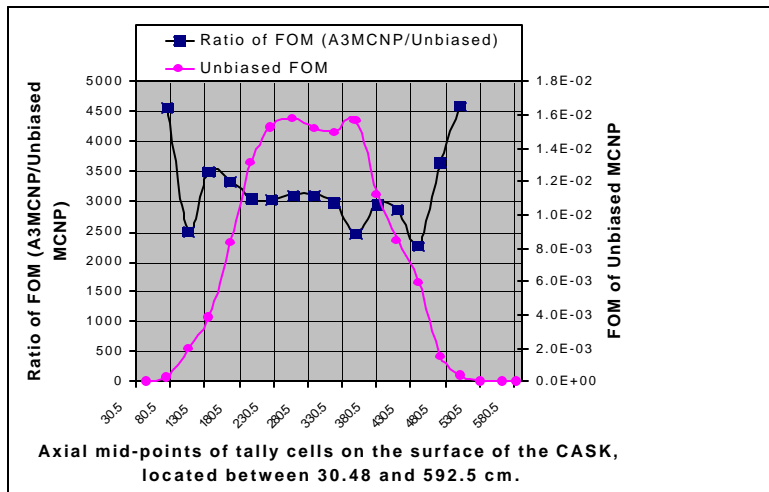
Biased Source



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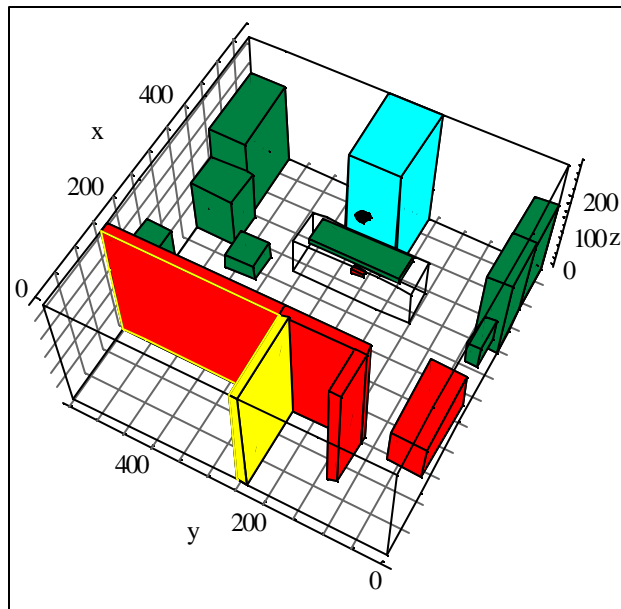
formance of A³MCNP
mpared to the MCNP
biased) calculations



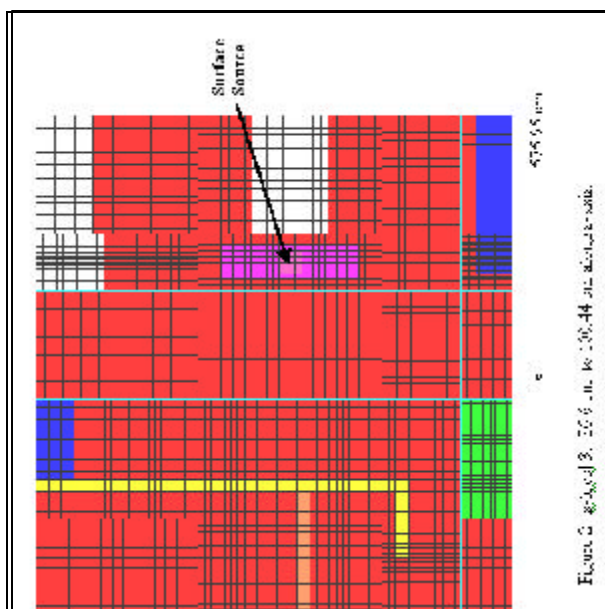
Determination of radiation dose in an x-ray room

An x-ray room with a physical size of 90 m³ is simulated using the PENTRAN code system on the SPARKY2 cluster.

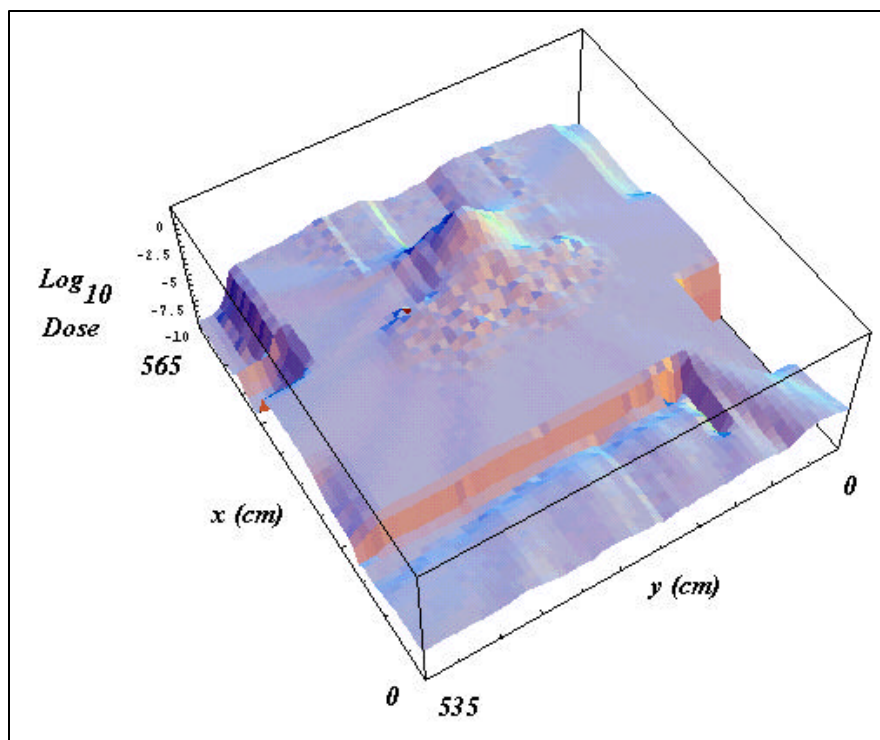
X-Ray room schematic



PENTRAN model



X-ray dose throughout the room



Simulation of an experimental setup for measurement of Fe cross-section

We are developing PENTRAN models for performing sensitivity studies in support of a joint project with NIST and Ohio University (DOE NERI).

The unique feature of this model is that neutrons are emanated from a very localized source, and detector is located at a distance of over 600 cm that is mostly occupied by air.

Physical model

Neutron source

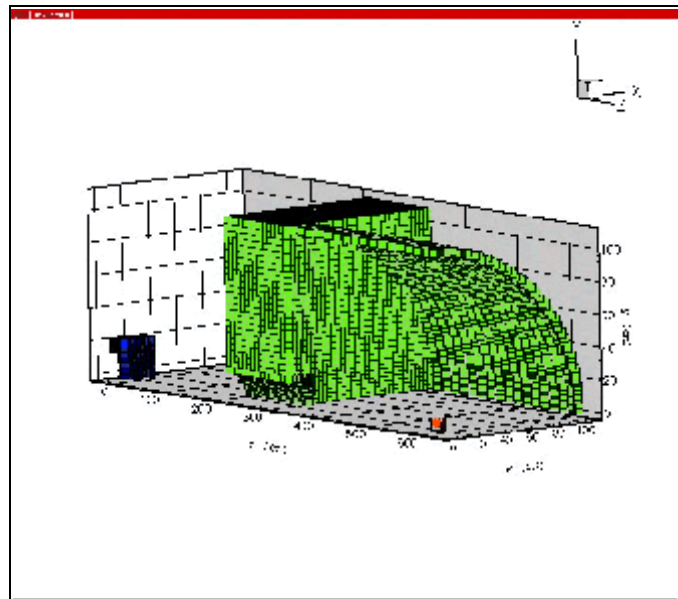
(Left/Front/Bottom corner)

Fe Shield (blue) ----->

Wall (green)

Tunnel (green)

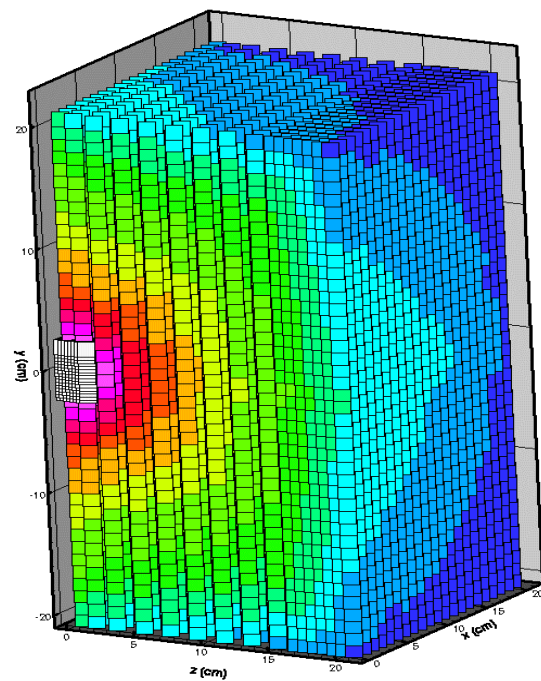
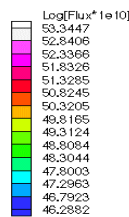
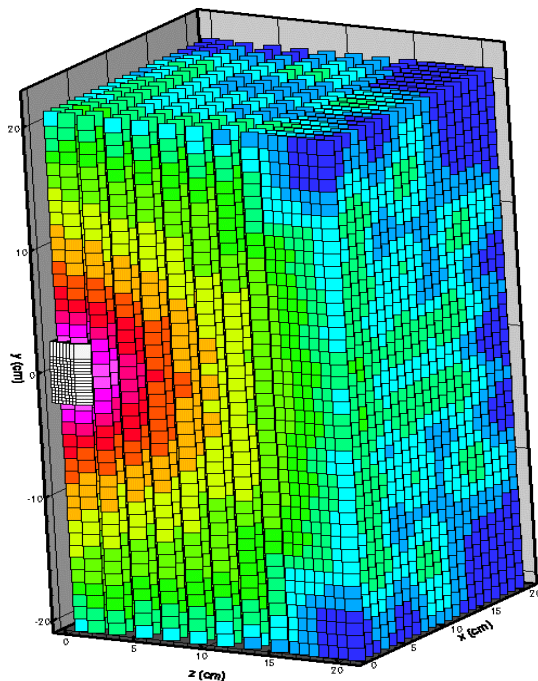
Detector (red)



Flux distribution

S20 level symmetric

S30 Pn-Tn with ordinate splitting



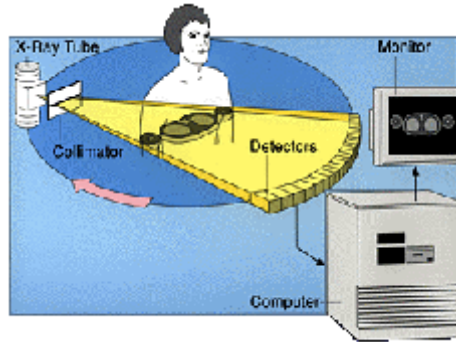
Simulation of a CT scanning device

A CT scan that uses γ -ray imagery is mostly modeled with empirical formulations that are obtained based on simple theoretical formulations adjusted by data from experiments on phantoms.

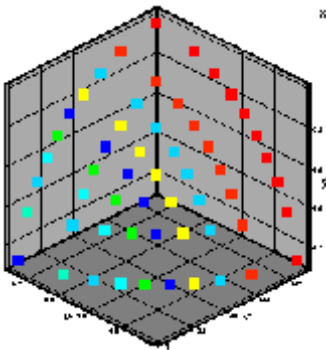
Some efforts have been devoted to using Monte Carlo methods for simulation of a CT scan. These methods, however, suffer from long running times.

PENTRAN with new quadrature sets has resulted in accurate results as compared to Monte Carlo predictions. We have demonstrated that our new quadrature sets are necessary for this type of simulation, and PENTRAN can solve for detailed flux distributions in a short (orders of magnitudes) time compared to the Monte Carlo calculations.

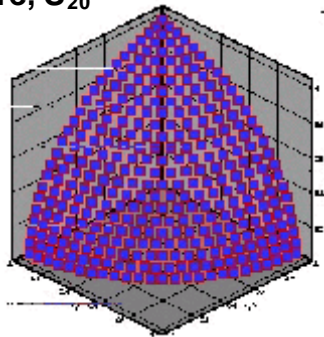
Schematic of a CT scan device



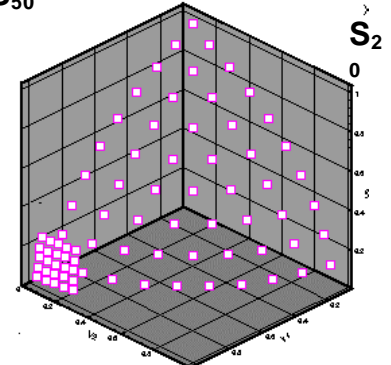
Level-symmetric



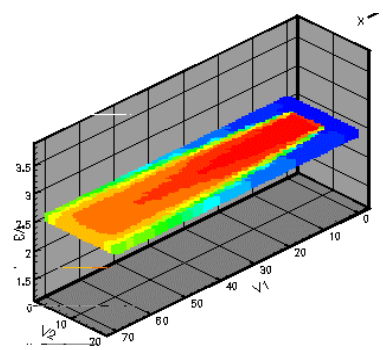
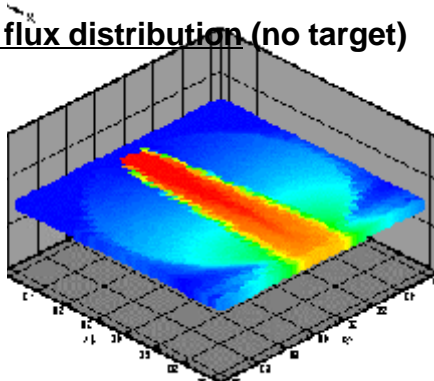
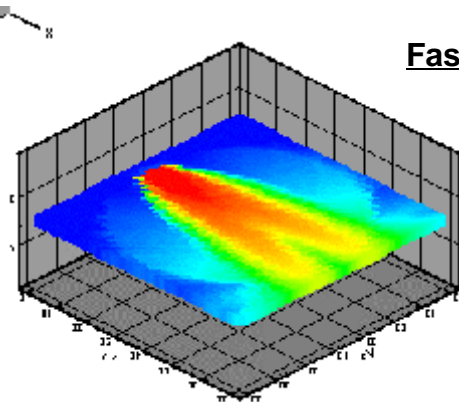
Equal-weight (EW) quadrature, quadrature, S_{20}



EW with Ordinate Splitting S_{50}



Fast flux distribution (no target)



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