UT-BATTELLE

MEDICAL APPLICATION OF DOORS

R. A. Lillie

Oak Ridge National Laboratory

P. O. Box 2008

Oak Ridge, Tennessee, 37831

(865) 574-6083 lilliera@ornl.gov

Presented at

Computational Medical Physics Working Group Meeting

October 26, 2005

Doors is a Collection of Codes Anchored by ANISN, DORT, & TORT

- **Discrete Ordinates Codes**
  - ANISN One-Dimensional
  - DORT Two-Dimensional
  - TORT Three-Dimensional
- **Semi-Analytic Uncollided Flux & 1st Collision Source Codes and Last Flight Estimation Code**
  - GRTUNCL & GRTUNCL3D and FALSTF
- **Coupling (Splicing) Codes**
  - Torsed (DORT to TORT)
  - Torset (TORT to TORT)
- **Graphics Codes**
  - ISOPLOT (Pre- and Post Processing), ASPECT, etc.

Simplistic Discrete Ordinates

$$H(\rho)\Phi(\rho) = S(\rho)$$

ρ	= phase space variable = (x,y,z,E,Ω,t)
$\Phi(\rho)$	= particle flux at ρ
$S(\rho)$	= source particle density at ρ
$H(\rho)$	= Boltzmann integral-differential operator
$H(\rho)\Phi(\rho)$	= particle losses at ρ (collisional loss and leakage from system)

[Above equation is a particle balance at ρ]

Simplistic Discrete Ordinates (cont. 1)

Discretize Balance Equation:

Subdivide angular domain into a finite number of directions and weights (quadrature set)

$$\sum_{m=1}^{M} \Phi_m w_m = \int_{\Omega} \Phi(\Omega)\, d\Omega, \; \Phi_m = \Phi(\Omega_m), \; w_m = \frac{1}{4\pi} \int_{\Delta\Omega_m} \Omega\, d\Omega$$

Subdivide energy domain into finite number of energy groups (multigroup approximation)

$$\sum_{g=1}^{G} \Phi_g = \int_E \Phi(E)\, dE, \quad \Phi_g = \int_{E_{g+1}}^{E_g} \Phi(E)\, dE$$

Simplistic Discrete Ordinates (cont. 2)

Subdivide spatial domain into a finite number of cells (voxels)

Introduce some type of spatial differencing (and interpolation) scheme to obtain a coupled set of M x G x N algebraic equations

Invert H iteratively and solve for Φ:

$$\Phi(\rho) \cong \Phi_{m,g,n} = \overline{H}^{-1}(\rho)S(\rho)$$

Dose Calculation 1) Fold flux with flux-to-dose factors - EASY

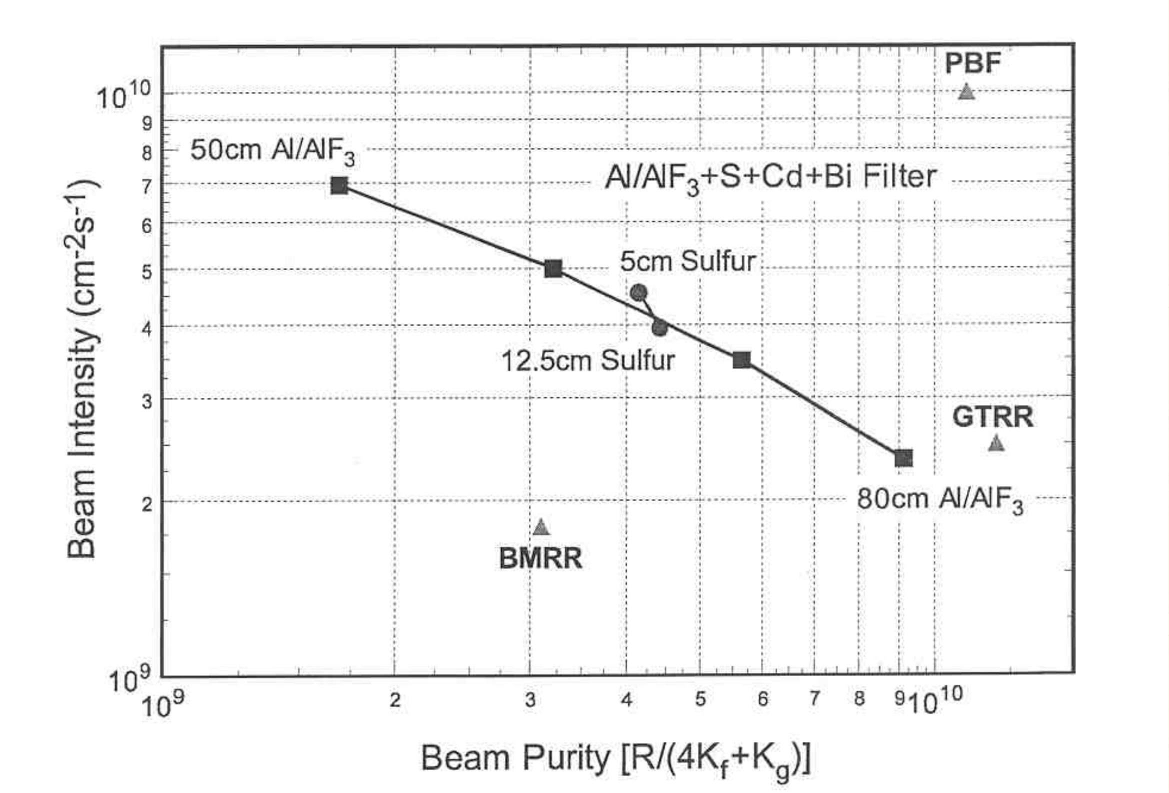
2) Calculate from energy balance - DIFFICULT

BNCT Facility Design Optimization

- BNCT is a bimodal therapy for treating tumors - in particular glioblastoma multiforme (GBM)
  - Patient given suitable boronated pharmaceutical that preferentially seeks malignant tissue
    - Tumor absorbs more than healthy brain tissue because of breakdown of blood-brain-barrier
  - Tumor region irradiated with epithermal or near epithermal neutron beam to generate thermal flux in diseased tissue
  - Due to high ^{10}B capture cross section - thermal neutrons are readily absorbed yielding ^{4}He & ^{7}Li
  - ^{4}He & ^{7}Li range out over cell dimensions leading to destruction of tumor tissue

TSR-II Brute Force Optimization
(Ingersoll, Slater, and Williams)

- **ANISN Calculations**
  - **Optimal filter**
    - **0.8 m Al/AlF3**
    - **92 mm sulfur**
    - **0.2 mm cadmium**
    - **0.1 mm bismuth**
- **DORT Calculations**
  - **Collimator**
    - **0.1 m lithiated polyethylene**



One-Dimensional Gradient Optimization
(Karni, Greenspan, Vujic, and Ludewigt)

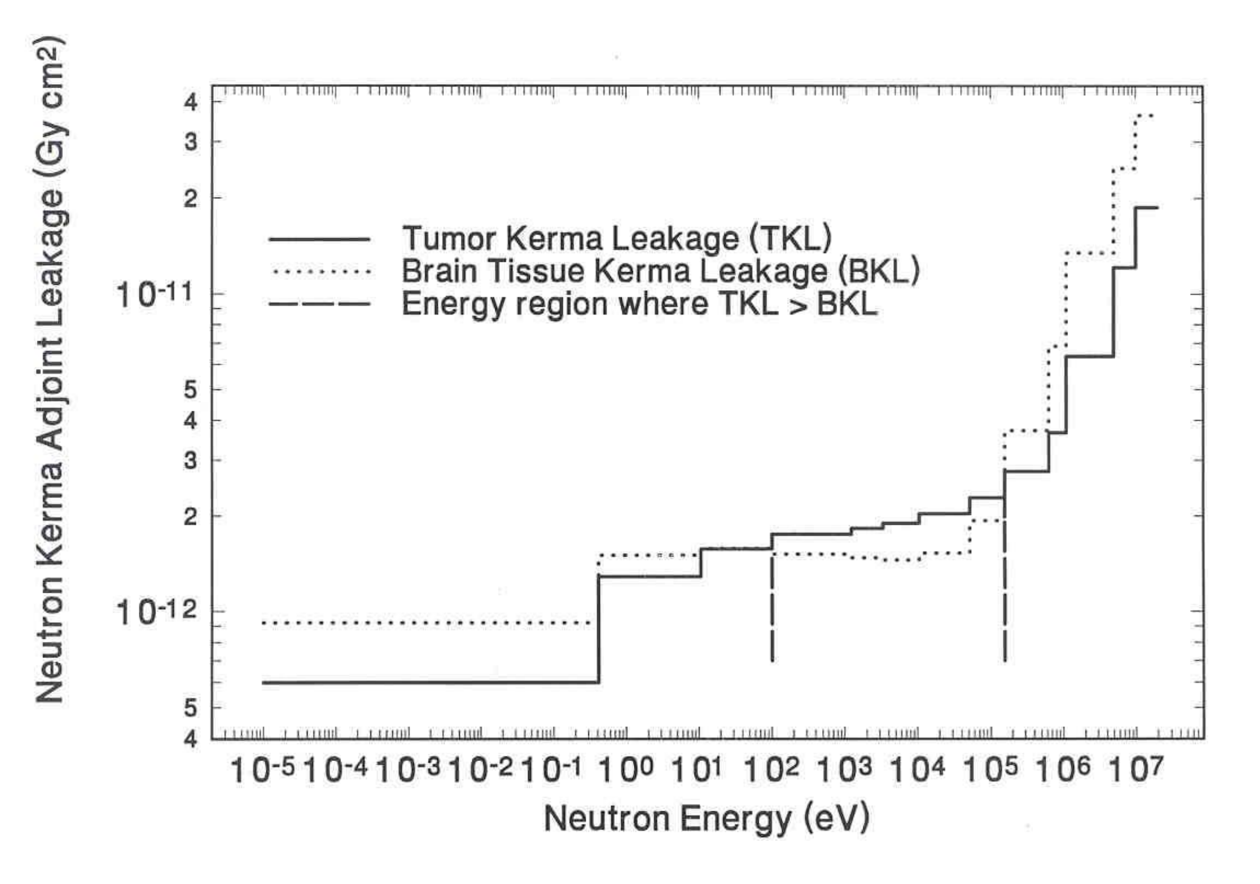
- **Employed SWAN optimization code to identify suitable source assemblies for BNCT**
  - SWAN uses gradient information to calculate material replacement effectiveness functions (REF's)
    - REF of material j relative to material k =
      change in a performance factor due to changing material j by equal amount of material k at same location
  - SWAN based on perturbation theory approach
    - Requires calculation of both forward and adjoint fluxes
- **Optimization of tumor/healthy tissue dose ratio**
  - Ratio REF = numerator EF - denominator EF
  - All fluxes calculated with ANISN

Multi-Dimensional Gradient Optimization
(Lillie)

- Three-dimensional model of patients head (TORT)
  - Calculate adjoint leakage due to healthy tissue KERMA
  - Adjoint leakage due boron loaded tumor KERMA
- Two-dimensional model of beam-tube-filter geometry (DORT)
  - Forward flux due to radiation source
  - Adjoint fluxes due to above adjoint leakages
- Calculate gradient of dose ratio with respect to filter materials
- Estimate new filter composition using gradient
- Repeat DORT calculations with new filter, ...

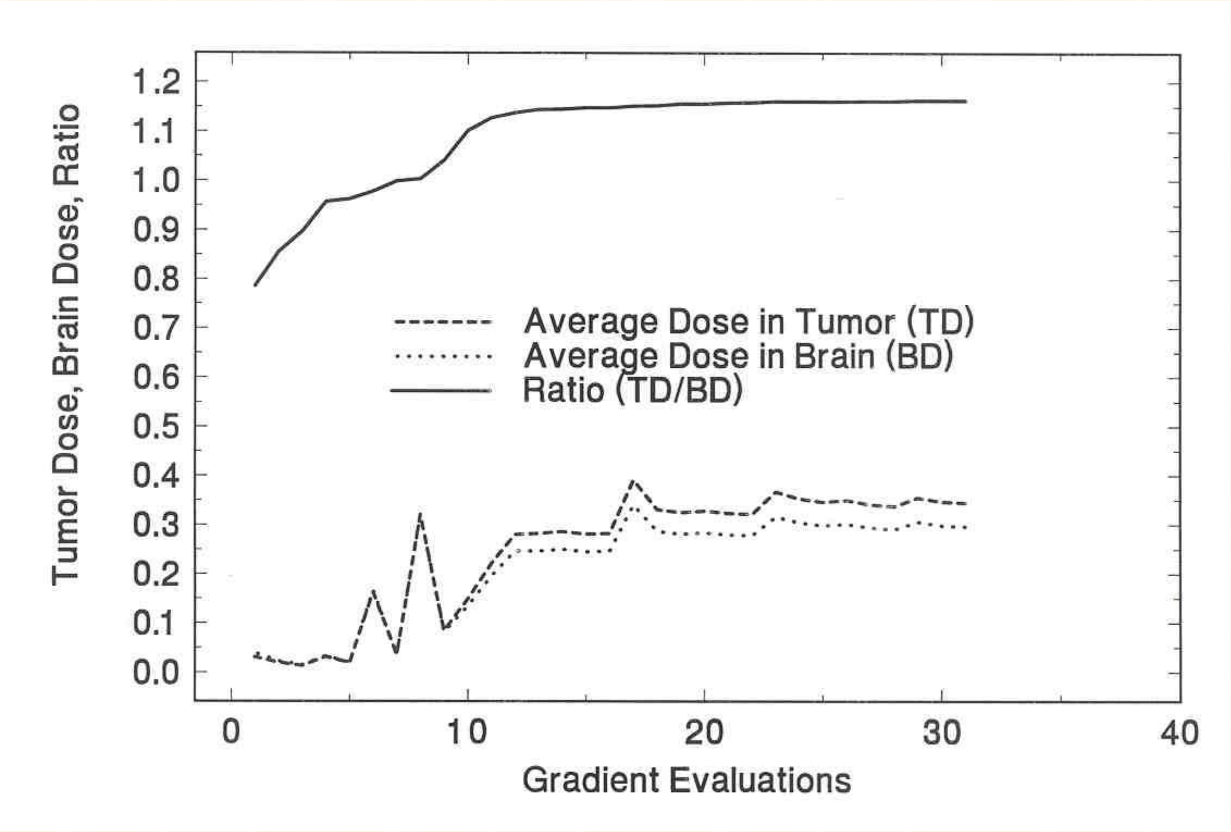
Multi-Dimensional Gradient Optimization
(Lillie)

- **Neutron Adjoint Leakage**
  - **TKL/BTL > 1.0 only between 100 eV & 180 keV**
  - **Maximum TKL/BKL from 10 to 40 keV (TKL/BKL = 1.33)**
- **Maximum Tumor to Healthy Tissue Dose Ratio = 1.33**



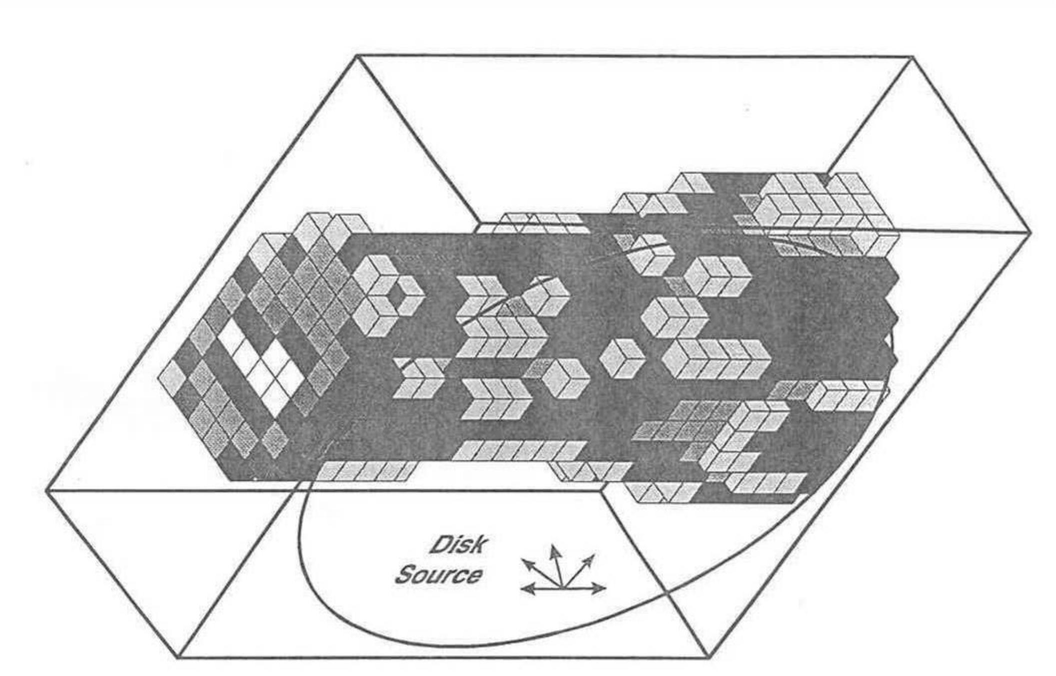
Multi-Dimensional Gradient Optimization
(Lillie)

- **Tumor dose increases**
  0.05 to 0.34
- **Healthy tissue dose increases**
  0.06 to 0.29
- **Dose ratio increases**
  0.78 to 1.17
- **Optimization increases dose ratio from 59% to 88 % of maximum possible dose ratio**

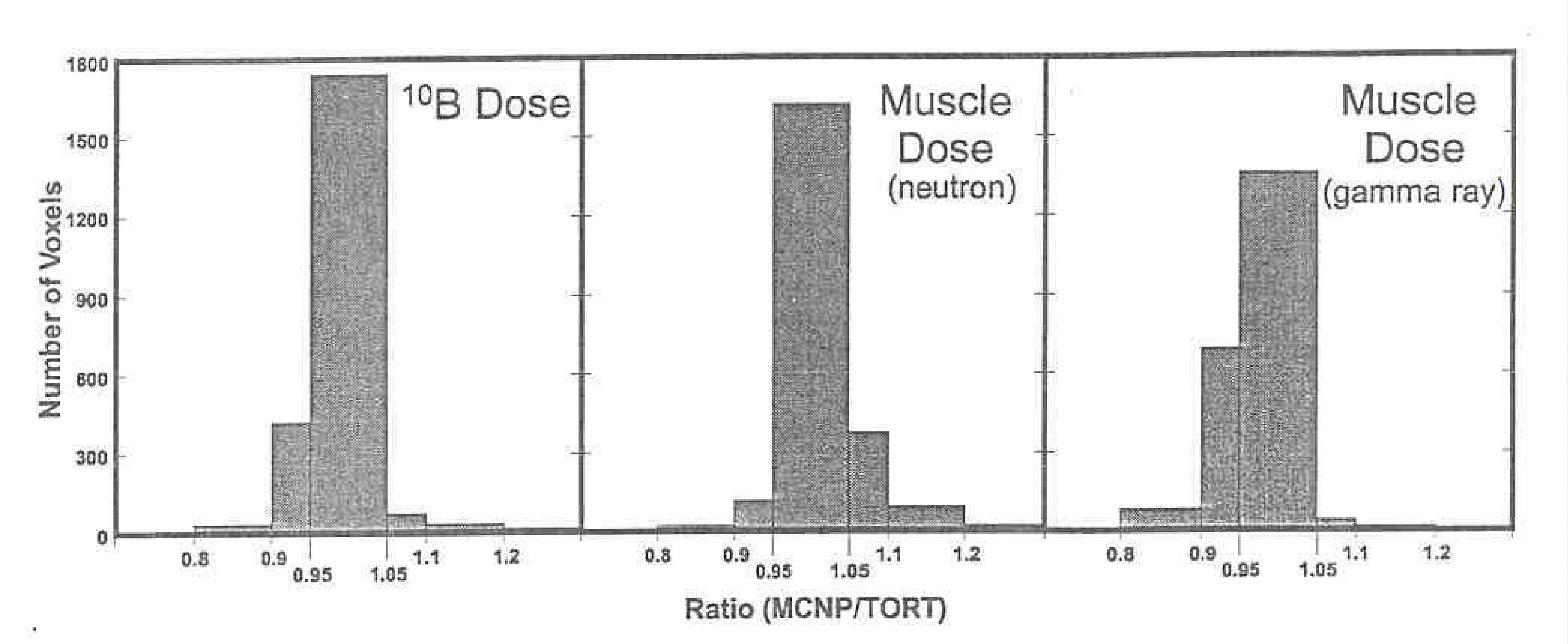


Lower Leg Dose Comparison
(Ingersoll, Slater, Williams, Redmond, and Zamenhof)

- **Lower leg voxel model built from CT scans**
  - TORT - 15,782 voxels
  - MCNP - 11,025 voxels
- **TORT results affected?**
  - ENDF data (V or VI) - no
  - Theta weight - yes
- **MCNP results affected (better agreement)?**
  - S(α,β) kernels - yes
  - Histories 3 $\rightarrow$ 10 M - yes



Lower Leg Dose Comparison
(Ingersoll, Slater, Williams, Redmond, and Zamenhof)

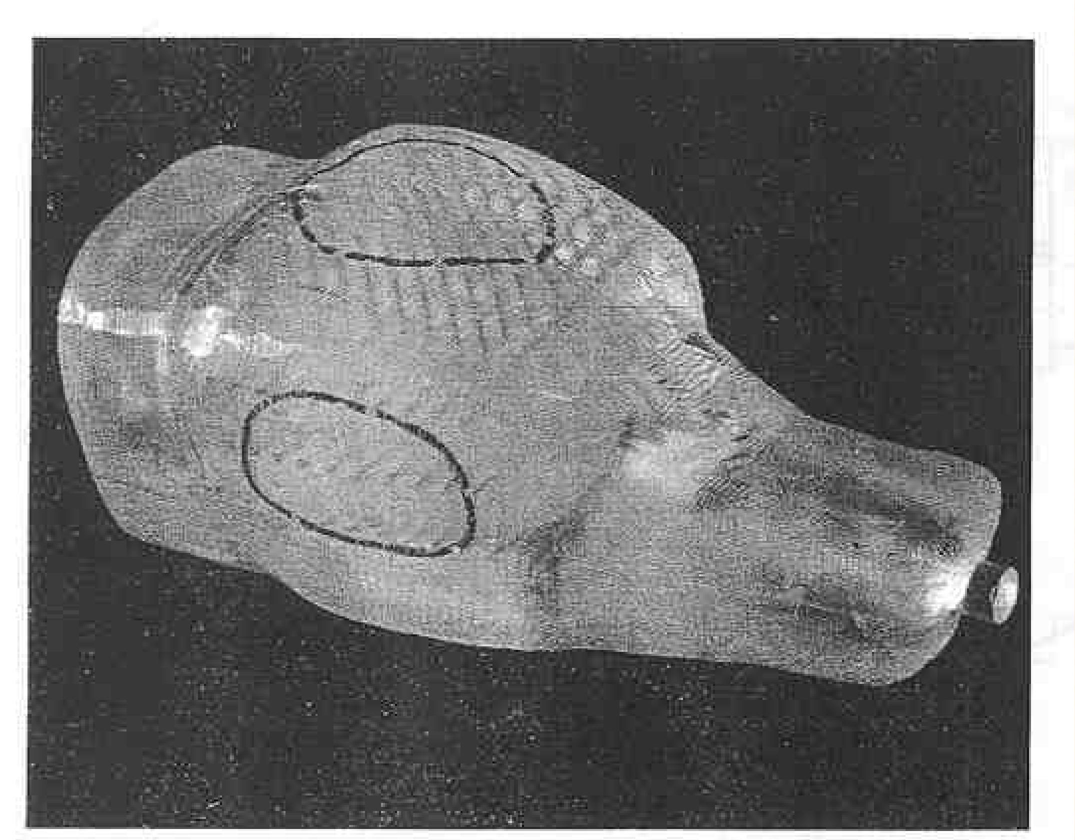


Better than 5% agreement found in more than 95% of comparable voxels

(not all TORT voxels in MCNP model)

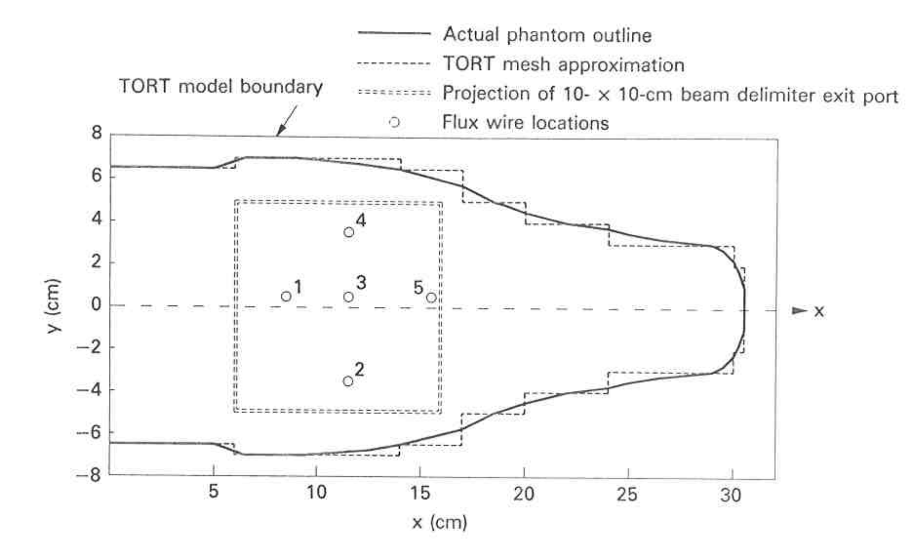
Phantom Dog Head Comparison
(Wheeler and Nigg)

- **Irradiated lucite dog head phantom at BMRR**
- **Activated copper-gold alloy wires**
  - **thermal flux measured separately from total**
- **Compared measured thermal flux with that calculated using**
  - **Monte Carlo (rtt_MC - INEL)**
  - **Deterministic (TORT - ORNL)**

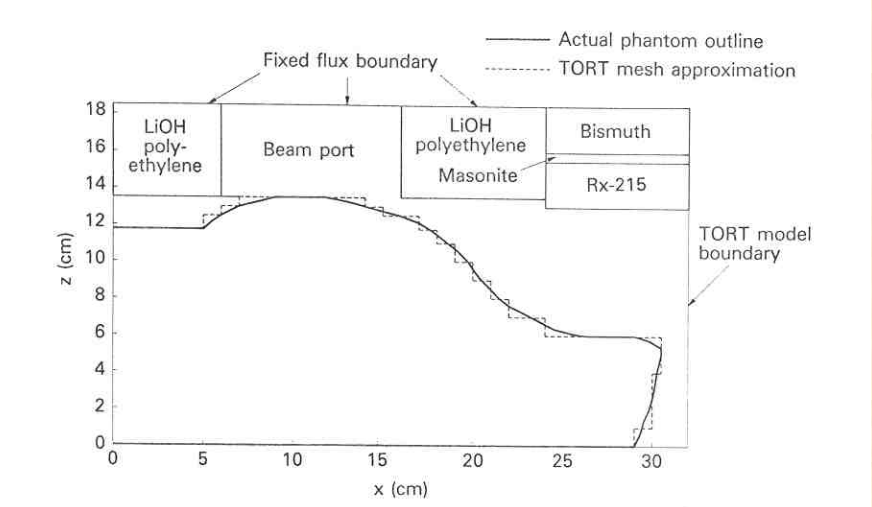


Phantom Dog Head Comparison
(Wheeler and Nigg)

Top View



Side View



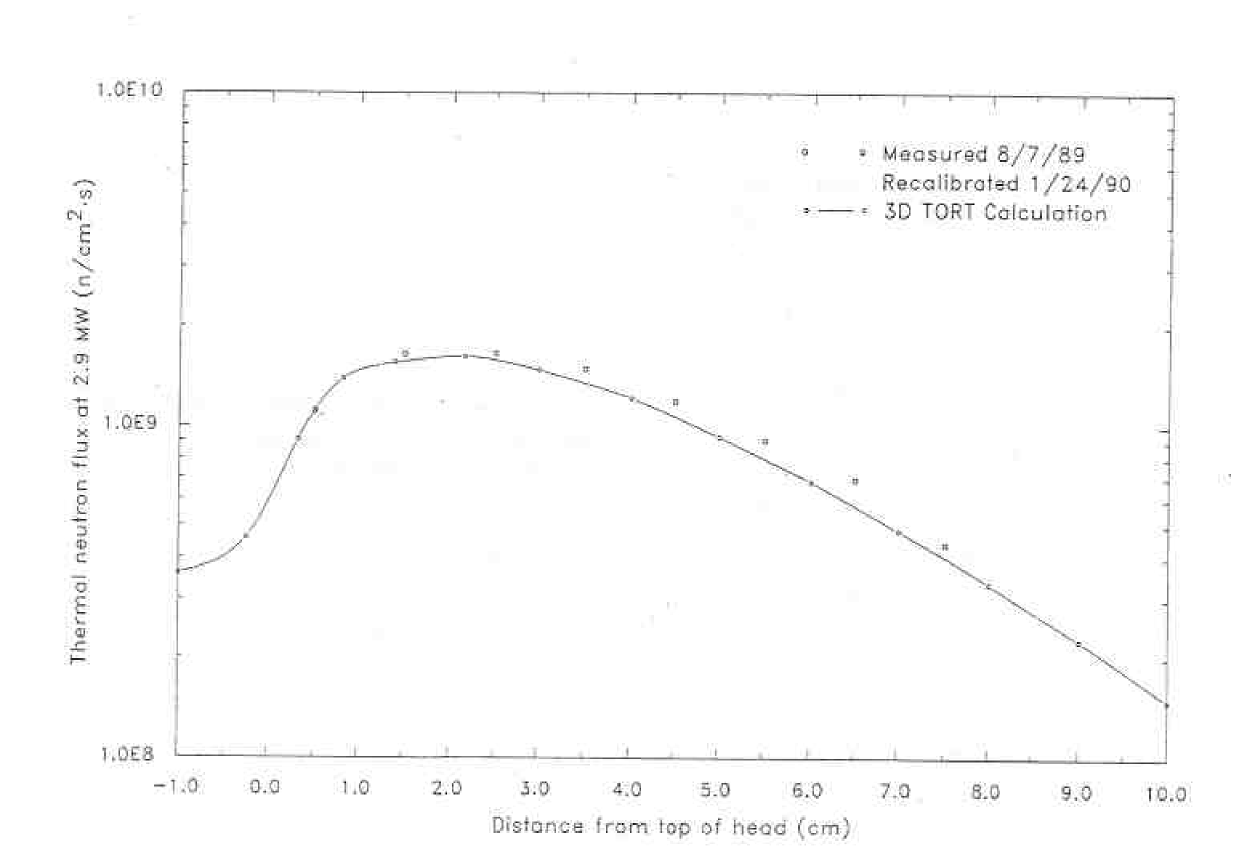
Mesh Representation of Dog Head in TORT Model

1 cm rectangular mesh - 32x16x22 x,y,z mesh intervals

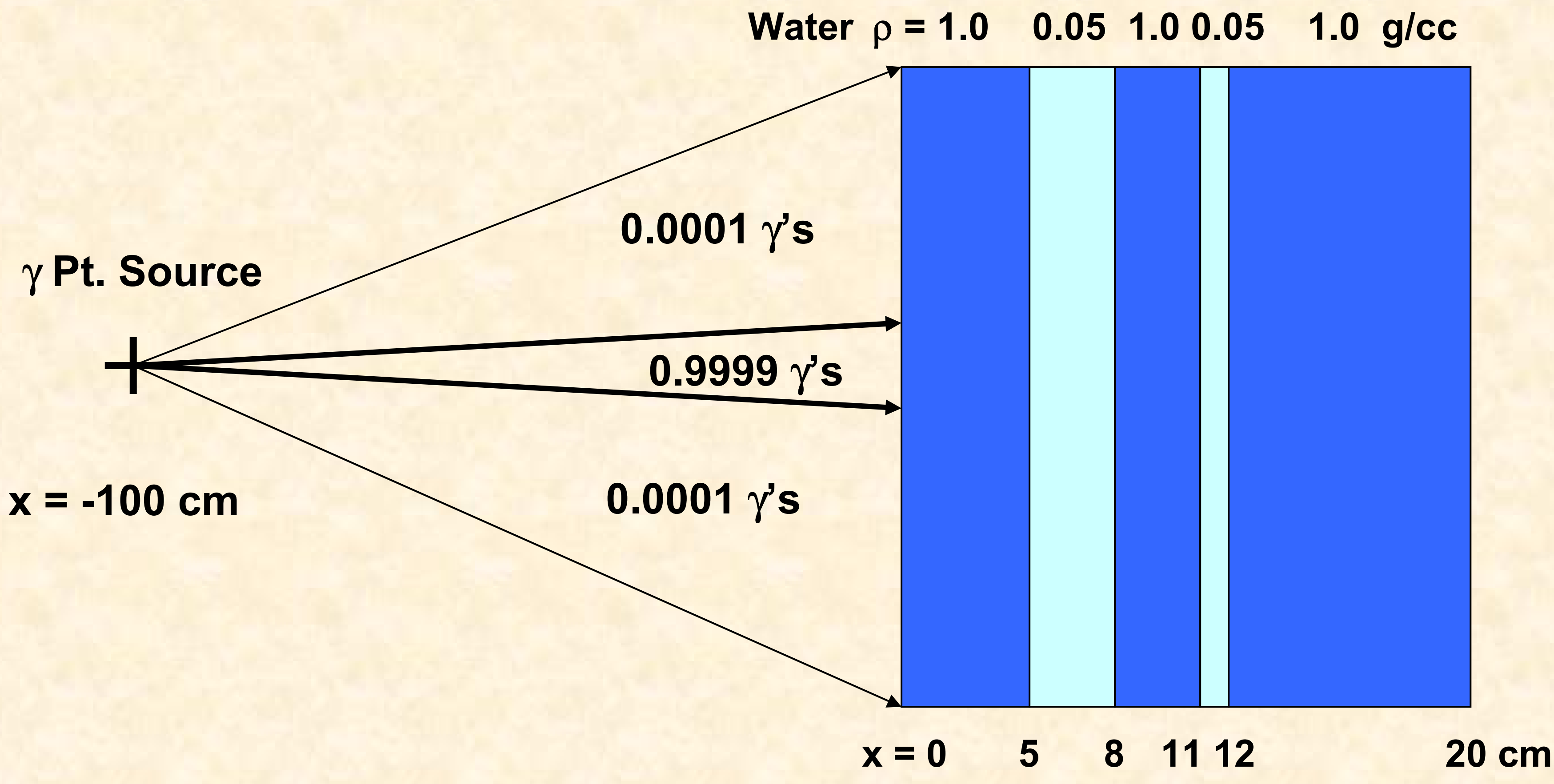
S_8 angular quadrature (96 angles), BUGLE80 47neutron-22gamma groups

Phantom Dog Head Comparison
(Wheeler and Nigg)

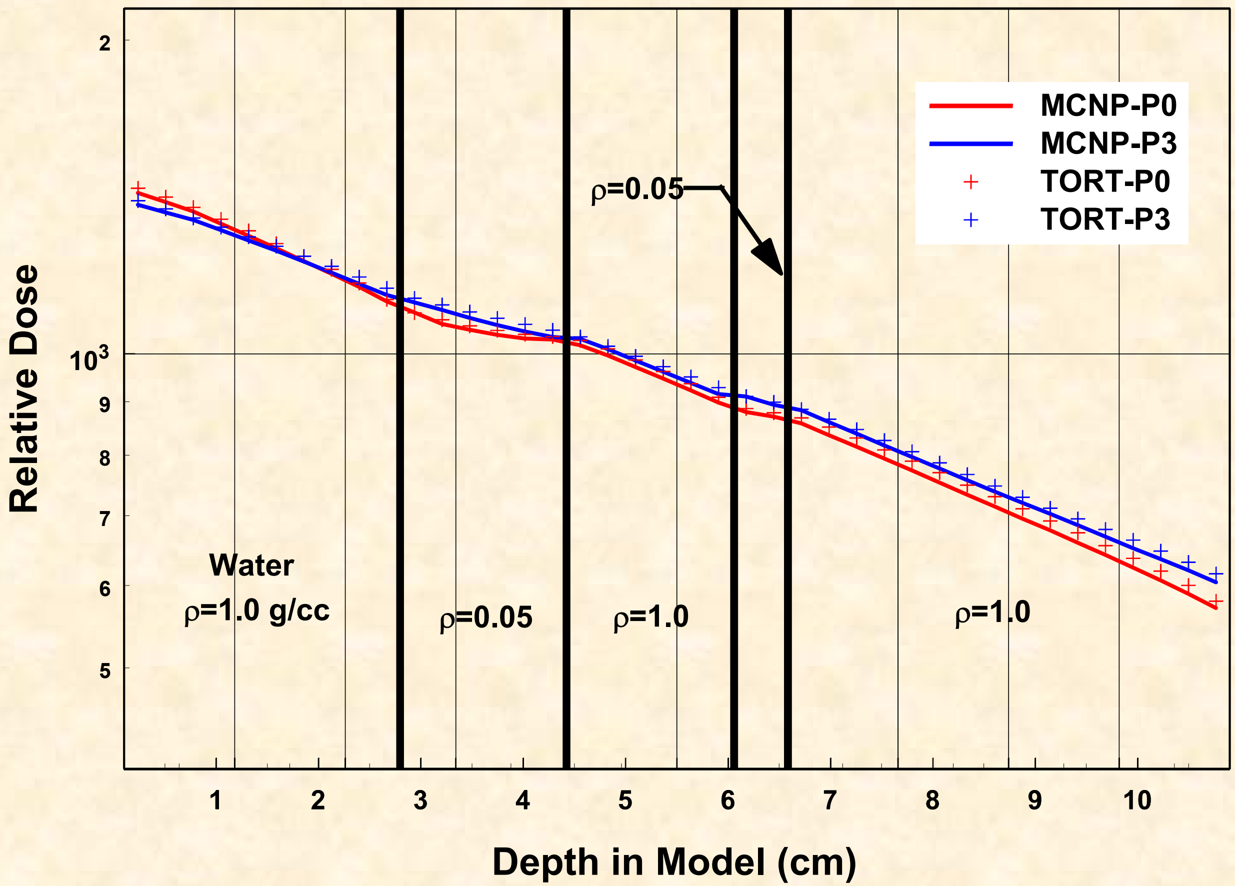
- **BMRR power**
  2.9 MW
- **Peak thermal flux**
  - **Measured (10%)**
    1.91 x 10^9 n/cm^2•s
  - **rtt_MC**
    2.13 x 10^9 n/cm^2 • s
  - **TORT**
    2.02 x10^9 n/cm^2 • s
- **TORT - 650 min.**
- **rtt_MC - 196 min**



MCNP and TORT Simulation Model
(Peplow and Lillie)

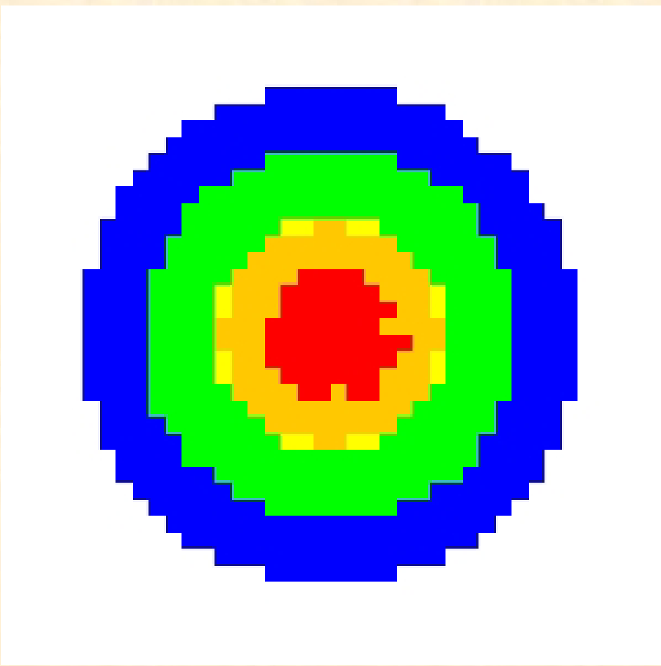


Comparison of Multigroup MCNP and TORT Dose Profiles (y = 10.25 cm, z =10.25 cm)
(Peplow and Lillie)



Multigroup P_3 Scattering MCNP & TORT Dose Contours (Perpendicular to Beam, x = 9.75 cm)

(Peplow and Lillie)

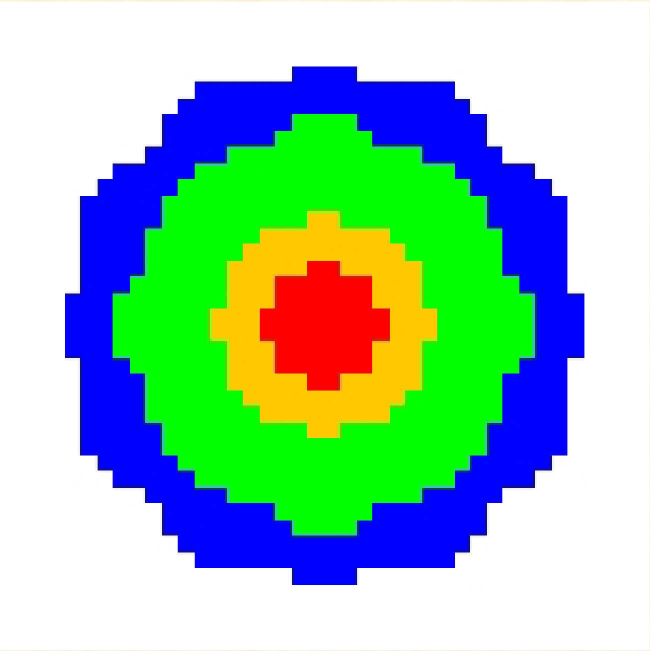


MCNP

Scale

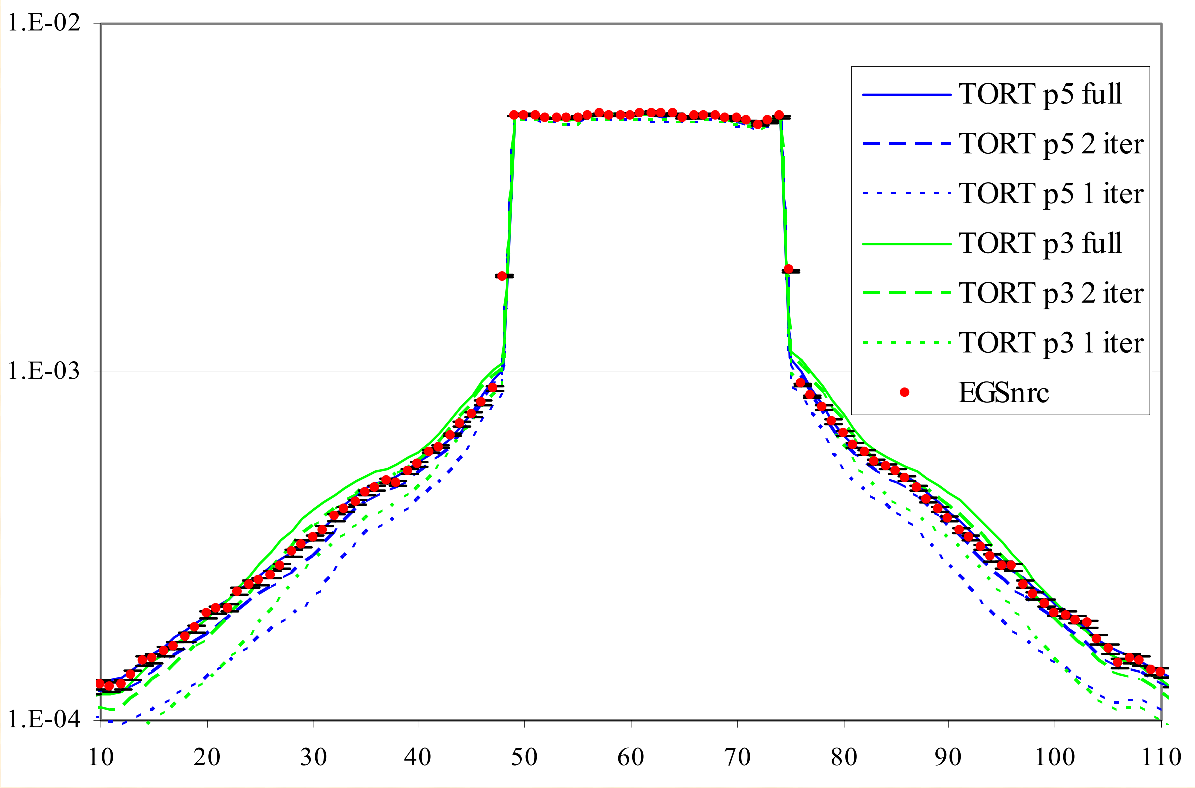
Red	0.99 - 1.0
Orange	0.5 - 0.99
Yellow	0.1 - 0.5
Green	0.01 - 0.1
Blue	0.005 - 0.01
White	< 0.005

9.5 cm < x < 10.0 cm



TORT

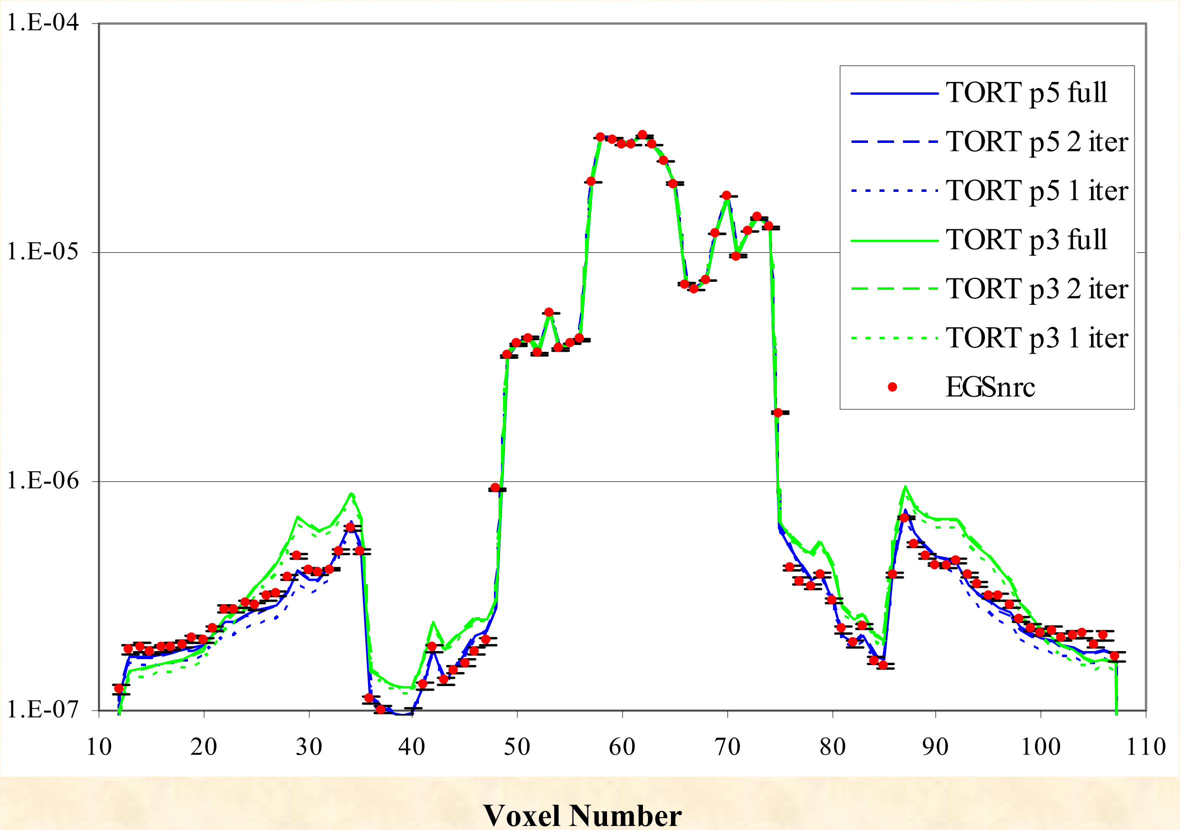
Photon Beam Transport in a Human Phantom Model: DORT vs EGSnrc
(Peplow and Lillie)



Voxel Number

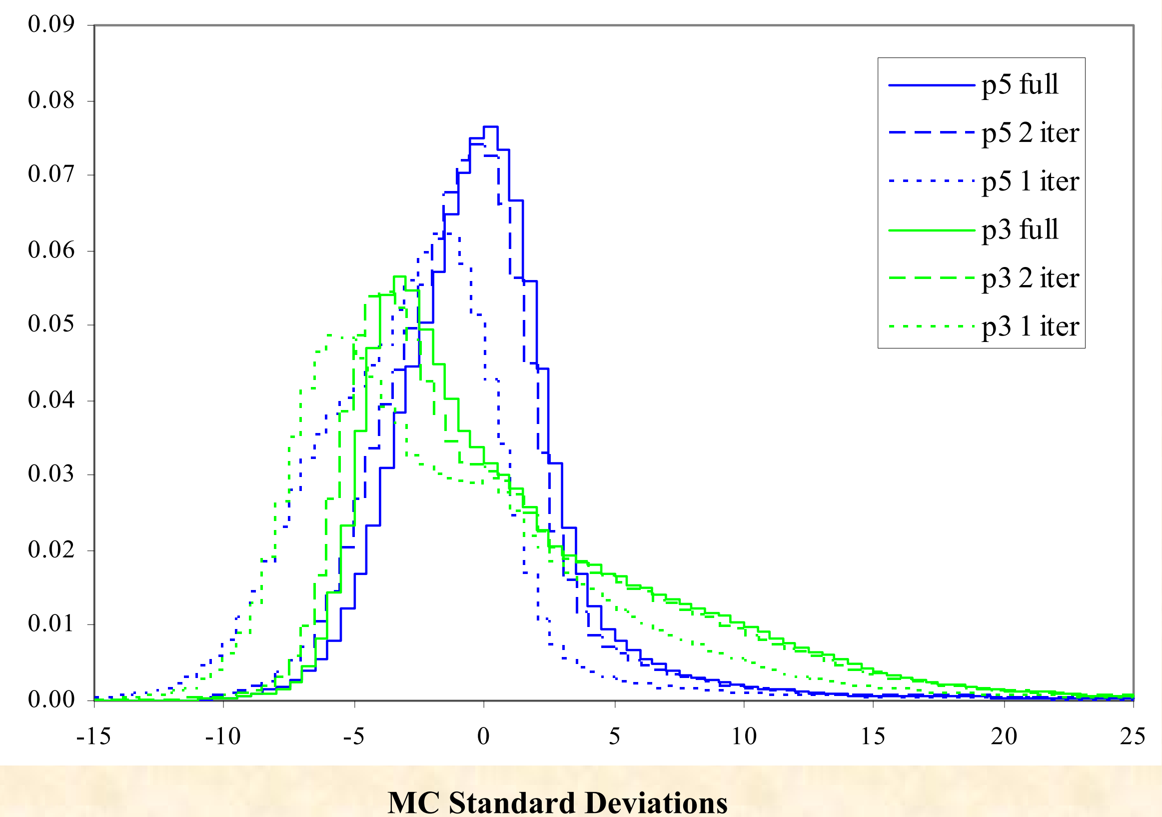
Discrete Ordintates vs Monte Carlo Flux Transverse Profiles on a Mid-plane Coronal Slice halfway between CT Isocenter and Beam Exit

Photon Beam Transport in a Human Phantom Model: TORT vs EGSnrc
(Peplow and Lillie)



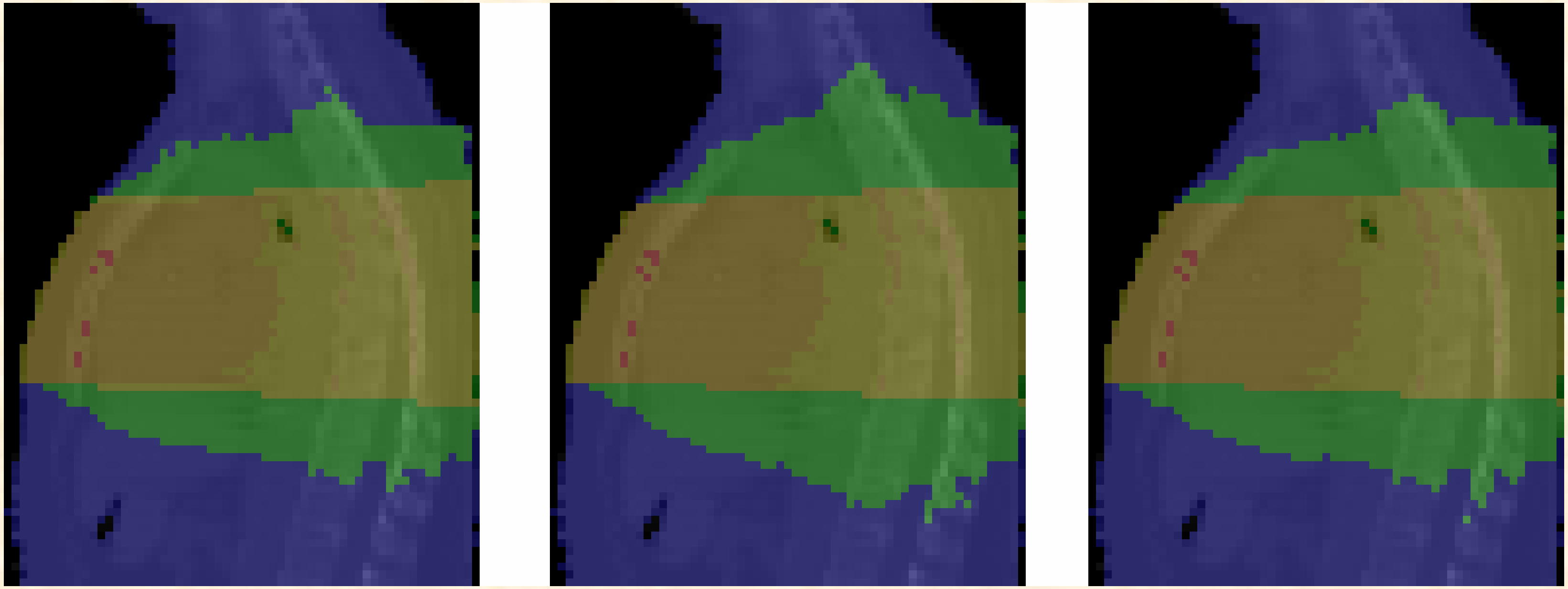
Discrete Ordintates vs Monte Carlo Energy Deposited Transverse Profiles on a Mid-plane Coronal Slice halfway between CT Isocenter and Beam Exit

Photon Beam Transport in a Human Phantom Model: TORT vs EGSnrc
(Peplow and Lillie)



Fractional Frequency Distribution of Voxel Energy Deposited Differences between Discrete Ordinates and Monte Carlo divided by MC Standard Deviation

Photon Beam Transport in a Human Phantom Model: TORT vs EGSnrc
(Peplow and Lillie)



EGSnrc TORT (p3 scattering) TORT (p5 scattering)

Energy Deposited Sagittal Profiles

blue: 0.1-1%, green: 1-10%, yellow: 10-50%, orange: 50-90%, and red: 90-100% of max

Photon Beam Transport in a Human Phantom Model: TORT vs EGSnrc

(Peplow and Lillie)

CPU Times Required for Discrete Ordinates and MC Calculations

Code	*Calculation*	*CPU Time (minutes)*
EGSnrc	Photon Flux	88
	Energy Deposited	5000
TORT[a]	P_3 1 iteration	23
	P_3 2 iteration	35
	P_3 fully converged	185
TORT[a]	P_5 1 iteration	62
	P_5 2 iteration	97
	P_5 fully converged	570

[a]Includes GRTUNCL3D CPU times of 5 and 12 minutes for P_3 and P_5 calculations, respectively.

Summary

- ANISN & DORT used for BNCT facility design - primarily filter optimization
  - Need fluence everywhere to obtain gradiants (difficult to do using Monte Carlo
- TORT
  - Lower Leg (neutrons) - Excellent agreement with Monte Carlo calculated dose rates
    - Suitable for anatomical voxel based models
    - Significantly less computational cost (single processor)
  - Phantom dog head (neutrons) - Very good agreement with measured thermal fluxes
  - Human Phantom Model (photons) – Good agreement using higher order scattering and only two iterations (reduced computation time)