Unique Formulations in TITAN and PENTRAN for Medical Physics Applications

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For presentation at ICRS12 & RPSD-2012, Nara, Japan, Sept 2-7, 2012

Contents

- Introduction to
  - TITAN
  - PENTRAN
- TITAN unique algorithm for SPECT
- PENTRAN unique algorithm for
- Conclusions

PENTRAN-MP Code System
(G. Sjoden and A. Haghighat, 1996)

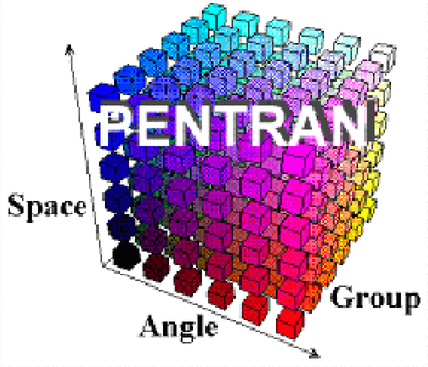
Pre-processing

GHOST-3D and DXS (**3-D General Collapsing Code** determines an effective phantom material distribution, **DXS** yields sources distributions)

PENMSH-XP (prepares mesh, source, and material distributions)

CEPXS (from SNL, prepares multi-groups Cross-section libraries)

S_N Transport Calculation



(Parallel Environment Neutral-particle TRANsport)

Post-processing

EDK-S_N (calculate total 3D-dose distributions for all Energy Groups based on Electron Dose Kernels generated by Monte Carlo Calculations)

PENTRAN^{TM} (cont.)

- **ANSI FORTRAN 90 with MPI library (Export classification 0D999B available for use in most countries)**

- **Coarse-mesh-oriented data structure** allowing localized meshing, differencing scheme

- **Parallel processing:** Hybrid domain decomposition (angle, energy, and/or space); Parallel I/O; Partition memory

- **Adaptive Differencing Strategy (ADS):** Diamond Zero (DZ) → Directional Theta-Weighted differencing (DTW) → Exponential-Directional Iterative (EDI)

- **Fully discontinuous variable meshing -** Taylor Projection Mesh Coupling (TPMC)

- **Angular quadrature set:** Level symmetric (up to S20) and Pn-Tn with OS

TITAN – A 3-D Parallel Hybrid Transport Code (C. Yi, A. Haghighat, 2006)

- Written in **Fortran 90 (**with some features in Fortran 2003 standard, such as dynamic memory allocation and object oriented23) and MPI library
- **Compiled** by Intel Fortran Compiler (ifc 8.0+) or PGI f90 compiler (pgf90 6.1)
- **Coarse-mesh-oriented data structure** allowing localized meshing, quadrature and solver.
- **Coarse-mesh based Hybrid Algorithms**
  - Sn and Characteristics
  - Sn with fictitious quadrature and ray tracing

TITAN (continued)

- Hybrid algorithms use fast and memory-efficient spatial and angular projections on the interfaces of coarse meshes by using sparse projection matrix

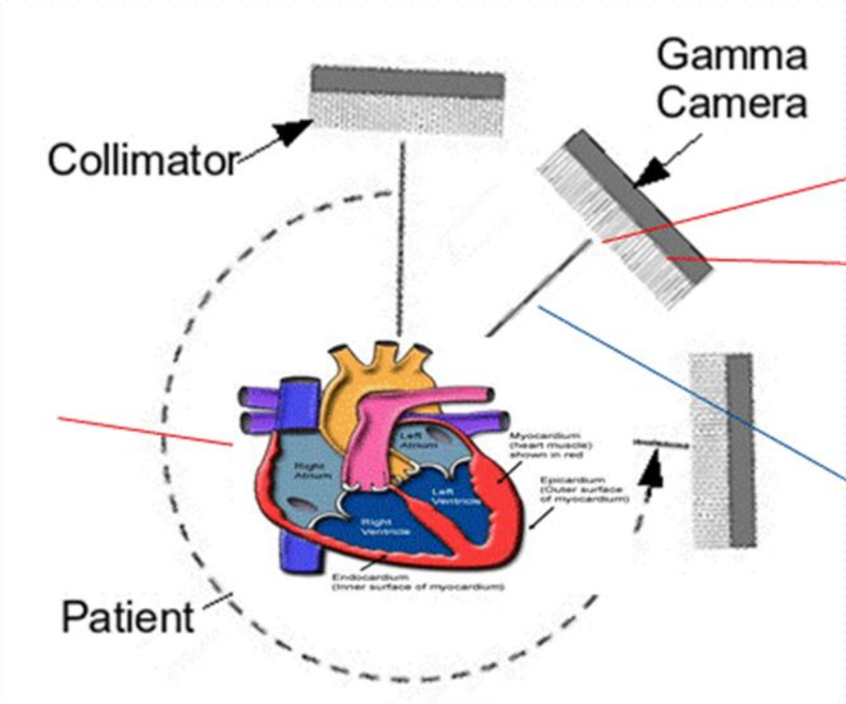
- Parallel processing: Angular and spatial domain decomposition; partition memory

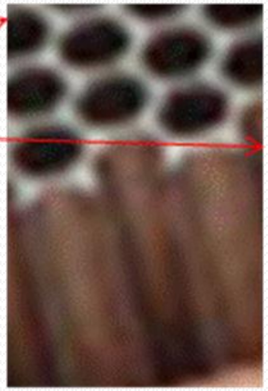
- Angular Quadrature:
  - Level-symmetric and Pn-Tn (arbitrary order) quadrature sets with Ordinate Splitting (OS)
  - Sn with *fictitious quadrature*

SPECT (Single Photon Emission Computed Tomography) device

- SPECT is a functional imaging device

Inject a radioactive material





<u>Example</u>
D~1.5 mm
L=23 mm
Aspect ratio=~15

A projection angle

Goal

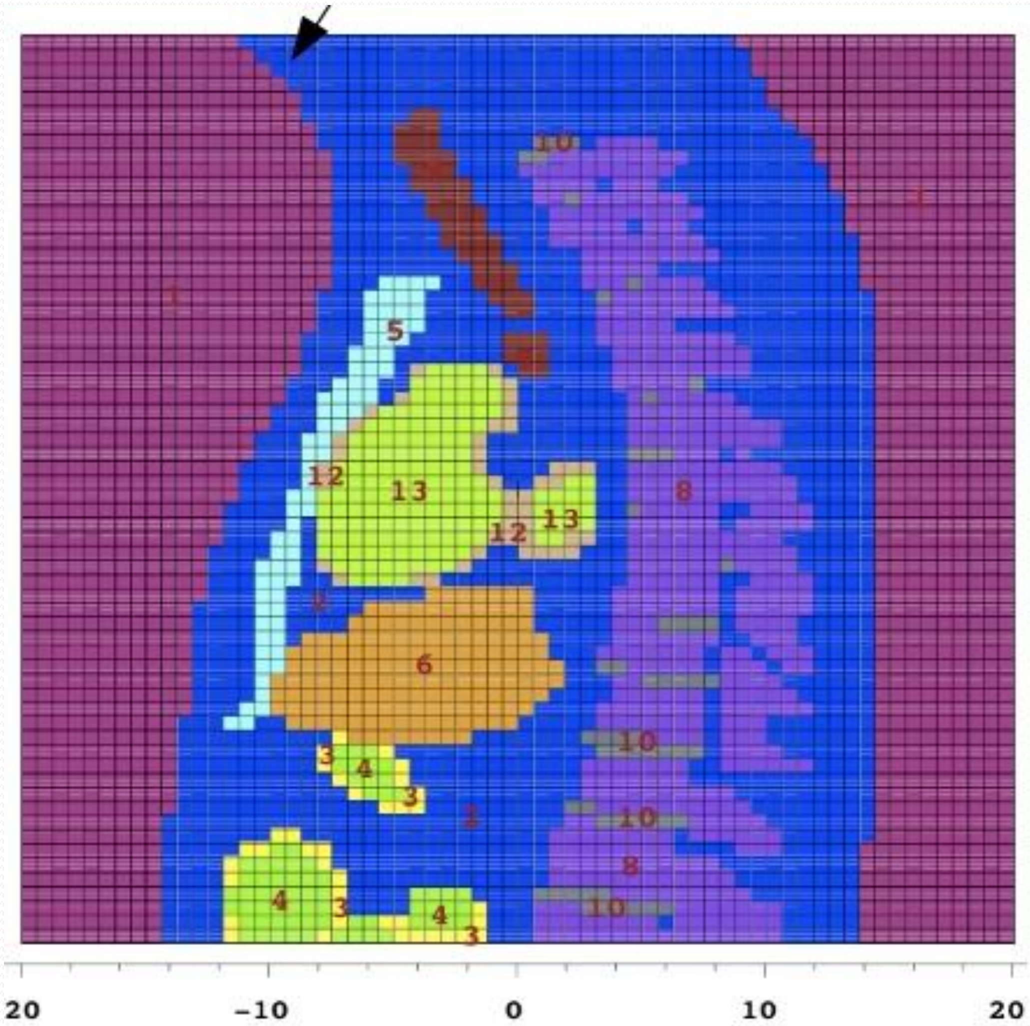
- Simulation of the SPECT (Single Photon Emission Computed Tomography) using accurate and fast hybrid deterministic formulation

- Why?
  - Improving the image quality
  - Reducing radioactive uptake

Reference Model

- A SPECT myocardial perfusion study with Technecium-99m (Tc-99m) was simulated.
- Tc-99m is absorbed by the heart wall where it emits 140.5 keV gamma rays.
- The NURBS-based cardiac-torso (NCAT) code was used to create a 64 x 64 x 64 voxel phantom with a Tc-99m source in the heart wall.

NCAT voxel phantom



Multigroup cross sections for TITAN

- Energy group structure

  Since source energy is 140.5 keV

Energy Group	Upper Bound (keV)	Lower Bound (keV)
1	154.55	126.45
2	126.45	98.35
3	98.35	10

- Used CEPXS multigroup photon cross sections (Sandia National Laboratories)

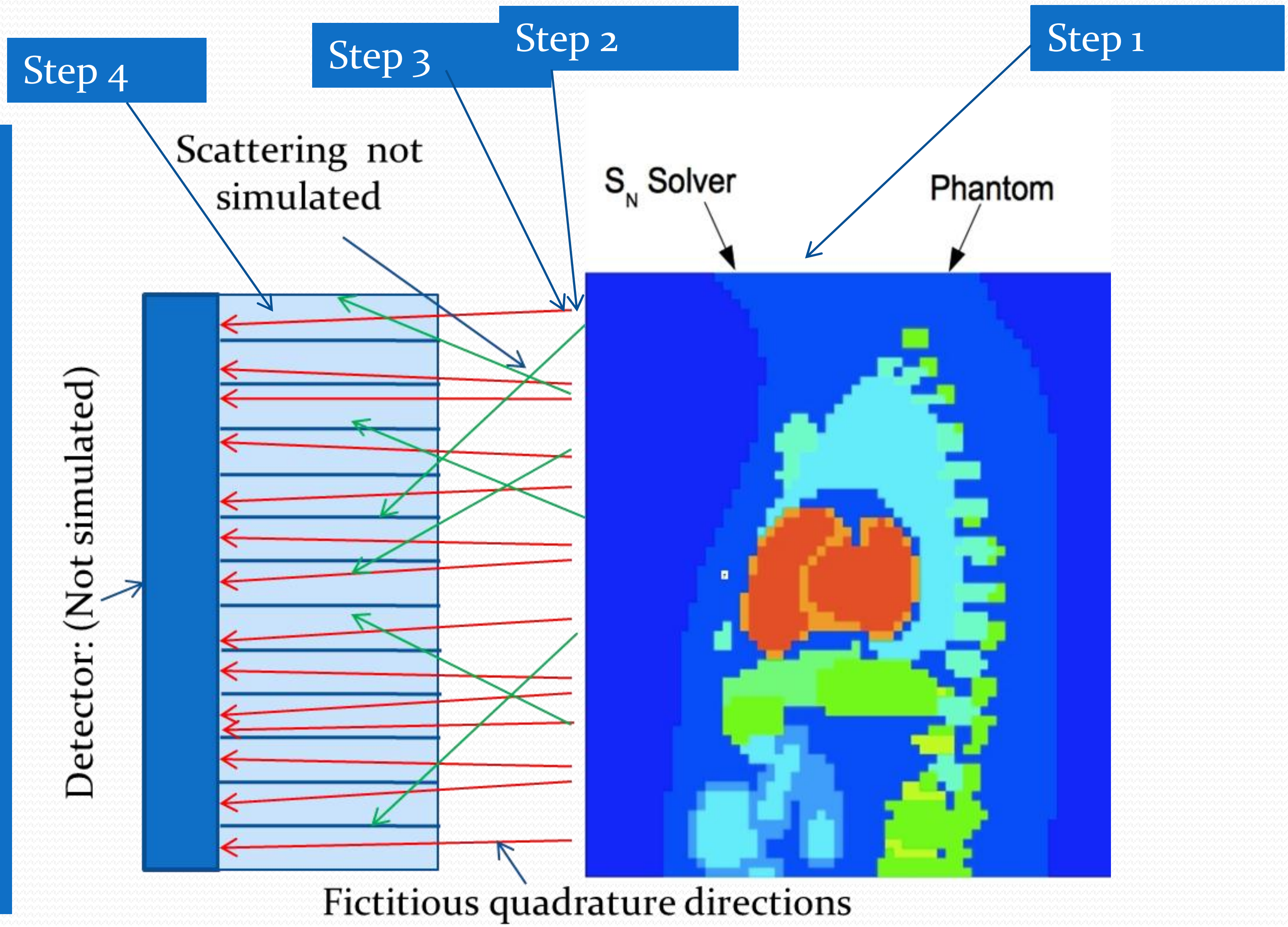
TITAN Hybrid formulation for SPECT simulation

Step 1- Sn calculation in phantom

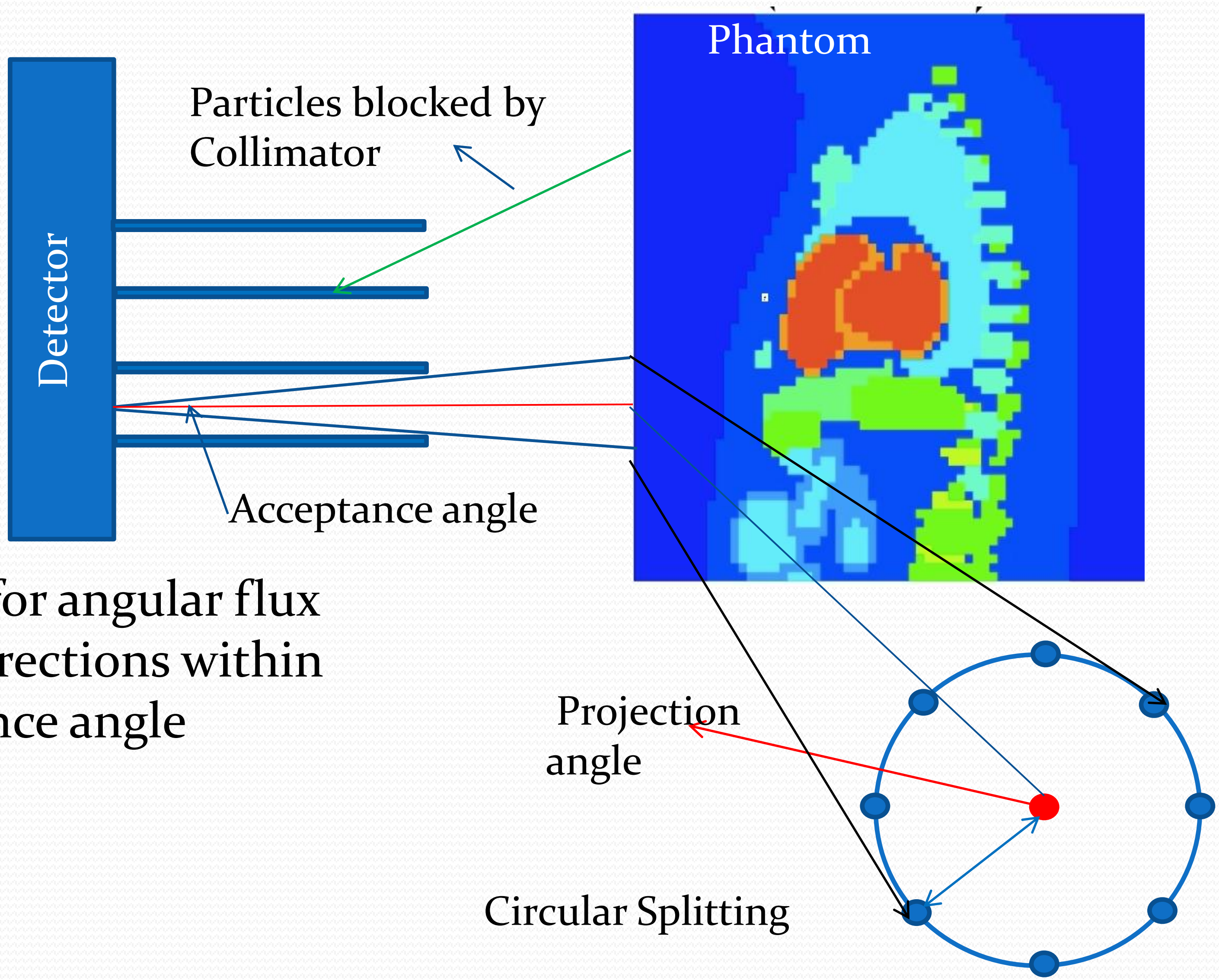
Step 2 – Selection of fictitious direction

Step 3 – Sn with fictitious quadrature

Step 4 – ray tracing



Step 2 – Selection of fictitious directions



- Solve for angular flux along directions within acceptance angle

Step 3 – Sn with fictitious direction

- To calculate angular fluxes along directions of interest, we revise the Sn algorithm for treating a fictitious quadrature set
  - Fictitious quadrature represents all the projection angles and directions created through circular splitting

Step 3 - Sn with Fictitious Quadrature

- To calculate the angular flux for the fictitious quadrature set on the surface of the phantom, we developed the following algorithm:
  - Obtain flux moments from step 1
  - Calculate Scattering Source for Extra Sweep along fictitious quadrature set

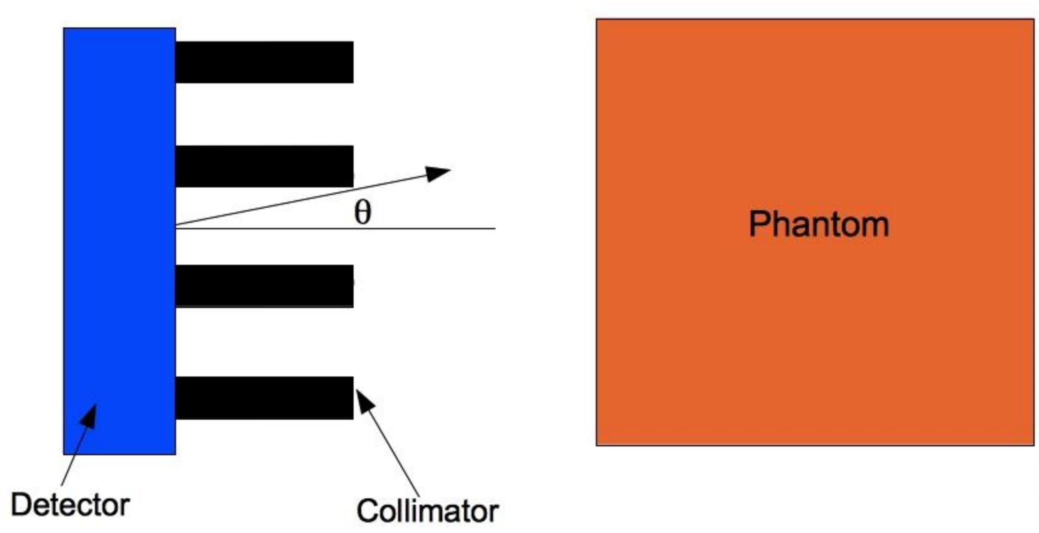
$$S_{scattering}^{(e.s.)} = \sum_{g'=1}^{G} \sum_{l=0}^{L} (2l+1)\sigma_{s,g'\to g,l} \{P_l(\mu_n^{(fic)}) \cdot \phi_{g',l}^{(con)} + 2\sum_{k=1}^{l} \frac{(l-k)!}{(l+k)!} P_l^k(\mu_n^{(fic)}) \cdot \left[\varphi_{C,g',l}^{k,(con)} \cdot \cos(k\varphi_n^{(fic)}) + \varphi_{S,g',l}^{k,(con)} \cdot \sin(k\varphi_n^{(fic)})\right]\}$$

  - Perform an extra sweep to obtain angular flux along the fictitious quadrature set.

Step 4 – Ray tracing along collimators

- Since the spatial meshing of the phantom is much coarser than the collimator opening
  - The characteristic rays are drawn from each pixel of the projection image backward to the phantom surface along the projection angle and the split directions circularly surrounding it
  - Using a bi-linear interpolation procedure, angular fluxes along the projection angle and its split directions are determine
- Using a ray-tracing formulation through vacuum - particles leaving the phantom surface are transported through a set of collimators normal to the SPECT camera.
- The intensity of each pixel in the projection images is evaluated by the integration of the angular flux at that pixel over the small collimator acceptance angle.

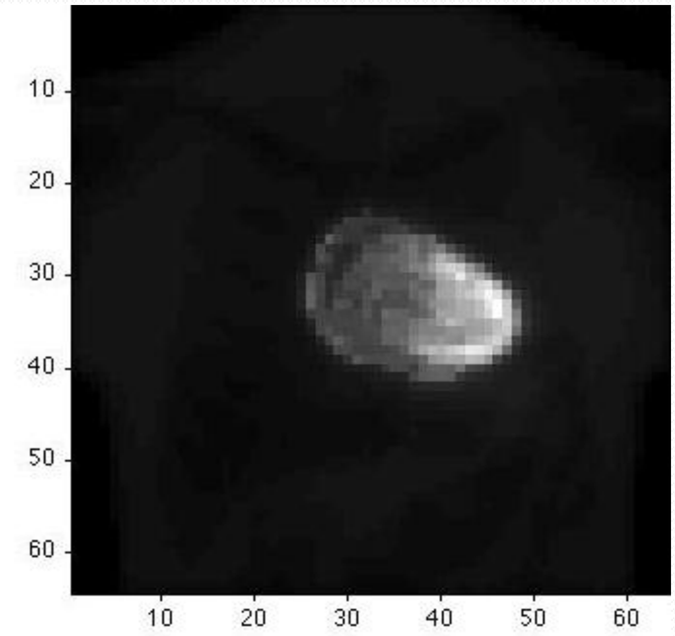
Collimator Cases



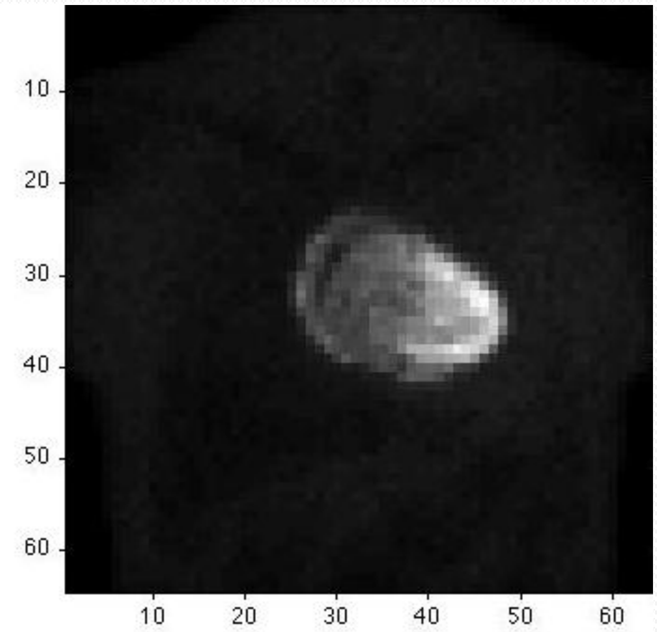
Case	Acceptance Angle	Aspect Ratio
1	2.97°	9.5
2	1.42°	20.1
3	0.98°	29.3

Collimator Case 3 (0.97º) Anterior Projection Images

(Based on 1st energy group)



TITAN



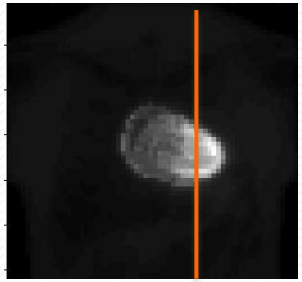
MCNP5

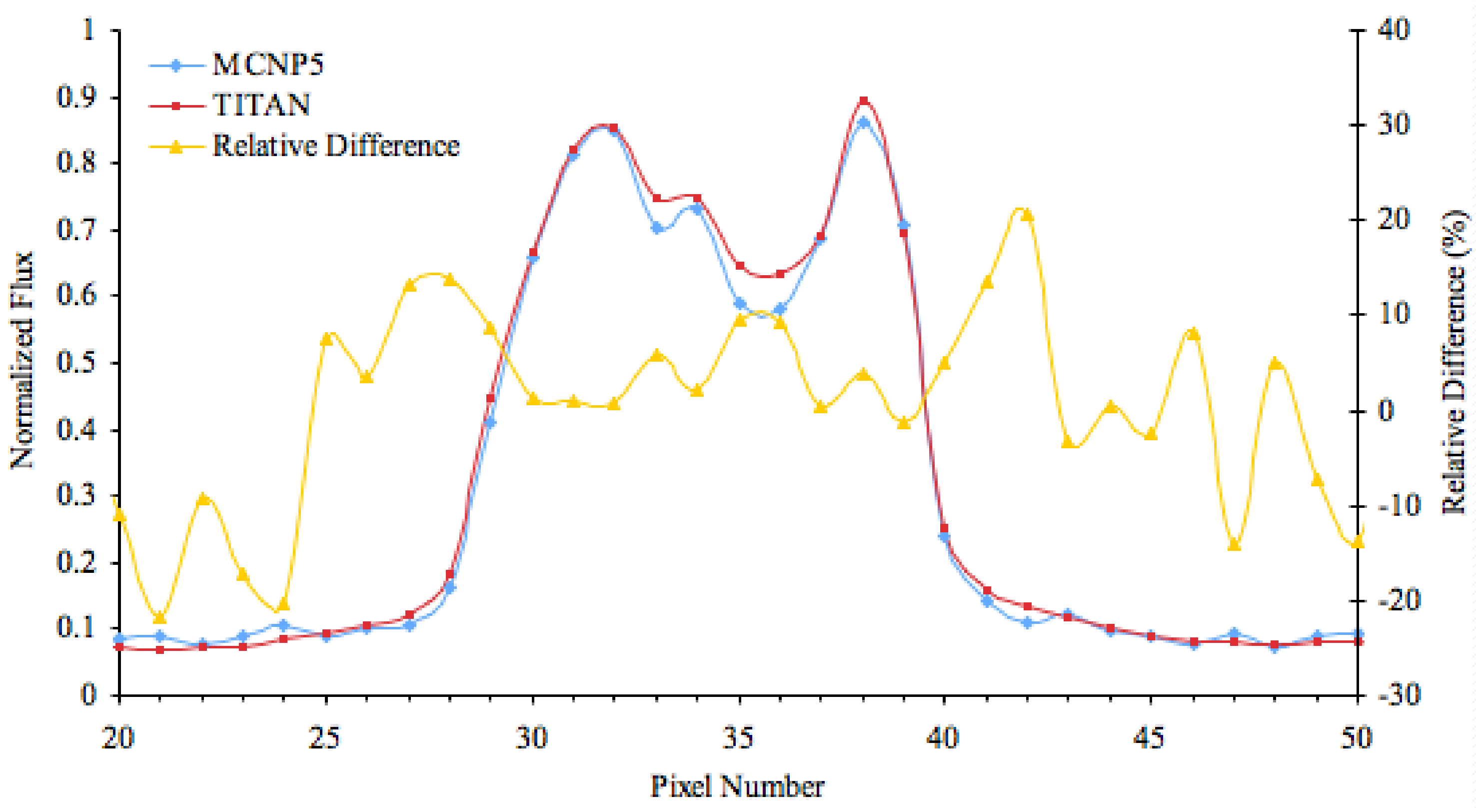
Maximum difference of TITAN results relative to MCNP5 results* in the heart for each collimator case

Case Number	Acceptance Angle (degrees)	Maximum Relative Difference (%)
1	2.97	21.3
2	1.42	11.9
3	0.98	8.3

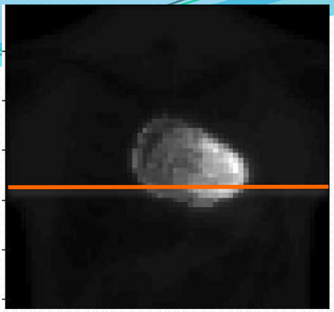
*All MCNP5 data had 1-σ uncertainty $\leq$3% in the heart

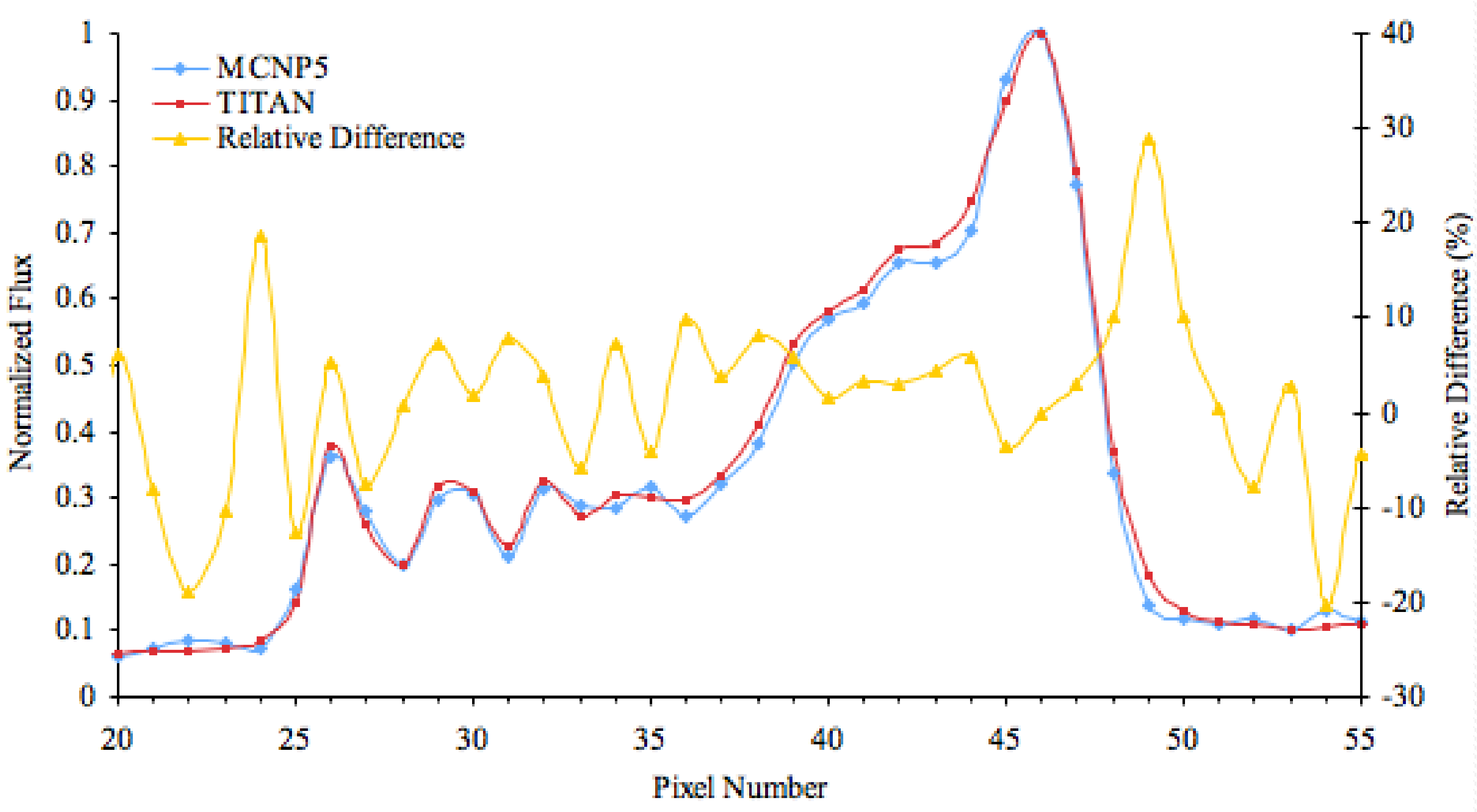
Profiles through column 44 of projection images





Profiles through row 33 of projection images





Timing

Case Number	Acceptance Angle (degrees)	Code		Speedup Factor (MCNP5/ TITAN)
		MCNP5 (min)*	TITAN (min)†	
1	2.97	313.8	0.82	382
2	1.42	1071.8	0.82	1304
3	0.98	2289.7	0.82	2787

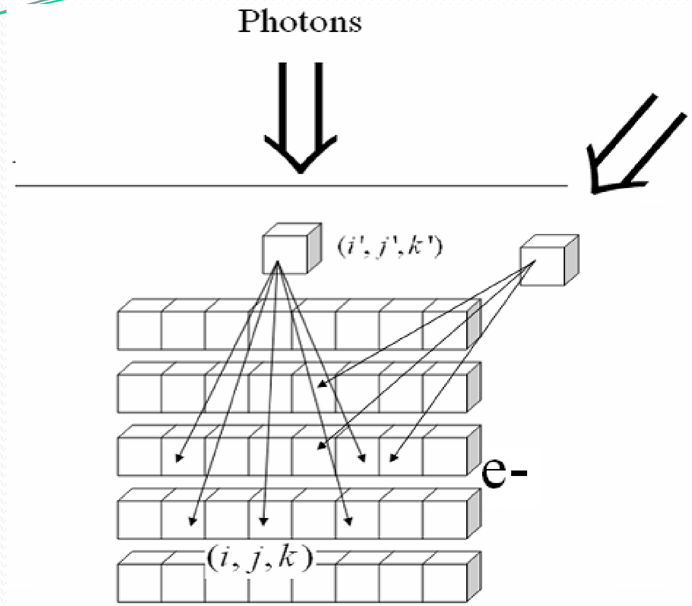
*Time to achieve 1-σ uncertainty of ≤3.0% in the heart
†180 projection angles

PENTRAN – Electron Dose Kernel-discrete ordinates (EDK-Sn)

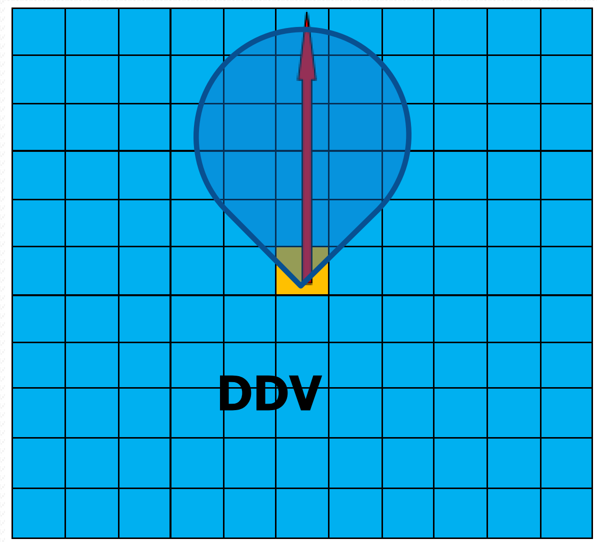
- EDK-Sn is developed for accurate and fast estimation of organ doses voxelized in the human body principally for applications in
  - High energy **external photon beam** therapy, accounting for both in-field and out-of-field doses.

A modern, digital medical linear accelerator (courtesy of Varian)

EDK-Sn Methodology



pre-determined photon energy groups in terms of the energy deposited in voxel (i, j, k) as a result of the incident primary photon beamlet in a given energy group g propagated from a Dose Driving Voxel, DDV(i', j', k')



1) Pre-compute (once) Electron Dose Fraction using the Monte Carlo MCNP5 code

$$EDF_g(i,j,k) = EDK_g(i,j,k) \Big/ \phi_{MC_g}(i',j',k')$$

Pre-computation of EDF's

- For a cube of 11x11x11 cm^3 and a mono-energetic beam of photons
- 8 MeV was partitioned into 16 even groups, and calculations performed for each energy interval using their mid-point value
- Three materials are considered including: soft tissue, bone and lung

Monte-Carlo Based Dose Kernels

2) Determine flux at the DDV as function of energy g using the PENTRAN code for a given beam of photons

3) Project *EDF* along the net current in DDV

4) Determine the dose rate

$$\dot{D}(i,j,k) = \sum_g \left(\sum_{\forall(i,j,k)} EDF_g(i,j,k)_S\right)\left(\phi(i^{'},j^{'},k^{'})_{S_N\,g}\right)\beta / M(i,j,k)$$

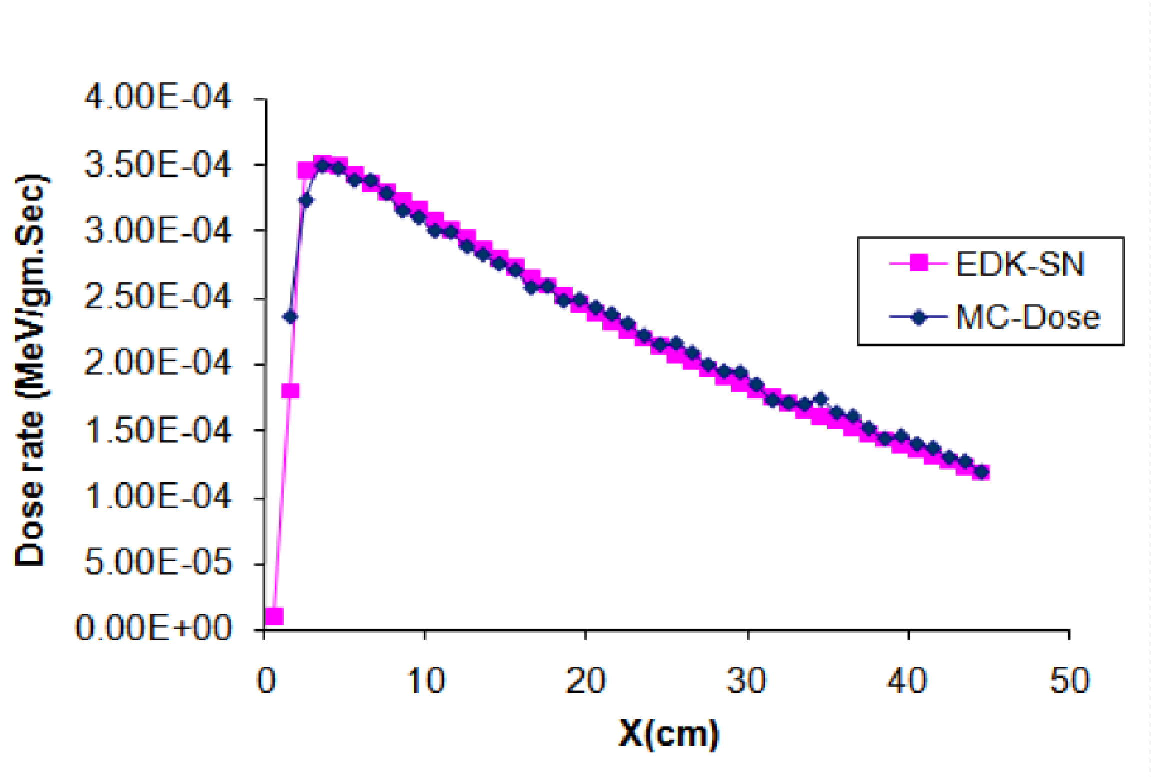
$EDF_g\,(i, j, k)$ - amount of energy deposited in voxel (i, j, k) in energy bin (s) per flux per source particle,

$M\,(i, j, k)$ - voxel mass

β - Meshing correction factor

Benchmarking

- slab phantoms using material specific absorbed dose kernels with 1 cm mesh densities. The dose rate in a soft-tissue phantom:



Human phantom (UF 15-year male)

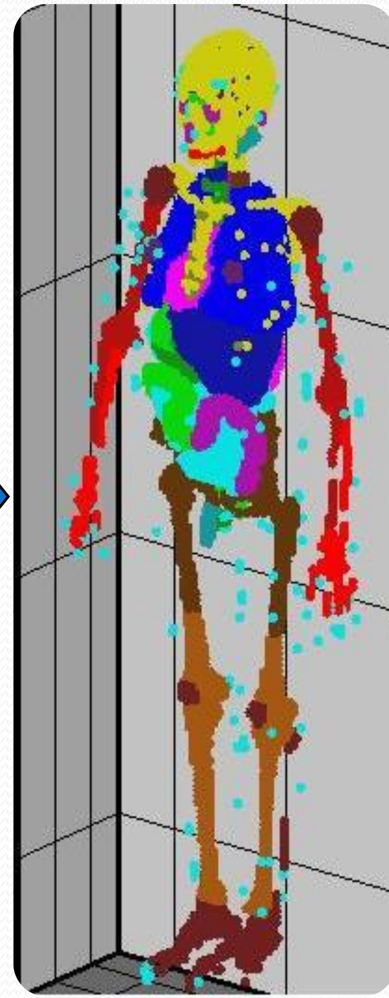
- Total dose delivered to the phantom from high energy volumetric ($20 \times 1 \times 17$ cm^3) flat weighted source [0, 8 MeV].

- 0-8 MeV was divided into 16 even groups, and 16-group cross-sections were generated using CPEX

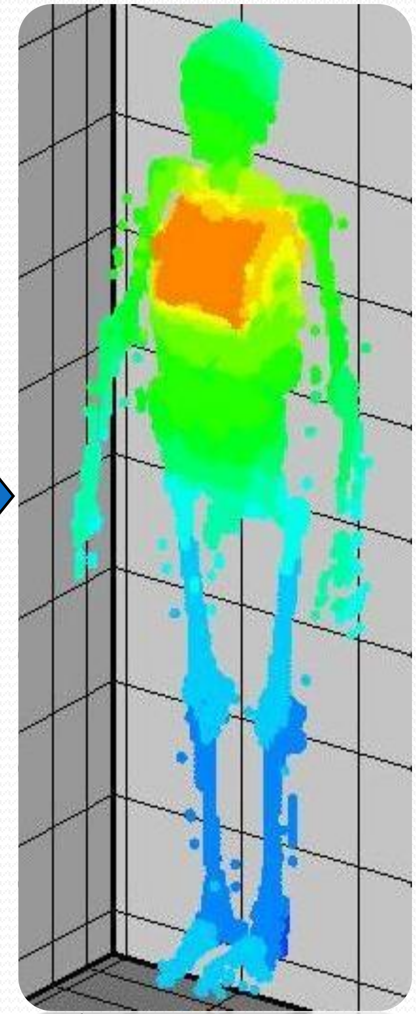
- The phantom, initially $2 \times 2 \times 2$ mm^3 ($302 \times 139 \times 836$ voxels), was down sampled to $1 \times 1 \times 1$ cm^3 ($60 \times 27 \times 167$ voxels), for total of 270,540 voxels

Simulation Methodology for Dose Computation

UF_15YR Nurbs Voxel Model

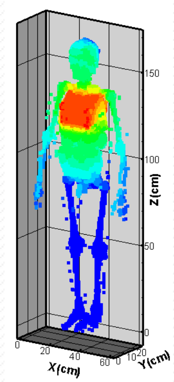


Phantom as a PENTRAN Input

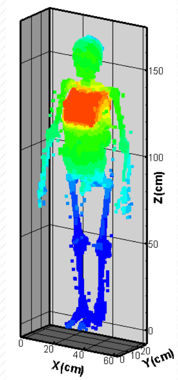


Phantom EDK-S_N Dose Distribution

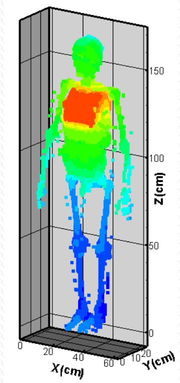
EDK-S_N Dose Computation for 15 Year Male



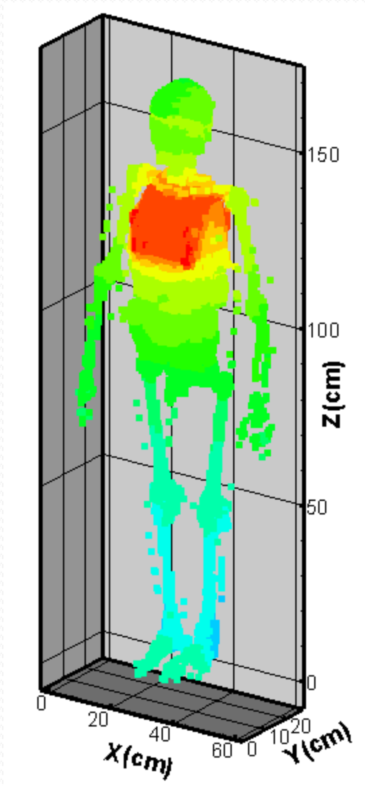
EG 1



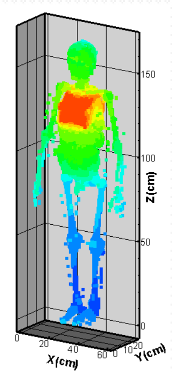
EG 4



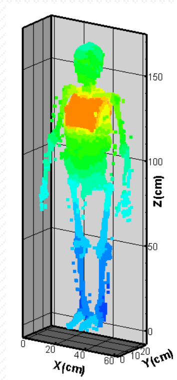
EG 7



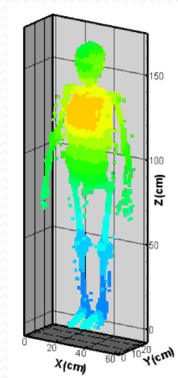
Total-Dose



EG 10



EG 13



EG 16

Comparison of organ absorbed dose rate (MeV/g.Sec) (EDK-S_N vs. MCNP) for test phantoms for a flat chest source of 8 MV X-ray [+]

Organ	MC(*F8) (MeV/g.Sec)	(2-sigma) MC Uncertainty	Sn-EDK (MeV/g.Sec)	(MC-EDK)/EDK
Right+ Left Lung	1.35E-01	6.80%	1.41E-01	4.56%
Pancreas	9.47E-05	4.14%	9.85E-05	4.02%
SI W	3.56E-05	4.00%	3.75E-05	5.43%
Spleen	1.11E-04	3.00%	1.18E-04	6.58%
Stomach W	1.86E-04	4.60%	1.94E-04	4.09%
Thyroid	1.41E-05	6.82%	1.38E-05	2.08%
Prostate	2.21E-08	44.00%	2.29E-08	3.62%

- **Above table reveals that all doses were comparable within a Monte Carlo (2σ) uncertainty, except for the spleen and prostate**
- **Additional MCNP simulation of ~40 h on 16 processors demonstrated the Monte-Carlo result was converging to the EDK-Sn result.**

Timing

- EDK-Sn calculation
  - Pre-calculation: 6 hrs per group for each tissue for achieving <0.1% 1-sigma (16 processors)
  - Routine calculation:
    - 1.5hr Sn (on 16 Processors)
    - 0.5hr EDK (on 16 processors)
- MCNP5 Monte Carlo calculation
    - 16 hr (on 16 Processors)
    - >> 40 hr for remote organs

Conclusions

- We have developed highly efficient and accurate algorithms for Medical Physics applications:
  - TITAN novel formulation for SPECT imaging
  - PENTRAN whole-body dose calculation from external photon beam