Unique Formulations in TITAN and PENTRAN for Medical Physics Applications

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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)*
- **CEPX5S** *(from SNL, prepares multi-groups Cross-section libraries)*

**S\textsubscript{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)*
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.
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

<table>
<thead>
<tr>
<th>Energy Group</th>
<th>Upper Bound (keV)</th>
<th>Lower Bound (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>154.55</td>
<td>126.45</td>
</tr>
<tr>
<td>2</td>
<td>126.45</td>
<td>98.35</td>
</tr>
<tr>
<td>3</td>
<td>98.35</td>
<td>10</td>
</tr>
</tbody>
</table>

➢ 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

Scattering not simulated

Detector: (Not simulated)

S<sub>N</sub> Solver

Phantom

Fictitious quadrature directions
Step 2 – Selection of fictitious directions

- Solve for angular flux along directions within acceptance angle

- Particles blocked by Collimator

- Acceptance angle

- Projection angle

- Circular Splitting
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

\[
S^{(e.s.,\text{scattering})}_{s, g' \rightarrow g, l} = \sum_{g'=1}^{G} \sum_{l=0}^{L} (2l + 1) \sum_{i=0}^{l} \left\{ P_{l} (\mu_{n}^{(\text{fic})}) \cdot \phi_{g', l}^{(\text{con})} + 2 \sum_{k=1}^{l} \frac{(l-k)!}{(l+k)!} \cdot P_{l}^{k} (\mu_{n}^{(\text{fic})}) \cdot \left[ \phi_{C, g', l}^{(\text{con})} \cdot \cos(k \phi_{n}^{(\text{fic})}) + \phi_{S, g', l}^{(\text{con})} \cdot \sin(k \phi_{n}^{(\text{fic})}) \right] \right\}
\]

- 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 determined

- 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

![Diagram of collimator cases with angles and aspect ratios](image)

<table>
<thead>
<tr>
<th>Case</th>
<th>Acceptance Angle</th>
<th>Aspect Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.97°</td>
<td>9.5</td>
</tr>
<tr>
<td>2</td>
<td>1.42°</td>
<td>20.1</td>
</tr>
<tr>
<td>3</td>
<td>0.98°</td>
<td>29.3</td>
</tr>
</tbody>
</table>
Collimator Case 3 (0.97°)  
Anterior Projection Images  
(Based on 1st energy group)
Maximum difference of TITAN results relative to MCNP5 results* in the heart for each collimator case

<table>
<thead>
<tr>
<th>Case Number</th>
<th>Acceptance Angle (degrees)</th>
<th>Maximum Relative Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.97</td>
<td>21.3</td>
</tr>
<tr>
<td>2</td>
<td>1.42</td>
<td>11.9</td>
</tr>
<tr>
<td>3</td>
<td>0.98</td>
<td>8.3</td>
</tr>
</tbody>
</table>

*All MCNP5 data had 1-σ uncertainty ≤3% in the heart
Profiles through column 44 of projection images
Profiles through row 33 of projection images
# Timing

<table>
<thead>
<tr>
<th>Case Number</th>
<th>Acceptance Angle (degrees)</th>
<th>Code</th>
<th>Speedup Factor (MCNP5/TITAN)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>MCNP5 (min)*</td>
<td>TITAN (min)†</td>
</tr>
<tr>
<td>1</td>
<td>2.97</td>
<td>313.8</td>
<td>0.82</td>
</tr>
<tr>
<td>2</td>
<td>1.42</td>
<td>1071.8</td>
<td>0.82</td>
</tr>
<tr>
<td>3</td>
<td>0.98</td>
<td>2289.7</td>
<td>0.82</td>
</tr>
</tbody>
</table>

*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, \(DDV(i', j', k')\)

\[
EDF_g (i, j, k) = \frac{EDK_g (i, j, k)}{\phi_{MC_g} (i', j', k')}
\]

1) Pre-compute (once) Electron Dose Fraction using the Monte Carlo MCNP5 code
Pre-computation of EDF’s

- For a cube of 11x11x11 cm³ 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

$$\dot{D}(i, j, k) = \sum_g \left( \sum_{\forall (i, j, k)} EDF_g (i, j, k) \right) \left( \phi(i', j', k') \right) \frac{\beta}{M(i, j, k)}$$

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

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

$\beta$ - 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 (20×1×17 cm³) 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 2×2×2 mm³ (302×139×836 voxels), was down sampled to 1×1×1 cm³ (60×27×167 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

- EG 10
- EG 13
- EG 16

Total-Dose
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:

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

- Above table reveals that all doses were comparable within a Monte Carlo (2\(\sigma\)) 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-\(S_N\) 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