Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo 2013
La Cité des Sciences et de l'Industrie, Paris, France, October 27-31, 2013

Performance of the New WCOS Technique for the TITAN SPECT Formulation

Katherine Royston & Alireza Haghighat

Nuclear Engineering Program, Virginia Tech, Arlington, Virginia, USA

VirginiaTech
Nuclear Engineering Program

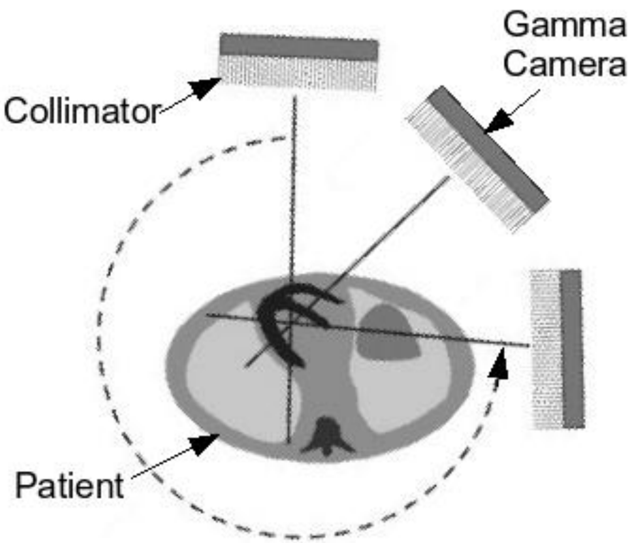
OUTLINE

- Research Objectives
- Introduction to SPECT
- The TITAN Code SPECT Formulation
- Development of the WCOS Algorithm
- Results – Accuracy & Parallel Performance
- Conclusions and Future Work

Research Objectives

- Exploit the advantages of deterministic codes over Monte Carlo methods
  - Statistical uncertainty
  - Computation time
- This work specifically seeks to:
  - Benchmark the TITAN code's collimator representation
  - Better comprehend sensitivity to parameters
  - Improve upon the collimator representation's accuracy
  - Examine the parallel behavior of the code

INTRODUCTION TO SPECT



- Single Photon Emission Computed Tomography
  - 17 million procedures in the US in 2010
  - Nuclear medicine imaging procedure used to examine myocardial perfusion, bone metabolism, thyroid function, etc.
  - *Functional* imaging modality
  - Radiopharmaceutical injected/ingested and localizes in a part of the body
  - Emitted radiation detected at a gamma camera to form 2D projection images at different angles
  - Collimator in front of the gamma camera provides spatial resolution
  - Projection images can be reconstructed to form a 3D image of the radionuclide distribution

The TITAN Code

- Deterministic transport code* to solve the linear Boltzmann equation (LBE)

$$H\psi = S \text{ in } V$$

$$H = \hat{\Omega}\cdot\nabla + \sigma_t(\vec{r},E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r},E' \rightarrow E,\hat{\Omega}' \rightarrow \hat{\Omega})$$

- Hybrid code allowing different solvers:
  - Discrete Ordinates (S_N) Method: discretize spatial domain into meshes (differencing scheme) and solve LBE in a discrete set of directions (quadrature set)
  - Characteristics Method (CM): discretize spatial domain into arbitrarily shaped regions and solve integral LBE along parallel directions (quadrature set)

*C. Yi and A. Haghighat, "A 3-D Block-Oriented Hybrid Discrete Ordinates and Characteristics Method," *Nucl. Sci. & Eng.*, **164**, pp. 221-247 (2010).

The TITAN SPECT Formulation

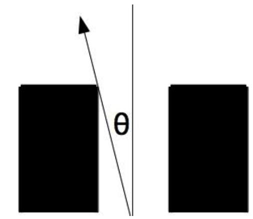
- Four-step hybrid S_N and simplified ray-tracing formulation:
  1. S_N transport calculation in the phantom with regular quadrature set
  2. Generation of fictitious quadrature set with circular ordinate splitting (COS) for a projection angle
  3. One extra transport sweep in the phantom with the fictitious quadrature set using the converged flux moments from *Step 1* to evaluate the scattering source:

$$S_s = \sum_{g'=1}^{G} \sum_{l=0}^{L} (2l+1) s_{s,g' \to g,l} \Big\{ P_l(m_n^{(fic)}) \cdot f_{g',l}^{(con)} + 2 \sum_{k=1}^{l} \frac{(l-k)!}{(l+k)!} P_l^k(m_n^{(fic)}) \cdot \Big[j_{C,g',l}^{k,(con)} \cdot \cos(k j_n^{(fic)}) + j_{S,g',l}^{k,(con)} \cdot \sin(k j_n^{(fic)}) \Big] \Big\}$$

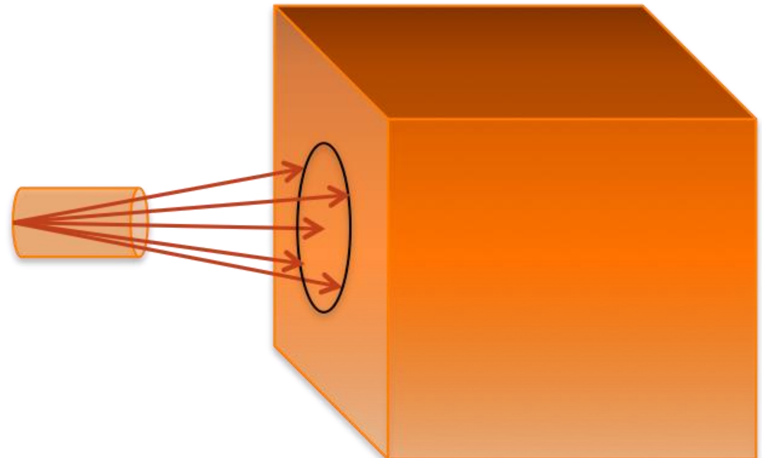
  4. Simulation of the projection image with the fictitious quadrature set using the simplified ray-tracing formulation outside of the phantom

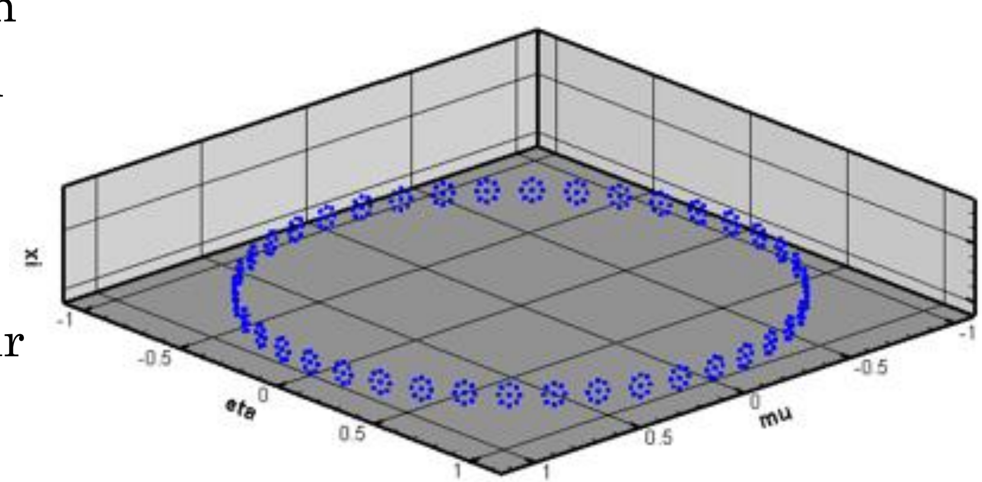
- *Step 1* is completed once and *Steps 2-4* are then repeated for each projection angle desired.

THE TITAN SPECT FORMULATION



- Circular Ordinate Splitting (COS)
  - TITAN feature to approximate the collimator
  - Represents an acceptance angleθabout the detector normal within which incoming photons reach the detector
  - Split directions made on a circle (or concentric circles) centered on the original projection direction
  - Backward ray-tracing from collimator to phantom surface
  - Average over original and split directions to approximate collimator blur





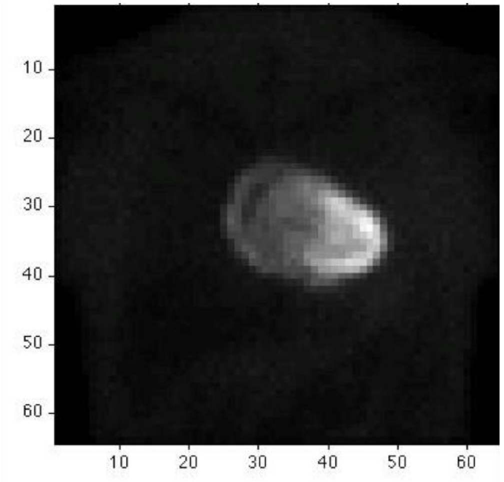
VirginiaTech
Nuclear Engineering Program

Previously Completed Work: Comparing TITAN Results for Different Collimators

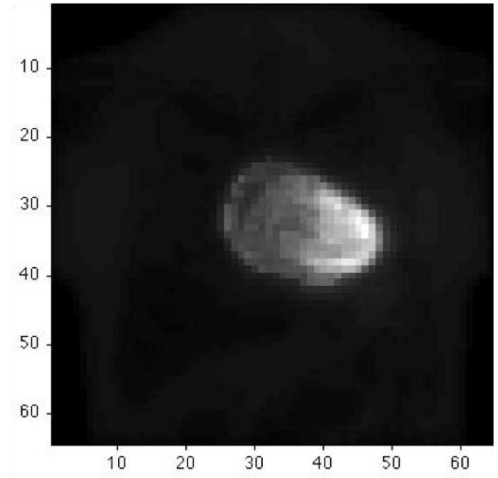
- TITAN comparison with MCNP5
  - using the NCAT voxel phantom
  - considering different collimator acceptance angles

Acceptance Angle	Maximum relative difference
2.97°	21.3%
1.42°	11.9%
0.98°	8.3%

*All MCNP5 data had 1-σ uncertainty ≤3% in the heart



MCNP5

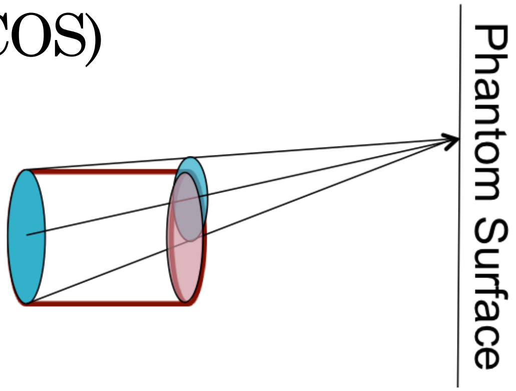


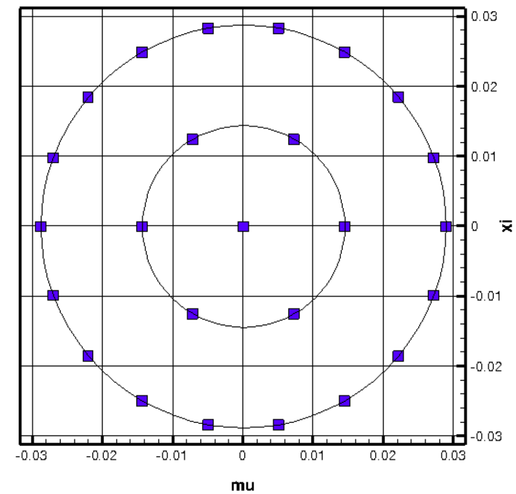
TITAN

Royston *et al.*, *Progress in Nuclear Science and Technology*, 2, 2011

THE WCOS ALGORITHM

- Weighted Circular Ordinate Splitting (WCOS)
  - Developed to improve upon the COS collimator representation (especially, for collimators with small aspect ratios)
  - Split directions used to calculate a geometry-based weighted average
    1. Project detector surface area to front of collimator
    2. Weight angular flux at phantom surface by overlapping area
  - Number of split directions in concentric circles scaled to area
  - User specifies collimator parameters (determines radius of outermost circle) and splitting order (i.e., number of directions on innermost circle)

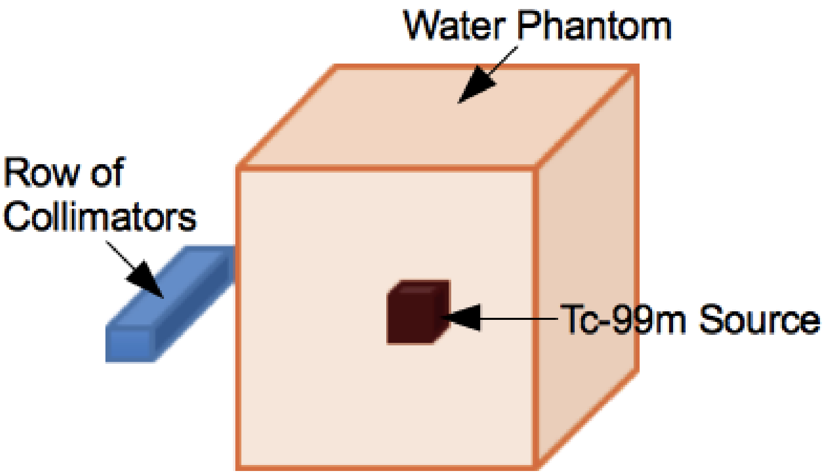




Example: splitting order of 6 with 2 circles

APPLICATION

- Cube of water with a cube of Tc-99m (140.5 keV) at the center
- Cross sections generated using the CEPXS code (20% energy window)
- Multigroup MCNP5 utilizing the CEPXS cross sections
- Model a Low Energy General Purpose (LEGP) collimator & a Low Energy High Sensitivity (LEHS) collimator



Collimator	Acceptance Angle	Detector Pixel Size	Aspect Ratio
LEGP	1.65°	0.210 cm	17.4:1
LEHS	4.29°	0.340 cm	6.7:1

RESULTS

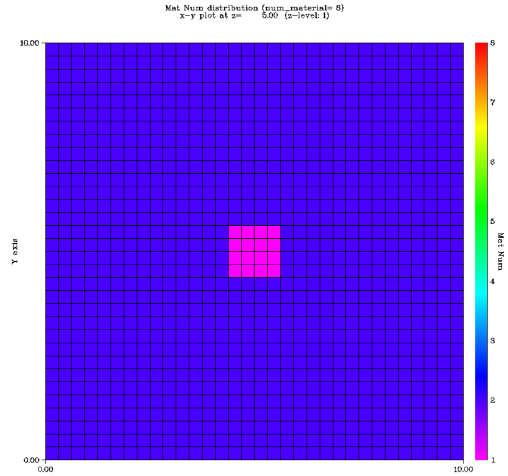
1. Phantom Modeling – Mesh and Quadrature Studies

2. Comparison with Monte Carlo

3. Computation Time & Parallel Performance

Results: Phantom Modeling – Mesh & Quadrature Studies

Mesh	Number of Meshes	Mesh Size
Coarse	16x16x16	0.6250 cm
Base	32x32x32	0.3125 cm
Fine	64x64x64	0.15625 cm



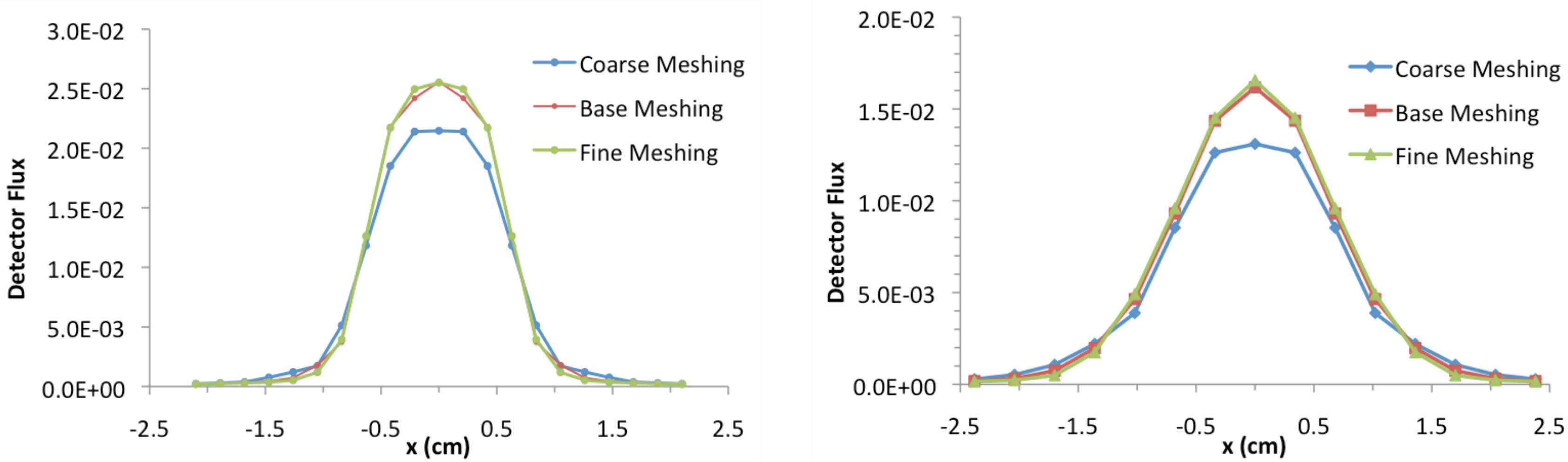
Base Meshing

VirginiaTech
Nuclear Engineering Program

Results: Phantom Modeling – Mesh & Quadrature Studies

LEGP collimator (1.65°)

LEHS collimator (4.29°)



Choose the fine meshing for LEGP and the base meshing for LEHS

Virginia Tech
Nuclear Engineering Program

Results: Phantom Modeling – Mesh & Quadrature Studies

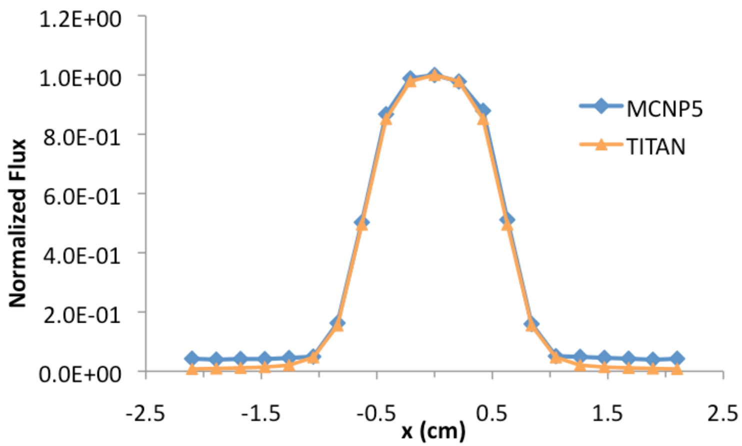
Difference in TITAN detector flux for LEHS collimator

Quadrature Order	Difference Relative to S_{60}	
	Average	Maximum
S_6 (48 directions)	-9.28%	-35.46%
S_{12} (168 directions)	-1.85%	-6.54%
S_{20} (440 directions)	-0.26%	-1.33%
S_{40} (1680 directions)	-0.02%	-0.06%

- Same behavior observed for LEGP collimator
- S_{20} level-symmetric quadrature used in all following results

Results: Comparison with Monte Carlo

- LEGP Collimator (1.65°)
  - MCNP5 1σ uncertainties 0.8-3.6%
  - For normalized fluxes >0.1, average difference of 2.3%
  - No significant difference between original COS and WCOS techniques

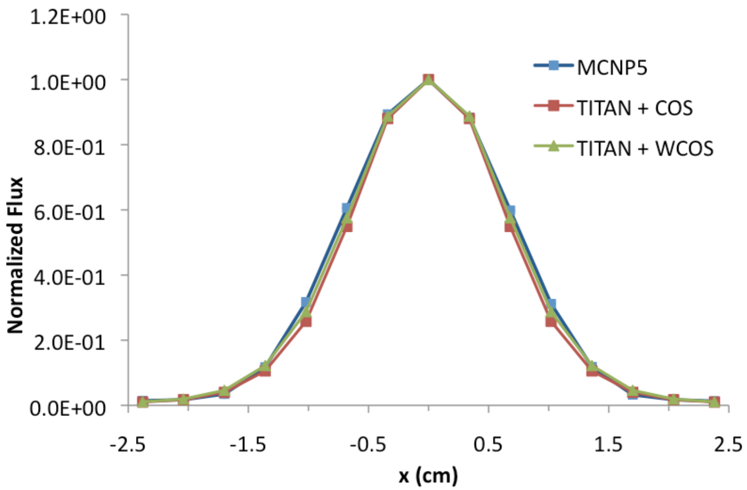


FWHM*		Difference
MCNP5	TITAN	
1.27 cm	1.25 cm	-1.2%

*Full Width at Half Maximum

Results: Comparison with Monte Carlo

- LEHS Collimator (4.29°)
  - MCNP5 1σ uncertainties 0.4-4.4%
  - The WCOS technique improves the TITAN solution



Code	FWHM (Relative Difference)	Average Relative Difference
MCNP5	1.60 cm	-
TITAN + COS	1.47 cm (-7.9%)	8.5%
TITAN + WCOS	1.54 cm (-4.0%)	3.8%

Results: Computation Time & Parallel Performance

- All studies were completed on a dedicated PC-cluster:
  - Intel Xeon 2.4 GHz processors
  - 3 compute nodes with 8 processors cores per node
  - 64 GB per node (8 GB per core)
  - 10 Gb network
- Detector dimensions chosen to cover model:
  - LEGP collimator – 42 by 42 detector array
  - LEHS collimator – 30 by 30 detector array
- Parallel Performance Metrics:

Parallel Speedup	$S_p = \frac{\text{Serial Computation Time}}{\text{Parallel Computation Time}}$
Parallel Efficiency	$E_p = S_p / P$
Parallelizable Fraction	$f_p = \frac{P(1-S_p)}{S_p(1-P)}$

P = number of processor cores

Results: TITAN-WCOS Computation Time & Parallel Performance

Computation times for LEGP Collimator Case with increasing number of projection images:

Serial Computation Times

Projections	S_N Time (s)	Projection Time (s)	Total Time (s)
4	435	25	455
45	-	298	729
90	-	557	985

Parallel Computation Times on 8 Processor Cores

Projections	S_N Time (s)	Projection Time (s)	Total Time (s)	Parallel Speedup
4	56	6	65	7.0
45	-	38	94	7.7
90	-	76	132	7.5

VirginiaTech
Nuclear Engineering Program

Results: TITAN-WCOS Computation Time & Parallel Performance

	Number of Processor Cores	Parallel Speedup	Parallel Efficiency	Parallelizable Fraction
1 Node	2	1.95	0.98	0.97
	4	3.87	0.97	0.99
	8	7.47	0.93	0.99
2 Nodes	12	10.97	0.91	0.99
	16	12.44	0.78	0.98
3 Nodes	24	17.07	0.71	0.98

Results for 90 projection angles

Results: Comparison of TITAN with MCNP5 Computation Time

Computation Times on 8 Processors

Collimator	MCNP5*		TITAN†
	Maximum Uncertainty (1σ)	Computation Time	Computation Time
LEGP	15.4%	46.9 hrs	132 sec
LEHS	9.9%	21.4 hrs	14 sec

*Time with source biasing towards a single detector array

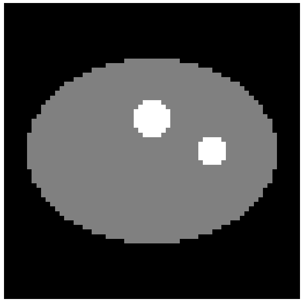
†Time to generate 90 projection images

Conclusions

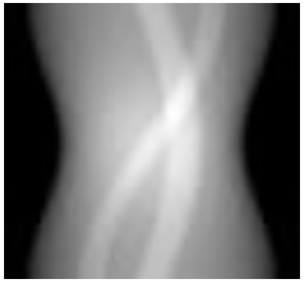
- The weighted circular ordinate splitting (WCOS) collimator representation has been implemented in the TITAN code
- Algorithm sensitivity to meshing & quadrature order studied
- Solutions benchmarked against MCNP5 for two collimator cases showed excellent agreement
- Parallel behavior was studied and a parallelizable fraction of 98% was found
- Computation times were shown to be on the order of minutes for TITAN and hours/days for MCNP5

Ongoing & Future Work

- An iterative reconstruction algorithm is being developed to utilize TITAN to model attenuation and scatter in the patient during the forward projection step



- Currently testing reconstruction of a 2-dimensional phantom using TITAN



Acknowledgment

The authors would like to thank Dr. Ce Yi of Georgia Tech for his assistance with the TITAN code

Thank you for your Attention!

Questions?

VirginiaTech
Nuclear Engineering Program