

MRT Methodologies for Real-Time Simulation of Nuclear Systems

Prof. Alireza Haghghat

Virginia Tech

Virginia Tech Transport Theory Group (VT³G)

Director of Nuclear Engineering and Science Lab (NSEL) at Arlington
Nuclear Engineering Program, Mechanical Engineering Department



Completed June 2011

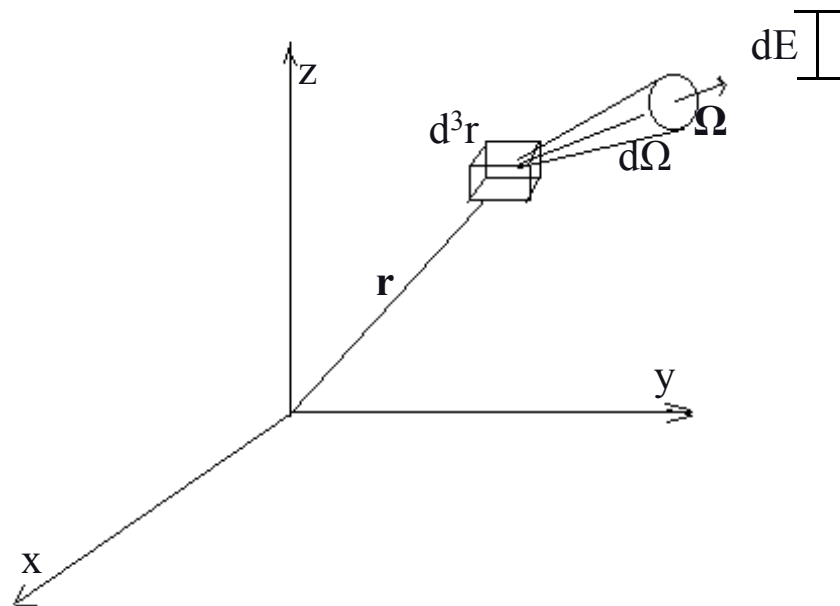
Mechanical and Aerospace Engineering Department, Sept 24-25, 2015

Particle Transport Theory

Objective

Determine the expected number of particles in a phase space $(d^3rdEd\Omega)$ at time t :

$$n(\vec{r}, E, \hat{\Omega}, t)d^3rdEd\Omega$$



Number density is used to determine angular flux/current, scalar flux and current density, partial currents, and reaction rates.

Simulation Approaches

- **Deterministic Methods**

- Solve the linear Boltzmann equation to obtain the expected flux in a phase space

- **Statistical Monte Carlo Methods**

- Perform particle transport experiments using random numbers (RN's) on a computer to estimate average properties of a particle in phase space

Deterministic – Linear Boltzmann Equation

- **Integro-differential form**

$$\begin{aligned}
 & \text{streaming} \quad \hat{\Omega} \cdot \nabla \Psi(\vec{r}, E, \hat{\Omega}) + \sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}) = \\
 & \quad \quad \quad \text{collision} \\
 & \quad \quad \quad \text{scattering} \\
 & \int_0^{\infty} dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \Psi(\vec{r}, E', \hat{\Omega}') + \\
 & \quad \quad \quad \text{fission} \quad \quad \quad \text{Independent source} \\
 & \frac{\chi(E)}{4\pi} \int_0^{\infty} dE' \int_{4\pi} d\Omega' \nu \sigma_f(\vec{r}, E') \Psi(\vec{r}, E', \hat{\Omega}') + S(\vec{r}, E, \hat{\Omega})
 \end{aligned}$$

- **Integral form**

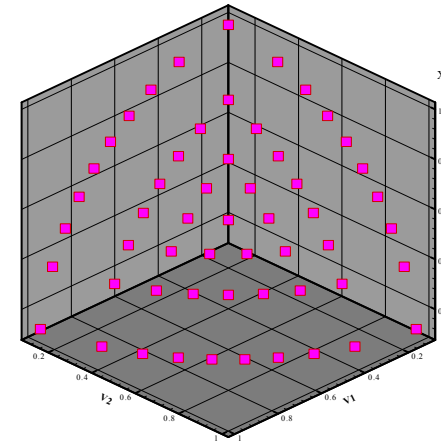
$$\psi(\vec{r}, E, \hat{\Omega}) = \int_0^R d|\vec{r} - \vec{r}'| Q(r') e^{-\tau_E(\vec{r}, \vec{r}')} + \psi(\vec{r}_s, E, \hat{\Omega}) e^{-\tau_E(\vec{r}, \vec{r}_s)}$$

Integro-differential - Solution Method

- **Angular variable: Discrete Ordinates (Sn) method:**

A discrete set of directions $\{ \hat{\Omega}_m \}$
and associated weights $\{ w_m \}$ are selected

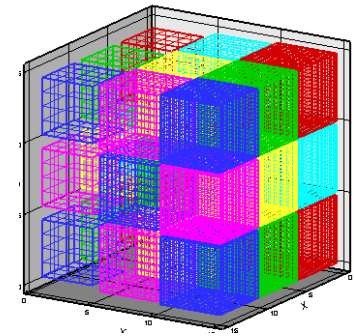
$$\hat{\Omega}_m \cdot \nabla \Psi(\vec{r}, E, \hat{\Omega}_m) + \sigma(\vec{r}, E) \Psi(\vec{r}, E, \hat{\Omega}_m) = q(\vec{r}, E, \hat{\Omega}_m)$$



- **Spatial variable**

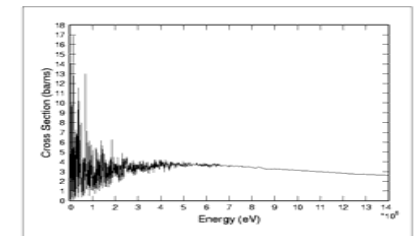
Integrated over fine meshes using FD or FE methods

$$\Psi_{m,g,A} = \frac{\int d^3r \Psi_{m,g}(\vec{r})}{\Delta V_{ijk}}$$



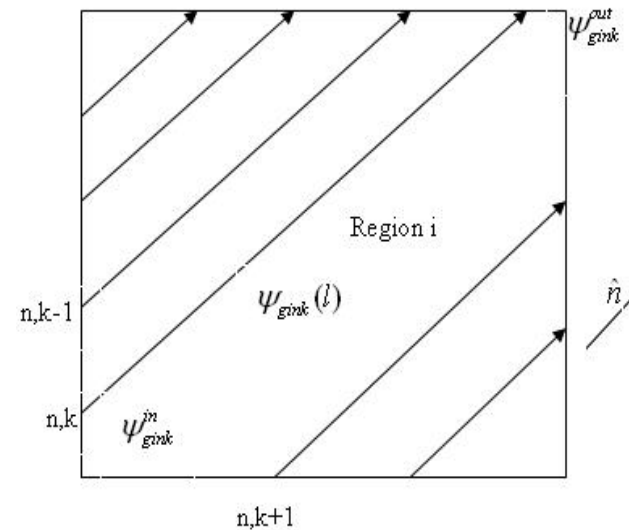
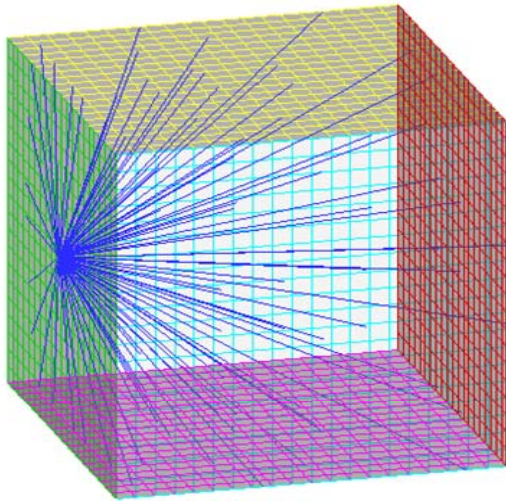
- **Energy variable**

Integrate over energy intervals to prepare multigroup cross sections, σ_g



Integral - Solution method

- **Method of Characteristic (MOC):** Model is partitioned into **coarse meshes** and transport equation is solved along the characteristic paths (k) (parallel to each discrete ordinate (n)), filling the mesh, and averaged



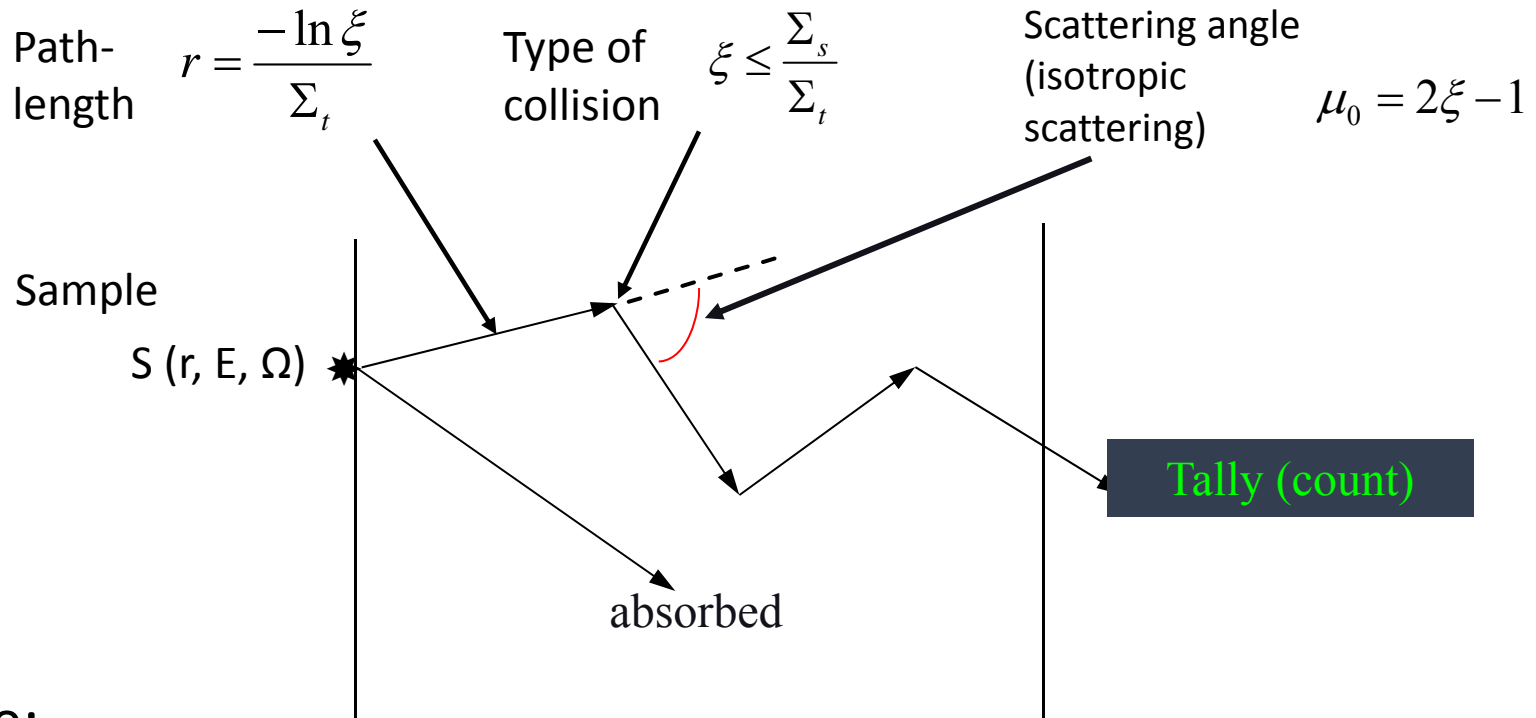
$$\psi_{g,m,i,k}(t_{m,i,k}) = \psi_{g,m,i,k}(0) \exp(-\sigma_{g,i} t_{m,i,k}) + \frac{Q_{g,m,i}}{\sigma_{g,i}} (1 - \exp(-\sigma_{g,i} t_{m,i,k}))$$

Deterministic - Issues/Challenges/Needs

- Robust numerical formulations (e.g., adaptive differencing strategy)
- Algorithms for improving efficiency (i.e., acceleration techniques – synthetic formulations and pre-conditioners)
- Use of advanced computing hardware & software environments
- Pre- and post-processing tools
- Multigroup cross section preparation
- Benchmarking

Monte Carlo Methods

- Perform an experiment on a computer; “exact” simulation of a physical process



Issue:

Precise expected values; i.e., small relative uncertainty, $R_{\bar{x}} = \frac{\sigma_{\bar{x}}}{\bar{x}}$

Variance Reduction techniques are needed for real-world problems!

Deterministic vs. Monte Carlo

Item	Deterministic	MC
Geometry	Discrete/ Exact	Exact
Energy treatment – cross section	Discrete	Exact
Direction	Discrete/ Truncated series	Exact
Input preparation	Difficult	simple
Computer memory	Large	Small
Computer time	Small	Large
Numerical issues	Convergence	Statistical uncertainty
Amount of information	Large	Limited
Parallel computing	Complex	Trivial

Why not MC only?

- Because of the difficulty in obtaining **detail information** with **reliable statistical** uncertainty in a **reasonable time**
- **Example situations**
 - Real-time simulations
 - Obtaining energy-dependent flux distributions,
 - Time-dependent simulations,
 - Sensitivity analysis,
 - Determination of uncertainties

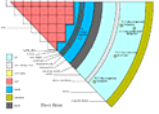
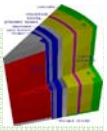
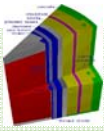
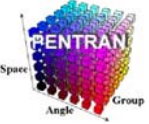
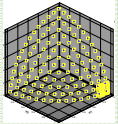
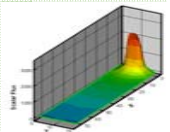
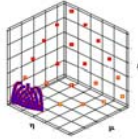
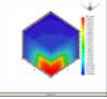

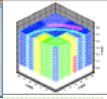



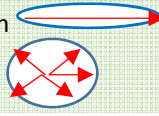
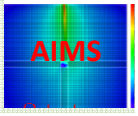
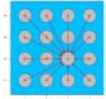

Why not use advanced hardware?

- VT³G has developed vector and parallel algorithms, and developed two large codes: PENTRAN (1996) and TITAN (2004)

Why not hybrid methods?

- **Deterministic-deterministic** (differencing schemes, different numerical formulations, generation of multigroup cross sections, generation of angular quadratures, acceleration techniques) (VT³G has developed various algorithms; a few have been implemented in PENTRAN and TITAN)
- **Monte Carlo-deterministic** (variance reduction with the use of deterministic adjoint) (VT³G has developed CADIS, A³MCNP in 1997; CADIS has become popular recently!)

VT³G Milestones & Contributing Current/Former Students (1986-2015)

1986-1989	<ul style="list-style-type: none"> Vector computing of 1-D Sn spherical geometry algorithm Development an adjoint methodology for simulation TMI-2 reactor 		Prof. Haghighat	
1989-1992	<ul style="list-style-type: none"> Vector and parallel processing of 2-D Sn algorithms Simulation of Reactor Pressure Vessel (RPV) 		Prof. R. Mattis, Pitt. Prof. B. Petrovic, GT	
1992-1994	<ul style="list-style-type: none"> Parallel processing of 2-D Sn algorithms & Acceleration methods Determination of uncertainties in the RPV transport calculations 		Dr. M. Hunter, W Prof. B. Petrovic, GT	
1994-1995	<ul style="list-style-type: none"> 3-D parallel Sn Cartesian algorithms Monte Carlo for Reactor Pressure Vessel (RPV) benchmark using Weight-window generator; deterministic benchmarking of power reactors 		Dr. G. Sjoden, DOD Dr. J. Wagner, ORNL	
1995-1997	<ul style="list-style-type: none"> Directional Theta Weight (DTW) differencing formulation PENTRAN (Parallel Environment Neutral Particle TRANsport) code system CADIS (Consistent Adjoint Driven Importance Sampling) formulation for Monte Carlo Variance Reduction A³MCNP (Automated Adjoint Accelerate MCNP) 		Dr. B. Petrovic Dr. G. Sjoden, DOD Dr. J. Wagner, ORNL	
1997-2001	<ul style="list-style-type: none"> Parallel Angular & Spatial Multigrid acceleration methods for Sn transport Hybrid algorithm for PGNNA device PENMSH & PENINP for mesh and input generation of PENTRAN Ordinate Splitting (OS) technique for modeling a x-ray CT machine 		Dr. V. Kucukboyaci, W Dr. B. Petrovi, GT Prof. Haghighat Prof. Hgahighat	
2001-2004	<ul style="list-style-type: none"> Simplified Sn Even Parity (SSn-EP) algorithm for acceleration of the Sn method RAR (Regional Angular Refinement) formulation Pn-Tn angular quadrature set FAST (Flux Acceleration Simplified Transport) PENXMSH, An AutoCad driven PENMSH with automated meshing and parallel decomposition CPXSD (Contributon Point-wise cross-section Driven) for generation of multigroup libraries 		Dr. G. Longonil, PNNL Dr. A. Patchimpattapong, IAEA Dr. A. Alpan, W	  
2004-2007	<ul style="list-style-type: none"> TITAN hybrid parallel transport code system & a new version of PENMSH called PENMSHXP ADIES (Angular-dependent Adjoint Driven Electron-photon Importance Sampling) code system 		Dr. C. Yi, GT Dr. B. Dionne, ANL	
2007-2011	<ul style="list-style-type: none"> INSPECT-S (Inspection of Nuclear Spent fuel-Pool Calculation Tool ver. Spreadsheet), a MRT algorithm TITAN fictitious quadrature set and ray-tracing for SPECT (Single Photon Emission Computed Tomography) FMBMC-ICEU (Fission Matrix Based Monte Carlo with Initial source and Controlled Elements and Uncertainties) 		W. Walters, PhD Cand. Dr. C. Yi, GT Dr. M. Wenner, W	
2011-2013	<ul style="list-style-type: none"> New WCOS (Weighted Circular Ordinated Splitting) Technique for the TITAN SPECT Formulation Adaptive Collision Source (ACS) for Sn transport AIMS (Active Interrogation for Monitoring Special-nuclear-materials), a MRT algorithm 		K. Royston, PhD Cand. W. Walters, PhD Cand.	
2014-2015	<ul style="list-style-type: none"> TITAN-SDM - includes Subgroup Decomposition Method for multigroup transport calculation TITAN-IR - TITAN with iterative image Reconstruction for SPECT RAPID - Real-time Analysis for spent fuel Pool <i>in situ</i> detection 		N. Roskoff, PhD Stud. K. Royston, PhD Cand. W. Walters, PhD Cand.	

Remarks

- Particle transport-based methodologies are need for real-time simulation
- Particle transport codes, even those parallel with hybrid algorithms, are **slow because of large number of unknowns**

Development of Transport Formulations for Real-Time Applications

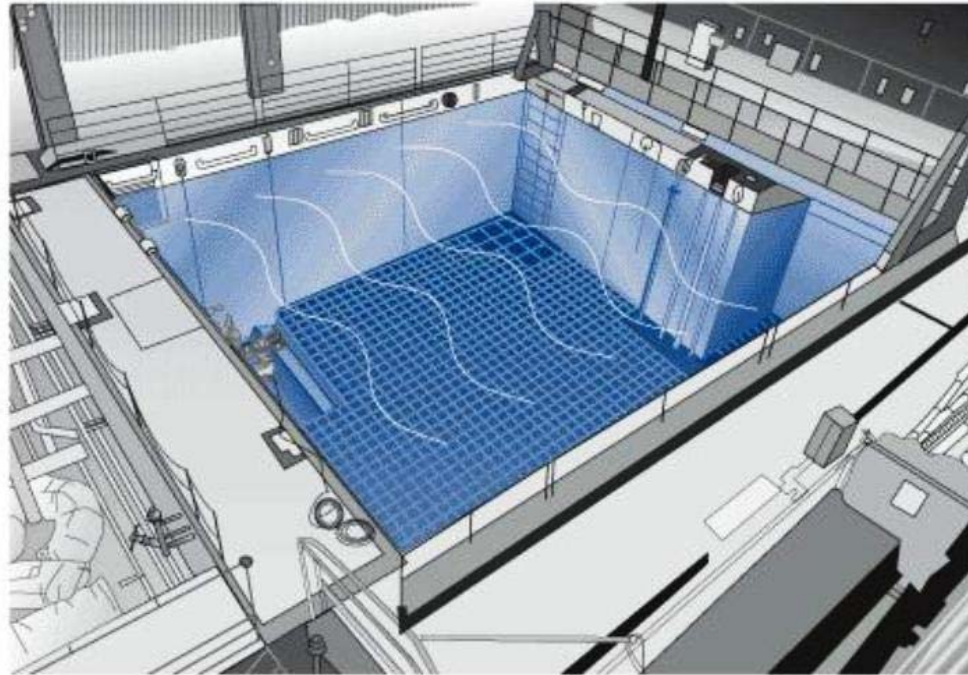
- *Physics-Based* transport methodologies are needed:
- Developed *Multi-stage, Response-function Transport (MRT) methodology*
 - Based on problem physics **partition** a problem into **stages** (sub-problems),
 - For each stage employ response method and/or adjoint function methodology
 - Pre-calculate response-function or adjoint-function using an accurate and fast transport code
 - Solve a linear system of equations to couple all the stages

Examples for *MRT Algorithms*

- **Nondestructive testing:** Optimization of the Westinghouse's PGNNA active interrogation system for detection of RCRA (Resource Conservation and Recovery Act) (e.g., lead, mercury, cadmium) in waste drums (partial implementation of MRT; 1999)
- **Nuclear Safeguards:** Monitoring of spent fuel pools for detection of fuel diversion (2007) (funded by LLNL)
- **Nuclear nonproliferation:** Active interrogation of cargo containers for simulation of special nuclear materials (SNMs) (2013) (in collaboration with GaTech)
- **Spent fuel safety and security:** Real-time simulation of spent fuel pools for determination of eigenvalue, subcritical multiplication, and material identification (partly funded by I²S project, led by GaTech) (Ongoing)
- **Image reconstruction for SPECT (Single Photon Emission Computed Tomography):** Real-time simulation of an SPECT device for generation of project images using an MRT methodology and Maximum Likelihood Estimation Maximization (MLEM) (filed for a patent, June 2015)

Real-time simulations for commercial spent fuel pools

Criticality Safety, Nonproliferation & Safeguards applications



Background

- **Standard approach - Full Monte Carlo calculations face difficulties in this area**
 - Convergence is difficult due to low coupling between regions (due to absorbers)
 - Convergence can also be difficult to detect
 - Computation times are very long, especially to get detailed information
 - Changing pool configuration requires complete recalculation
- **Fission Matrix (FM) approach – It can address the above issues**
 - Fission matrix coefficients are pre-calculated using Monte Carlo
 - Computation times are much shorter, with no convergence issues
 - Detailed fission distributions are obtained at pin level
 - Changing pool assembly configuration does not require new pre-calculations
 - No additional Monte Carlo

Derivation of Fission Matrix (FM) Formulation

- Eigenvalue formulation in operator form is expressed by

$$H\psi(\bar{p}) = \frac{1}{k} F\psi(\bar{p})$$

Where,

$$\bar{p} = (\bar{r}, E, \hat{\Omega})$$

$$H = \hat{\Omega} \cdot \nabla + \sigma_t(\bar{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\bar{r}, E' \rightarrow E, \mu_0)$$

$$F = \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \nu \sigma_f(\bar{r}, E')$$

FM Derivation (cont)

- We may rewrite above equation as

$$S(\bar{p}) = \frac{1}{k} AS(\bar{p})$$

Where,

$$S = \tilde{F}\psi, \quad A = \tilde{F}H^{-1}\chi, \quad \&$$

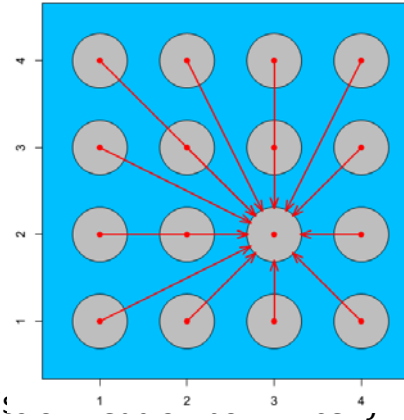
$$\tilde{F} = \frac{1}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' v\sigma_f(\bar{r}, E')$$

Fission Matrix (FM) Formulation

- Eigenvalue

$$F_i = \frac{1}{k} \sum_{j=1}^N a_{i,j} F_j$$

- k is eigenvalue
- F_j is fission source, S_j is fixed source in cell j
- $a_{i,j}$ is the number of fission neutrons produced in cell i due to a fission neutron born in cell j .



- Subcritical multiplication

$$F_i = \sum_{j=1}^N (a_{i,j} F_j + b_{i,j} S_j^{Intrinsic}),$$

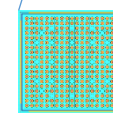
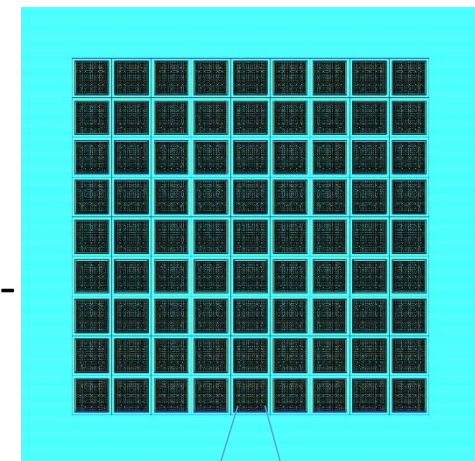
$$M = \frac{\sum_{j=1}^N (F_j + S_j^{intrinsic})}{\sum_{j=1}^N S_j^{intrinsic}}$$

- $b_{i,j}$ is the number of fission neutrons produced in cell i due to a source neutron born in cell j .

Developed a Multi-stage methodology for determination of FM coefficients

- As the computational size (for I²S reactor design)
 - $N = 9 \times 9 \times 336 = 27,216$ total fuel pins/ fission matrix cells
 - Considering 24 axial segments per rod, then
 - $N = 653,184$
- Standard FM would require $N = 653,184$ separate fixed-source calculations to determine the coefficient matrix
 - A matrix of size $N \times N = 4.26649E+11$ total coefficients (> 3.4 TB of memory is needed)
- The standard approach is clearly NOT feasible
- We have developed a multi-stage approach to obtain detailed FM coefficients (*in the process of filing for a patent*)

9x9 array of assemblies in a pool



Assembly with 19x19 lattice;
25 positions are reserved for control rods

RAPID tool

- **Developed the RAPID (Real-time Analysis spent fuel Pool *In situ* Detection) tool for determination of**
 - Eigenvalue
 - Subcritical multiplication
 - Pin-wise, axial fission density
- With application to
 - Criticality safety
 - Safeguards
 - Nonproliferation and materials accountability

RAPID code system - Structure

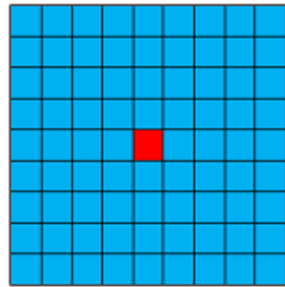
Pre-Calculation (one time):

1. Burnup Calculation – to obtain material composition
2. Fission Matrix Coefficient Generation

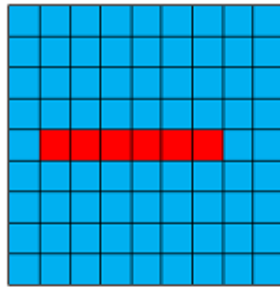
Real-time Analysis:

1. Run Fission Matrix Code
2. Process Results

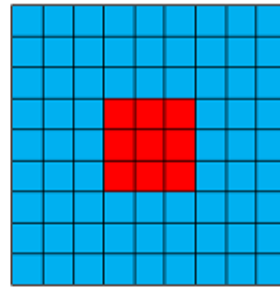
Test Problems (9x9 assemblies)



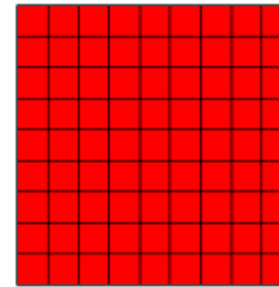
(a) Case 1



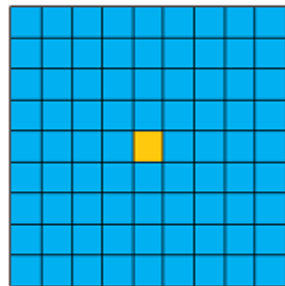
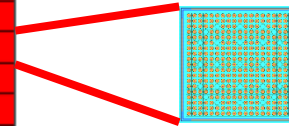
(b) Case 2



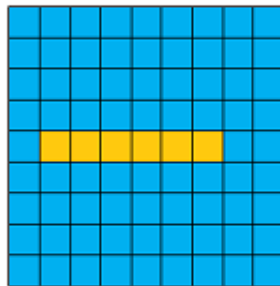
(c) Case 3



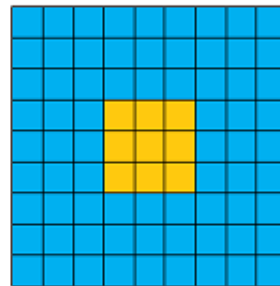
(d) Case 4



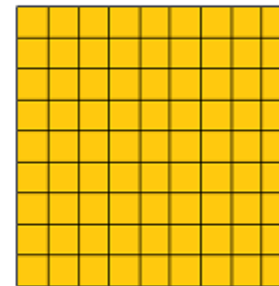
(e) Case 5



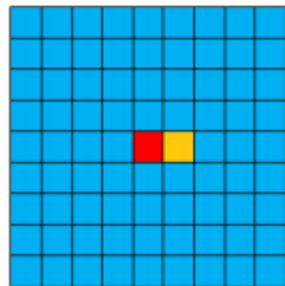
(f) Case 6



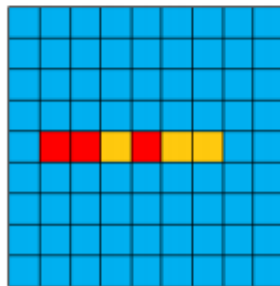
(g) Case 7



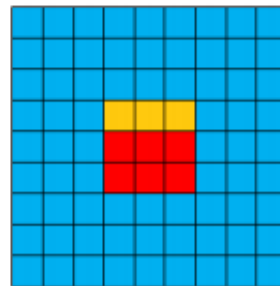
(h) Case 8



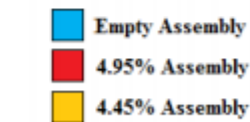
(i) Case 9



(j) Case 10



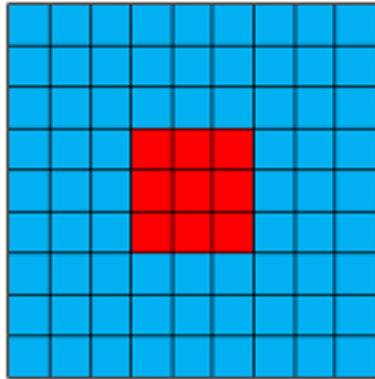
(k) Case 11



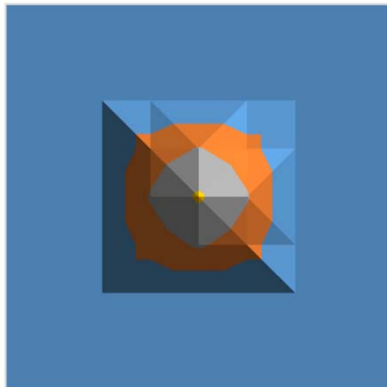
(l) Material Legend

Case #	Number of Assemblies	Fuel Type
1	1x1	4.95%
2	6x1	4.95%
3	3x3	4.95%
4	9x9	4.95%
5	1x1	4.45%
6	6x1	4.45%
7	3x3	4.45%
8	9x9	4.45%
9	2x1	Mixed
10	6x1	Mixed
11	3x3	Mixed

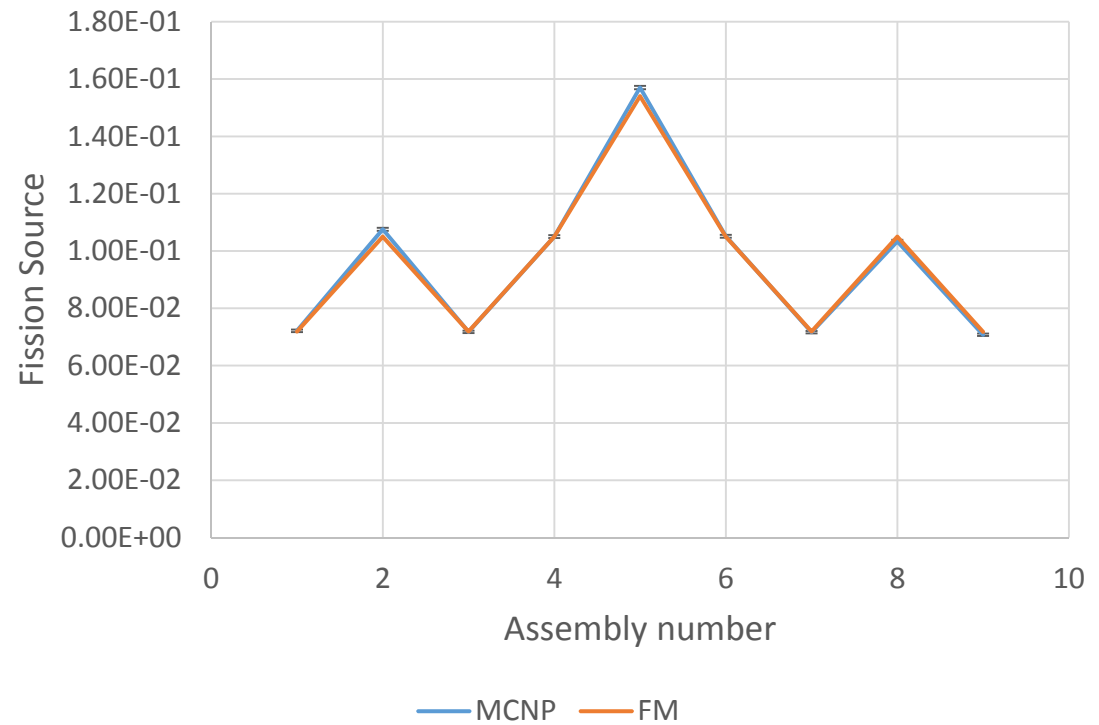
Case 3 Eigenfunction



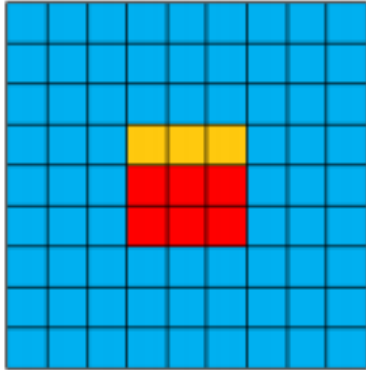
Reference Solution



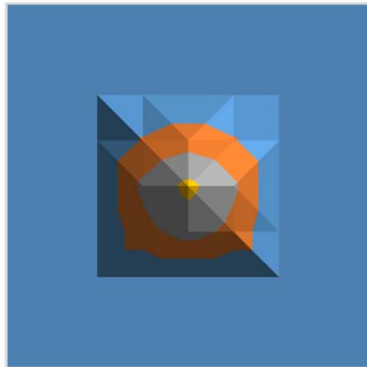
Comparison of RAPID with MC



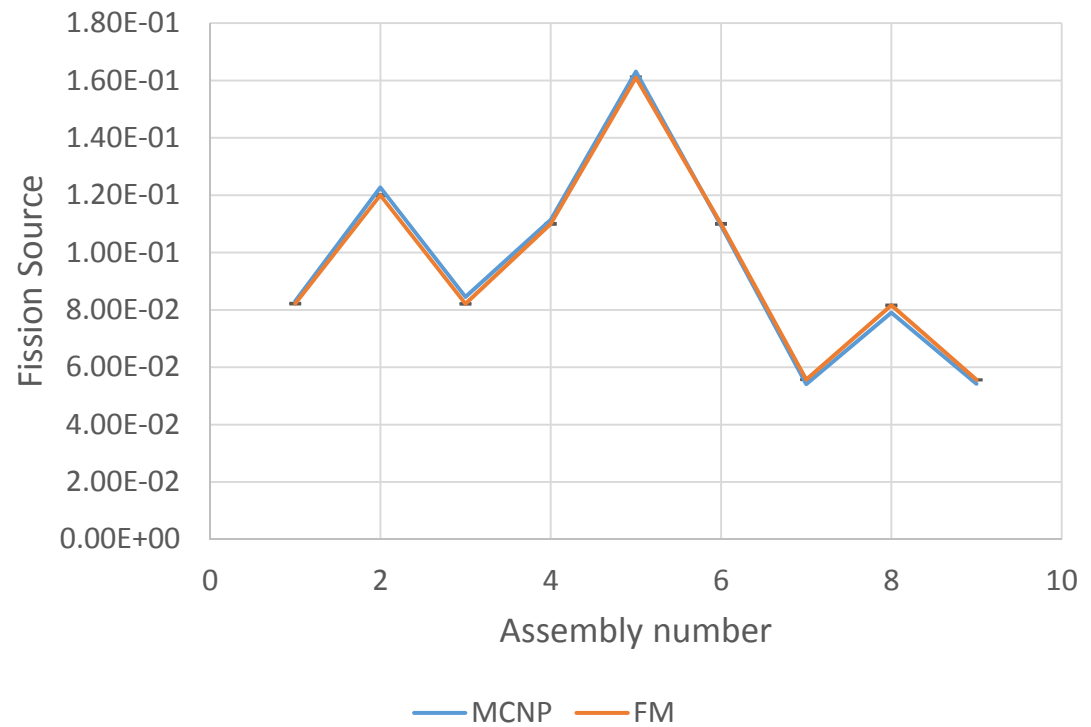
Case 11 Eigenfunction



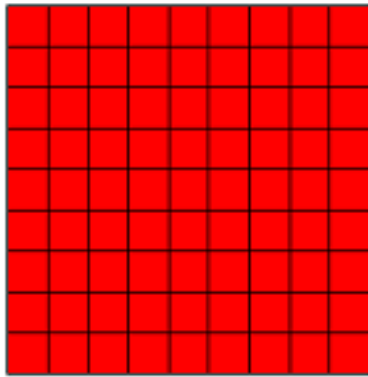
Reference Solution



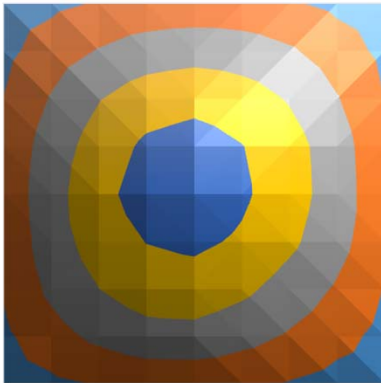
Comparison with RAPID with MC



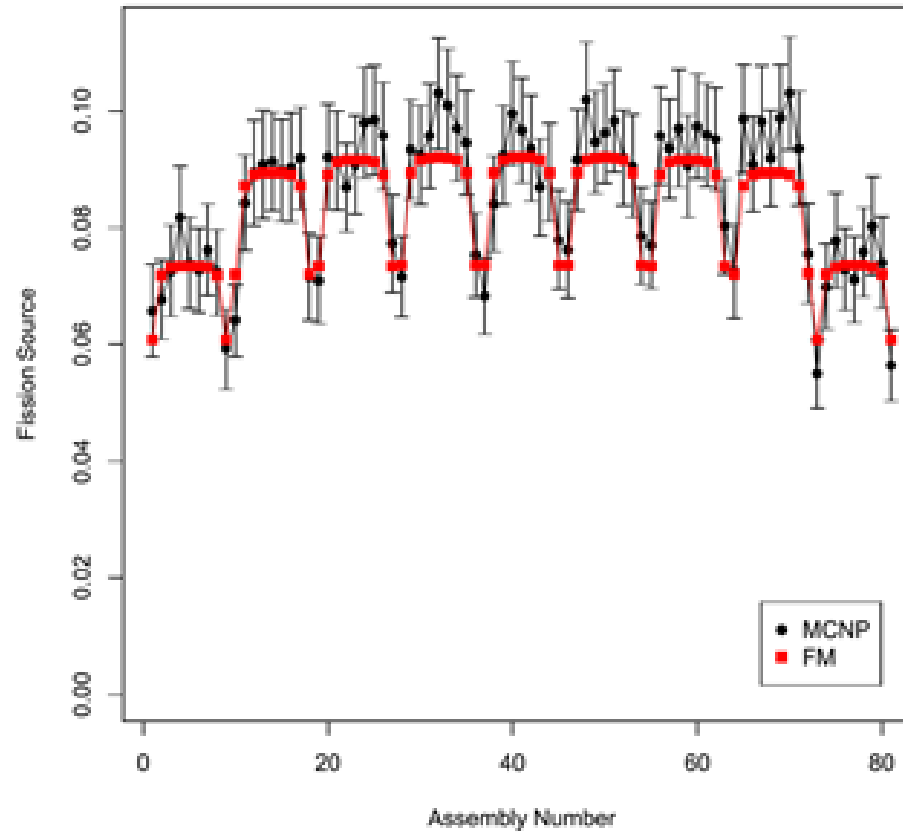
Case 4 Eigenfunction distribution



Reference Solution



Comparison with RAPID with MC



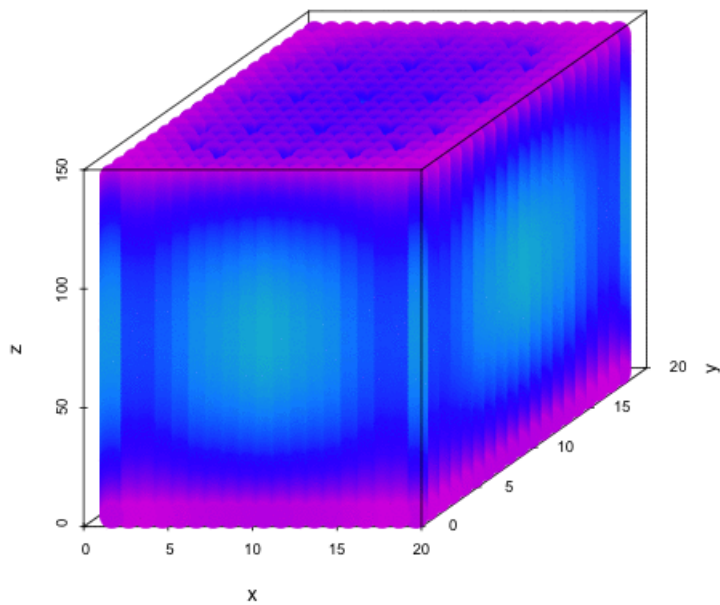
Comparison of calculated M - RAPID vs. MCNP

Case	FM		MCNP			Error in M (FM vs MCNP)	Speedup (FM vs MCNP)
	M	Time (min)	M	Time (min)	1- σ Uncertainty		
1x1	3.343353	0.092	3.33155	925	0.0010	0.35%	10062
6x1	4.328244	0.213	4.31336	1198	0.0010	0.35%	5613
3x3	5.428051	0.965	5.40992	1502	0.0011	0.35%	1558
9x9	6.697940	8.17	6.67674	1928	0.012	0.32%	236

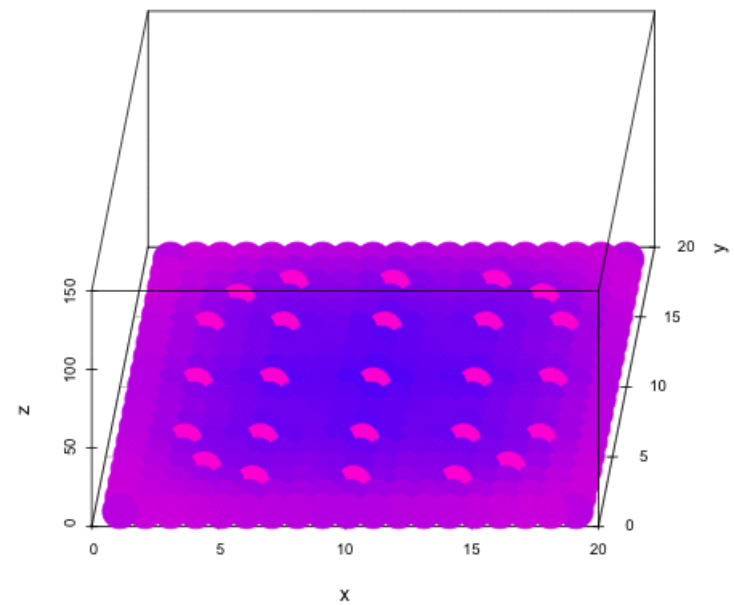
*Note that the FM technique also provide pin-wise, axial-dependent fission source or power.

3-D Fission Density

Y-LEVEL ANIMATION

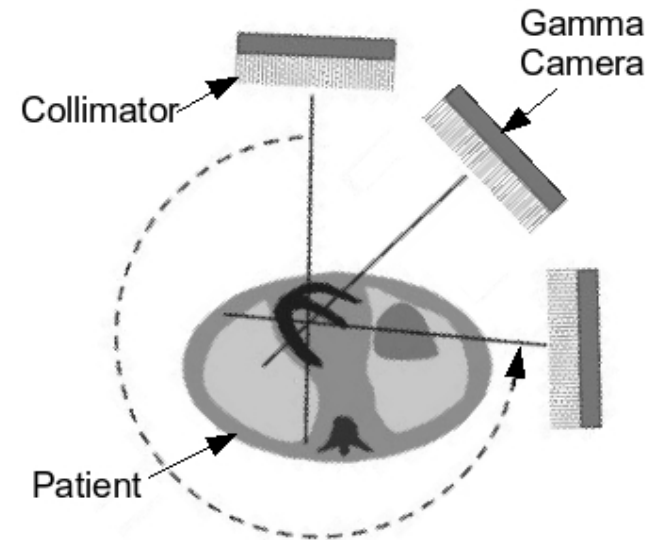


Z-LEVEL ANIMATION



Introduction to Single Photon Emission Computed Tomography (SPECT)

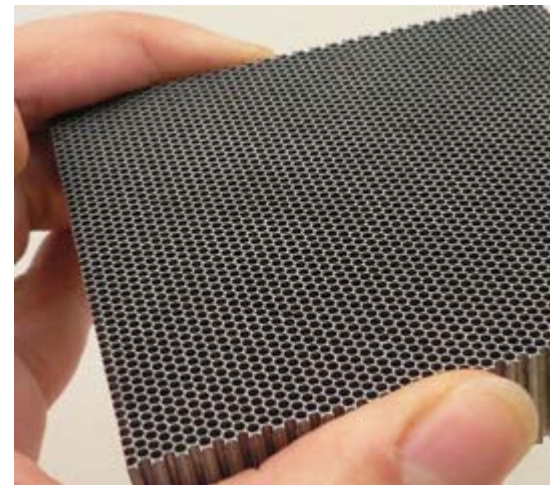
- 17 million procedures in the US in 2010
- Nuclear medicine imaging procedure used to examine myocardial perfusion, bone metabolism, thyroid function, etc.
- *Functional* imaging modality
- Radiopharmaceutical injected/ingested and localizes in a part of the body
- Emitted radiation detected at a gamma 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



TITAN Deterministic SPECT Simulation

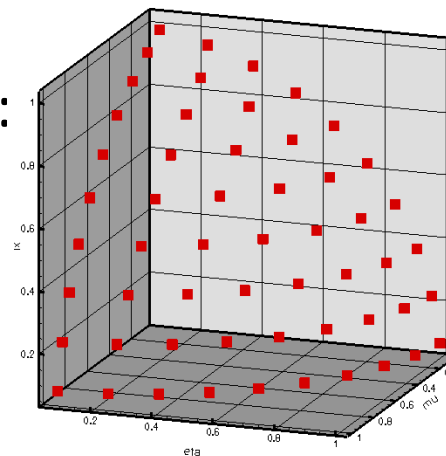
- The collimator in SPECT poses a challenge for deterministic modeling:

- Spatial discretization
- Angular discretization

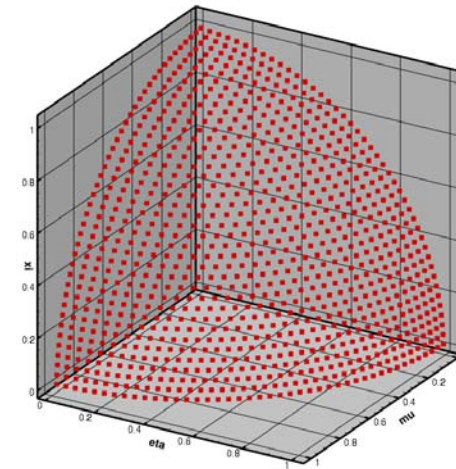


- Typical dimensions include:

- Hole diameter ~ 0.18 cm
- Septa thickness ~ 0.02 cm
- Length ~ 3.3 cm
- Acceptance Angle $\sim 1.6^\circ$



S_{20} Quadrature Set
(440 directions)

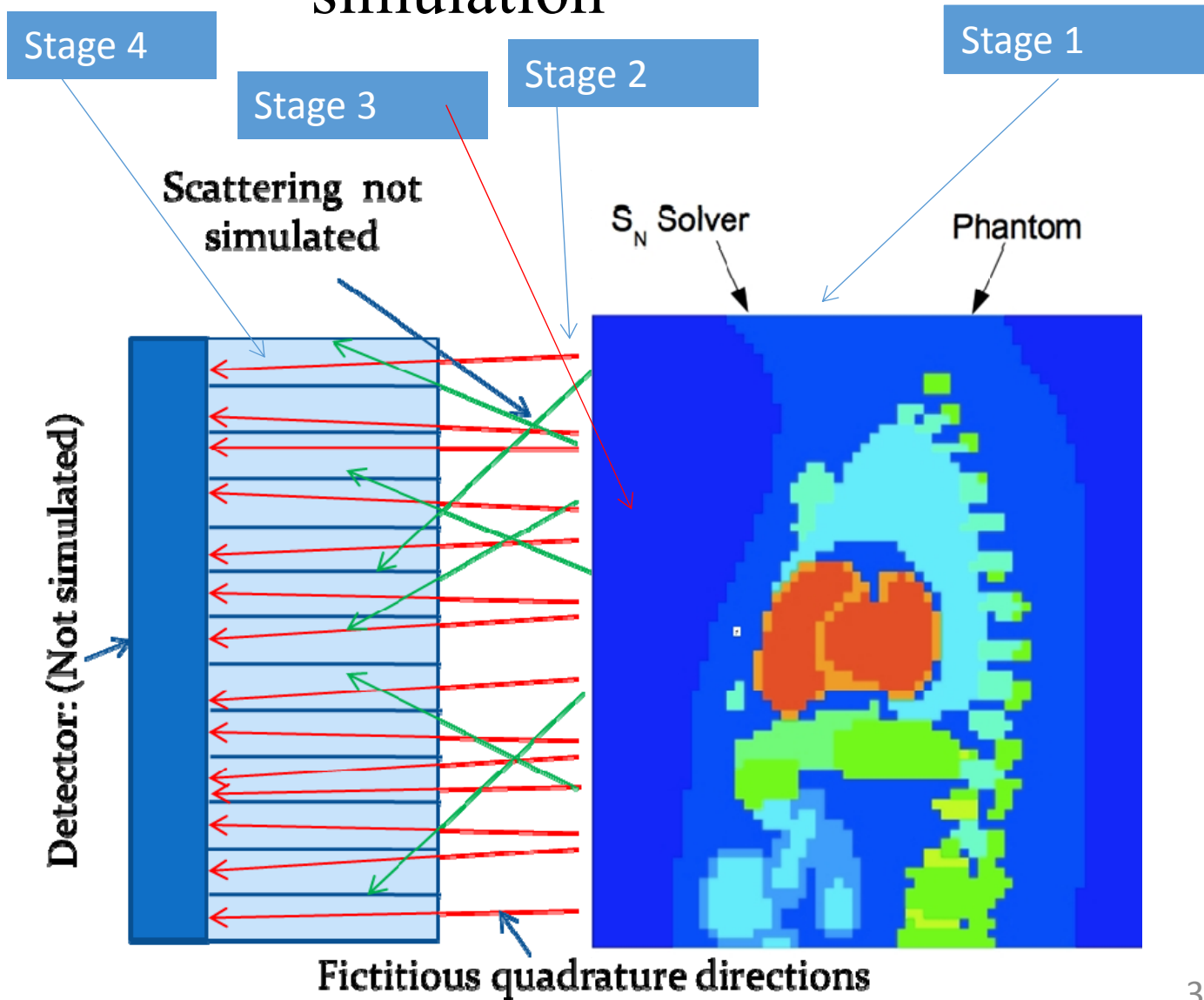


S_{86} Quadrature Set
(7568 directions)

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4-Stage TITAN Hybrid formulation for SPECT simulation

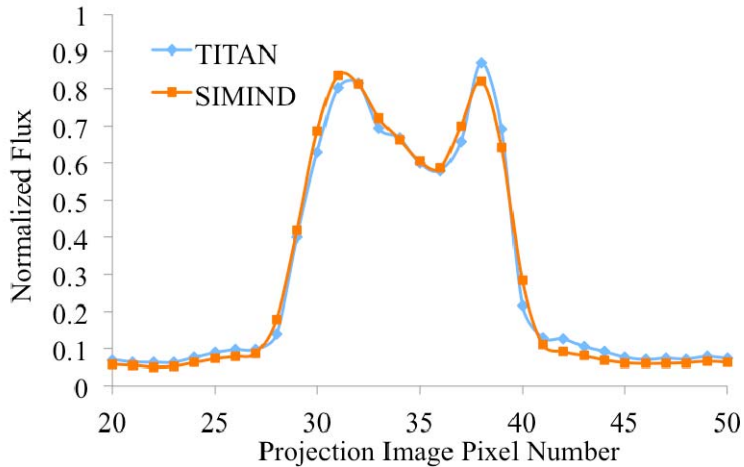
- Stage 1- S_n calculation in phantom
- Stage 2 – Selection of fictitious angular quadrature & Circular OS (COS) directions
- Stage 3 – S_n with fictitious quadrature
- Stage 4 – ray tracing



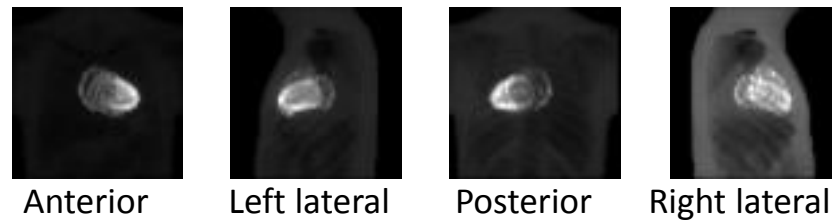
Example of Benchmarking TITAN Projection Images

SIMIND Comparison

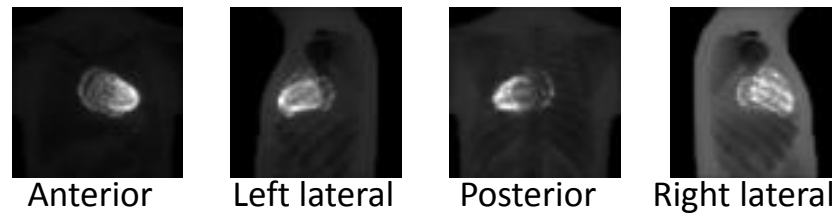
NURBS-based cardiac-torso (NCAT) phantom with Tc-99m (140 keV)



SIMIND generated projection images



TITAN generated projection images



Number of Projection Images	1	4	8	45	90
SIMIND Time (sec)	17	67	140	754	1508
TITAN Time (sec)	200	202	212	274	352

Times are for a single processor

Image Reconstruction

- Filtered backprojection (FBP) (Cormack 1963)
 - Analytic image reconstruction
 - Traditional standard for reconstruction due to speed and simplicity
 - Issues: filter choice, amplification of high-freq. noise, streak artifacts, cannot incorporate system details
- Algebraic reconstruction technique (ART) (Gordon *et al.* 1970)
 - Iterative constraint-based reconstruction
 - Allows the incorporation of prior knowledge
 - Issues: noisy, computationally expensive
- Maximum likelihood expectation maximization (ML-EM) (Shepp & Vardi 1982)
 - Iterative statistical reconstruction
 - For emission tomography, has recently surpassed FBP in popularity
 - Advantages include: Poisson statistics, nonnegativity constraint, incorporation of system details
 - Issues: increasing noise, computationally expensive

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ML-EM Brief Derivation

Mean number of photons detected in detector bin d :

$$\bar{n}_d = \sum_{b=1}^B p_{b,d} \hat{\lambda}_b$$

$p_{b,d}$: probability that photon emitted in voxel b is detected in bin d (system matrix)
 $\hat{\lambda}_b$: mean number of emissions in voxel b

Number of detected particles is a Poisson random variable, so the probability of detecting n_d^* photons in detector bin d :

$$P(n_d^*) = e^{-\bar{n}_d} \frac{\bar{n}_d^{n_d^*}}{n_d^*!}$$

Likelihood function:

$$L(\hat{\lambda}) = P(n_d^* | \hat{\lambda}) = \prod_{d=1}^D P(n_d^*) = \prod_{d=1}^D \frac{e^{-\bar{n}_d} \bar{n}_d^{n_d^*}}{n_d^*!}$$

Log-likelihood will have the same maximum location:

$$\begin{aligned} \ln(L(\hat{\lambda})) &= \sum_{d=1}^D \left(-\bar{n}_d + n_d^* \ln(\bar{n}_d) - \ln(n_d^*!) \right) \\ &= \sum_{d=1}^D \left[-\sum_{b=1}^B p_{b,d} \hat{\lambda}_b + n_d^* \ln\left(\sum_{b=1}^B p_{b,d} \hat{\lambda}_b\right) - \ln(n_d^*!) \right] \end{aligned}$$

Take derivative and set to zero to find maximum:

$$\frac{\partial \ln(L(\hat{\lambda}))}{\partial \hat{\lambda}_d} = -\sum_{d=1}^D p_{b,d} + \sum_{d=1}^D \frac{n_d^*}{\sum_{b'=1}^B p_{b',d} \hat{\lambda}_{b'}} p_{b,d} = 0$$

Multiply by $\hat{\lambda}_b$ and solve:

$$\hat{\lambda}_b^{(i+1)} = \frac{\hat{\lambda}_b^{(i)}}{\sum_{d=1}^D p_{b,d}} \sum_{d=1}^D \frac{n_d^*}{\sum_{b'=1}^B p_{b',d} \hat{\lambda}_{b'}^{(i)}} p_{b,d}, \quad b = 1, \dots, B$$

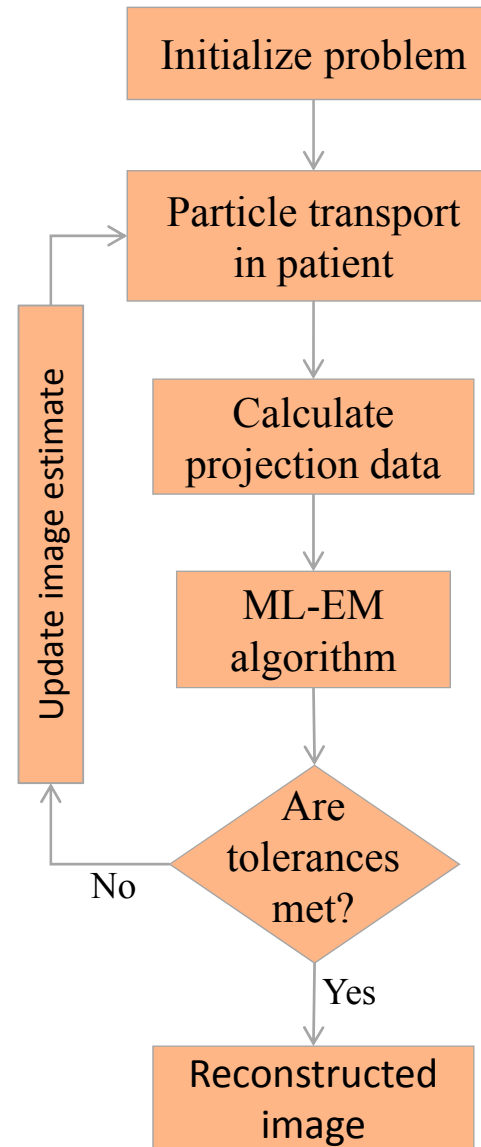
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Deterministic Reconstruction for SPECT (DRS)

- Projection data calculated by deterministic transport code
- Particle transport fully modeled in patient for forward projection
- Detailed system matrix never needs to be created
- Backprojection uses simple system matrix

$$\hat{\lambda}_b^{(i+1)} = \frac{\hat{\lambda}_b^{(i)}}{\sum_{d=1}^D p_{b,d}} \sum_{d=1}^D \frac{n_d^*}{\hat{n}_d^{(i)}} p_{b,d}, \quad b = 1, \dots, B$$

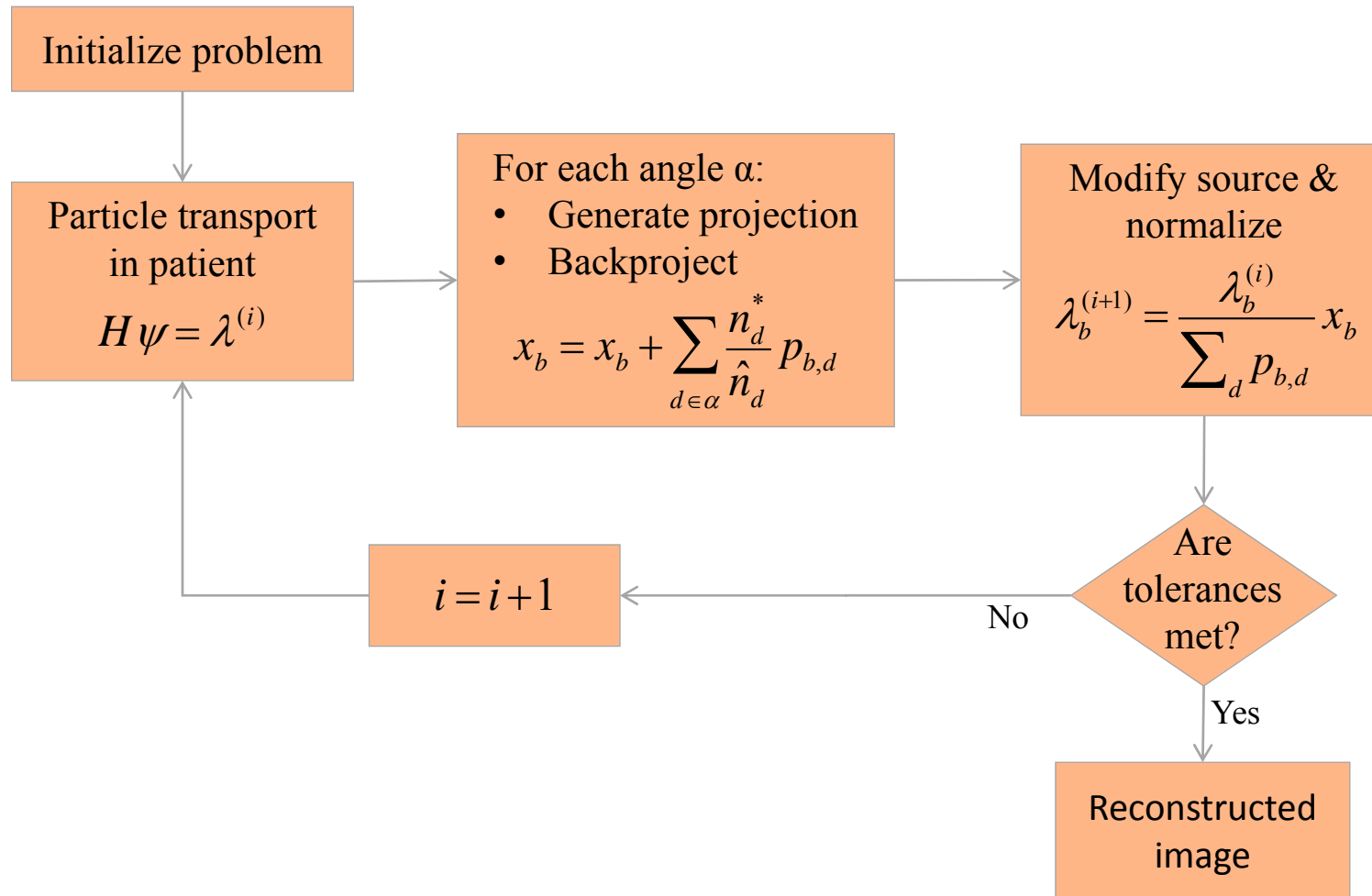
- A script was developed to allow anyone to use this method with any code that creates projection data for a given source distribution



TITAN with Image Reconstruction (TITAN-IR)

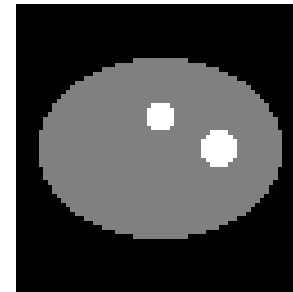
- Incorporate DRS methodology into TITAN code to take advantage of:
 - Fast generation of SPECT projection images
 - Parallel features
- Implement:
 - ML-EM reconstruction
 - Parallel image reconstruction
 - Image quality metrics (contrast and noise in reconstruction, mean relative error and mean squared error in projection data)
 - Post-reconstruction filtering

TITAN with Image Reconstruction (TITAN-IR)

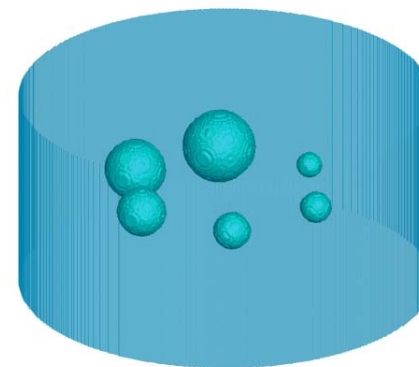


Analyzing TITAN-IR

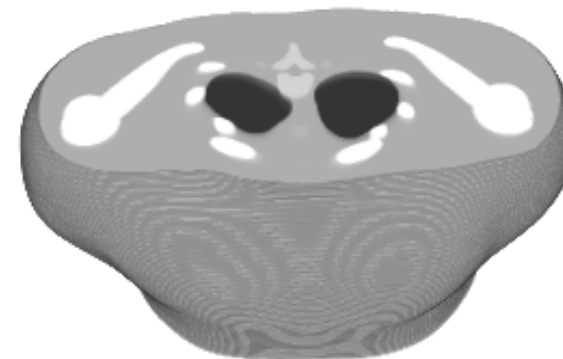
- 1) 2-D elliptical water phantom with two circles of high intensity source (i.e., lesions)



- 2) Jaszczak: 3-D quality assurance phantom, cold sphere region



- 3) NCAT: NURBS-based cardiac-torso, 3-D heterogeneous phantom



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Reconstruction Analysis

- Visually display reconstructed images
- Plot profiles through important areas of reconstructed images
- Quality metrics:

- Mean relative error (MRE)

$$\text{MRE} = \frac{1}{N_d} \sum_{d=1}^{N_d} \frac{|\hat{n}_d^{(i)} - n_d^*|}{n_d^*}$$

- Mean squared error (MSE)

$$\text{MSE} = \frac{1}{N_d} \sum_{d=1}^{N_d} (\hat{n}_d^{(i)} - n_d^*)^2$$

$\hat{n}_d^{(i)}$ = counts in detector bin d at iteration i

n_d^* = measured counts in detector bin d

- Contrast

$$C_l = \frac{\bar{I}_l - \bar{I}_0}{\bar{I}_0}$$

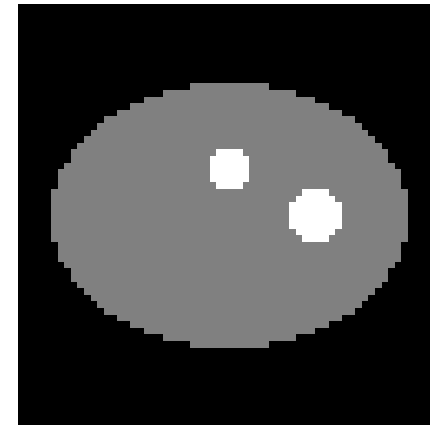
- Noise = $\frac{1}{\bar{I}_0} \left(\frac{\sum_{i=1}^{N_V} (I_i - \bar{I}_0)^2}{N_V - 1} \right)^{1/2}$

\bar{I}_l = average source intensity in lesion

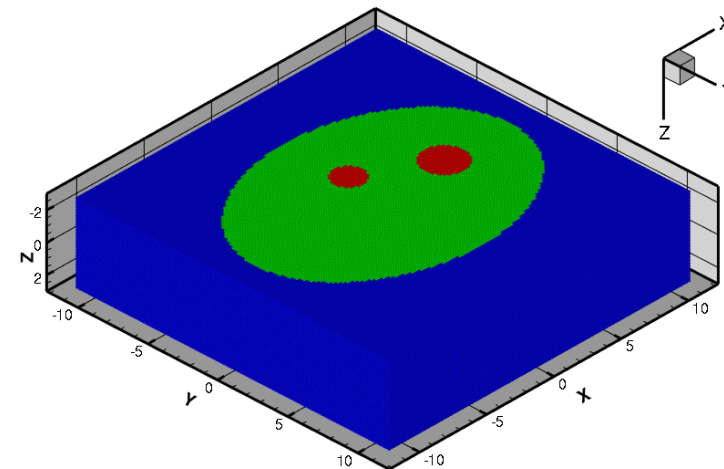
\bar{I}_0 = average reference background intensity

1) 2-D Phantom

- 2-dimensional, homogeneous, elliptical water phantom
- Tc-99m source (140 keV)
- Source strength of 2 in circles and 1 in rest of phantom
- 64 x 64 voxels (0.35 x 0.35 cm²)
- System matrix $p(b,d)$ generated by Prof. Fessler's Image Reconstruction Toolbox* in MATLAB (models attenuation only)
- Reference projection images obtained at 120 angles over 360° using the SIMIND Monte Carlo code
- Initial guess is a uniform source distribution



Reference source distribution



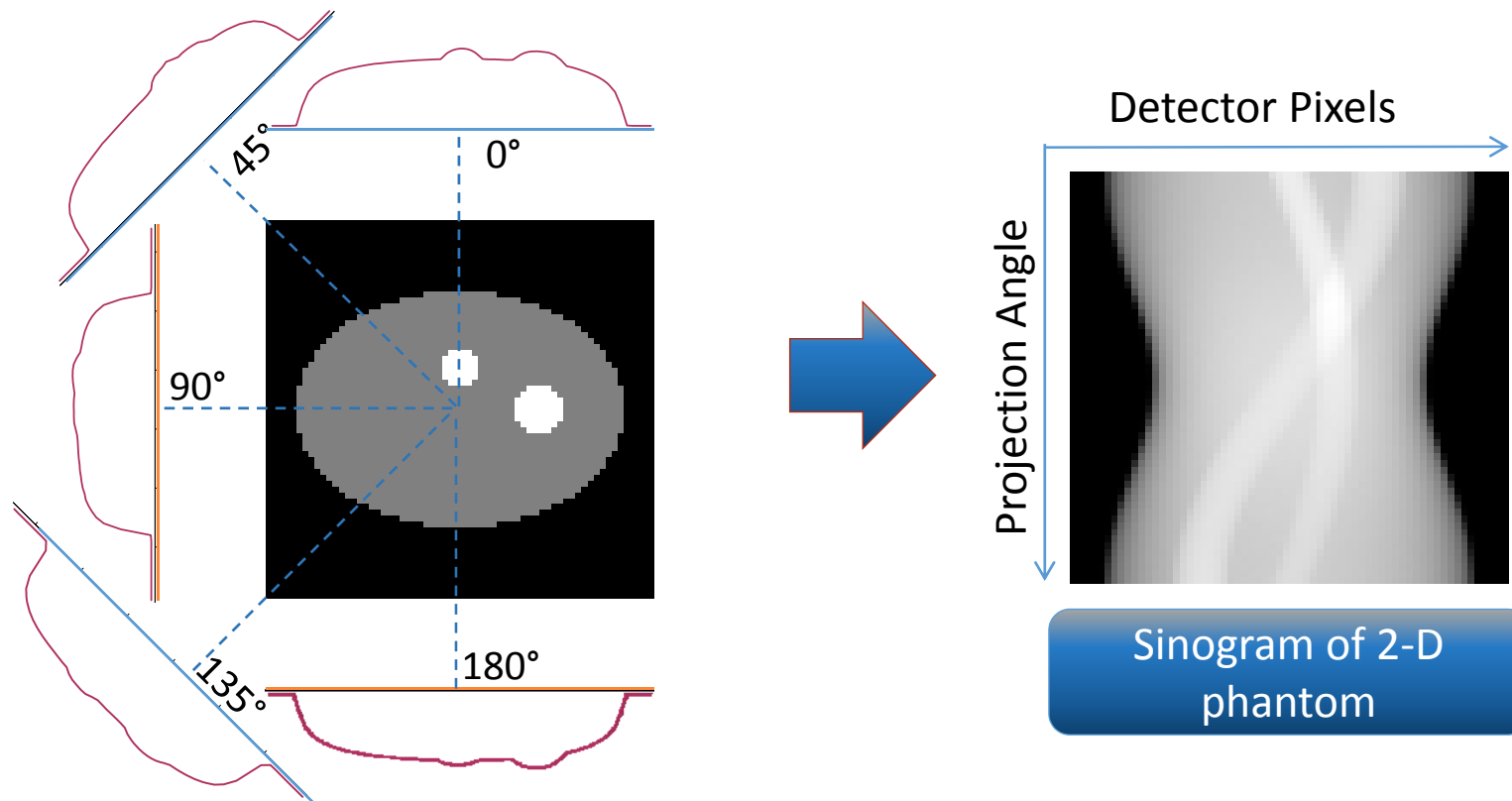
TITAN Model

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*J. A. Fessler, "Image reconstruction toolbox," University of Michigan

2-D Phantom

Reference projection data generated by the SIMIND Monte Carlo code* with no noise and a perfect collimator

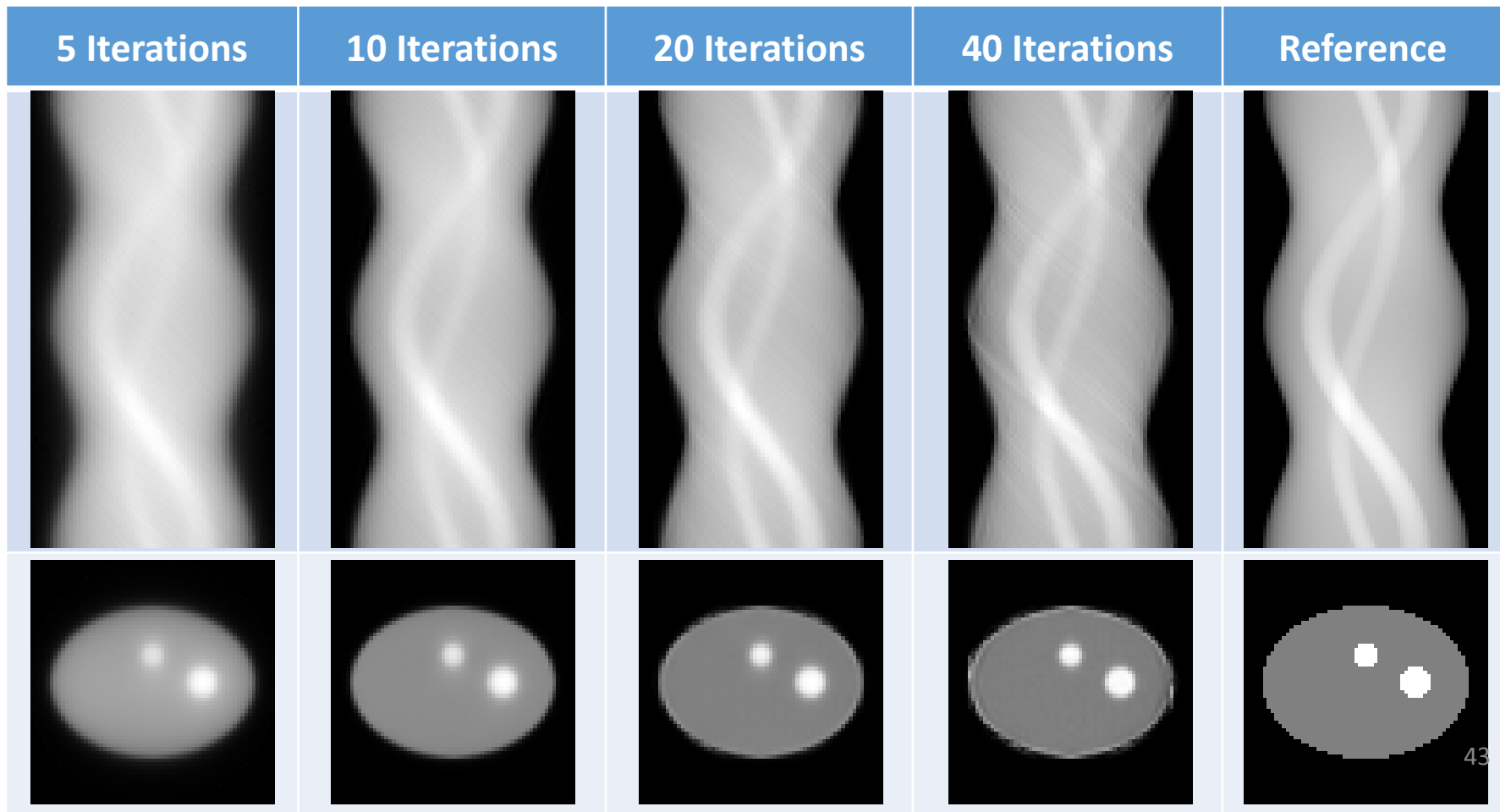


*M. Ljungberg and S.-E. Strand, *Comp Meth Progr Biomed*, 29, 257-272 (1989).

2-D Phantom

Image Reconstruction with TITAN

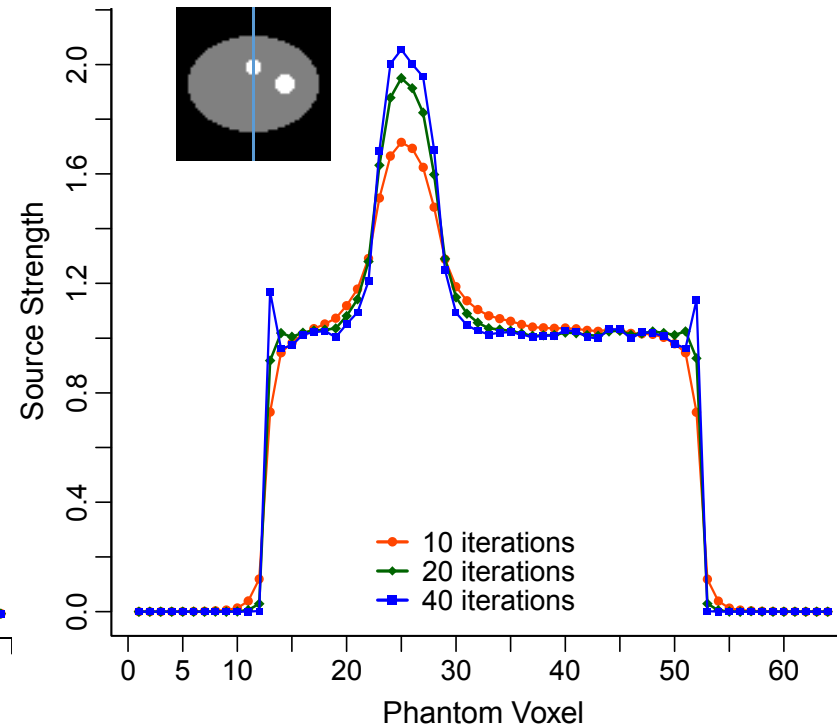
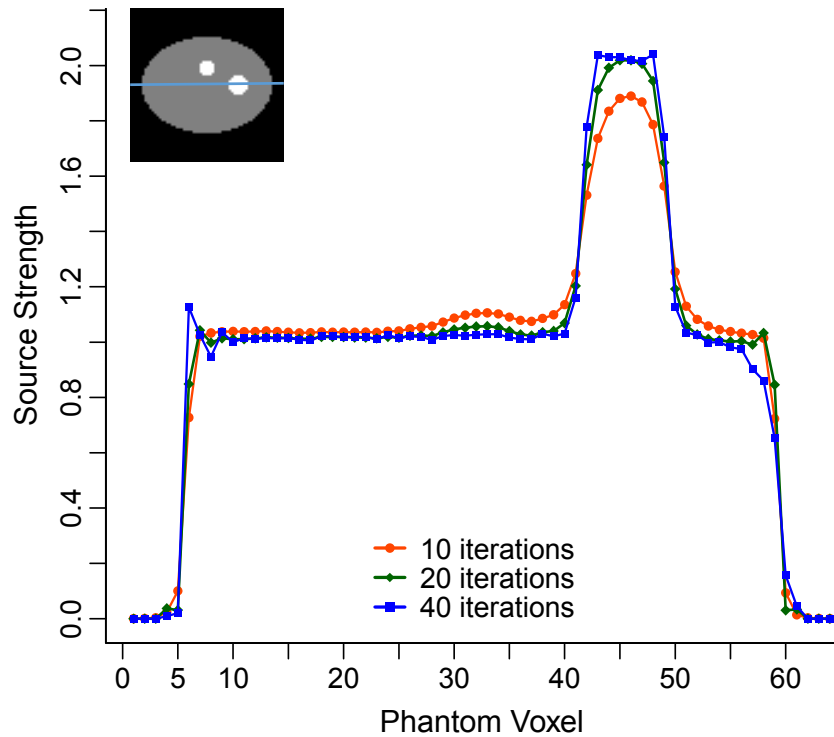
Reconstructed sinograms and images using TITAN for forward projection of 120 angles over 360°



Royston and Haghighat, *ANS RPSD 2014*, Knoxville, TN

2D Phantom: Profiles Through Reconstruction with TITAN

Profiles through the reconstructed source distributions for different numbers of iterations



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2D Phantom: Comparing Reconstructed Images

Contrast (C_l) and Log-likelihood (l) as a function of number of iterations

$$C_l = \frac{\bar{I}_l - \bar{I}_0}{\bar{I}_0}$$

\bar{I}_l = average source intensity in large circle

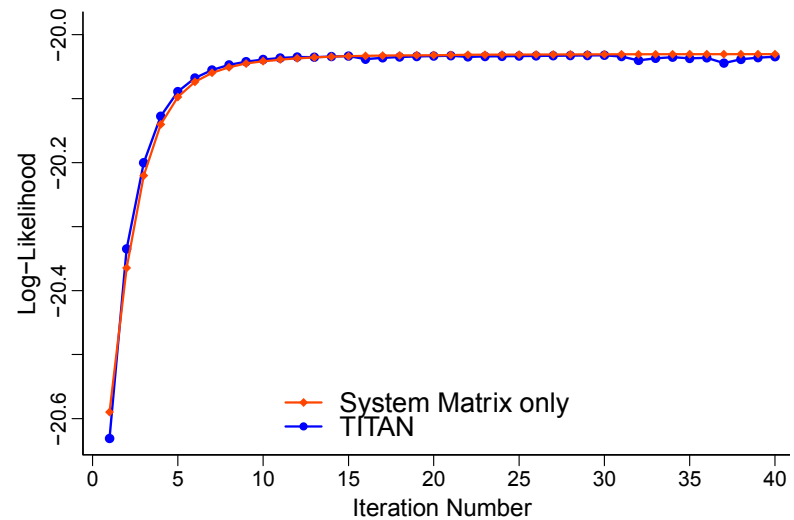
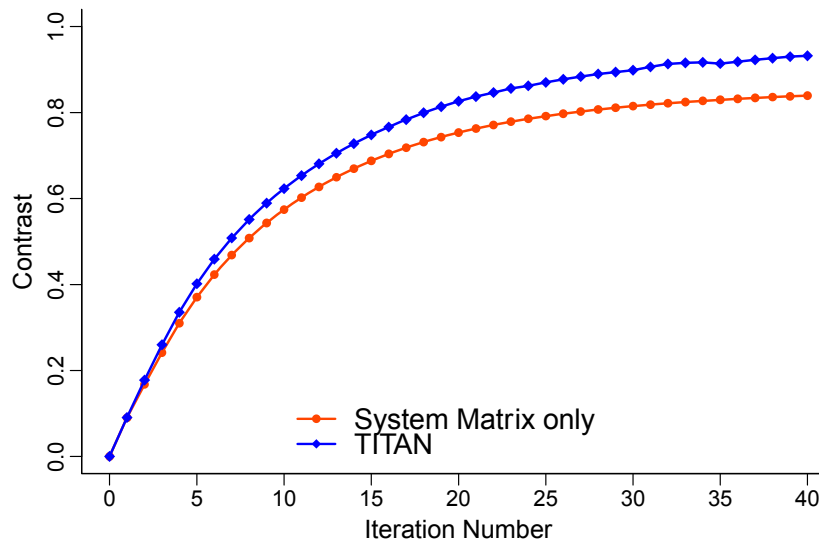
\bar{I}_0 = average reference background intensity

$$\text{Likelihood} = L(\hat{\lambda}) = \prod_{d=1}^D \frac{e^{-\bar{n}_d} \bar{n}_d^{n_d^*}}{n_d^*!}$$

$$l(\hat{\lambda}) = \sum_{d=1}^D n^*(d) \log(\hat{n}(d)) - \sum_{d=1}^D \hat{n}(d)$$

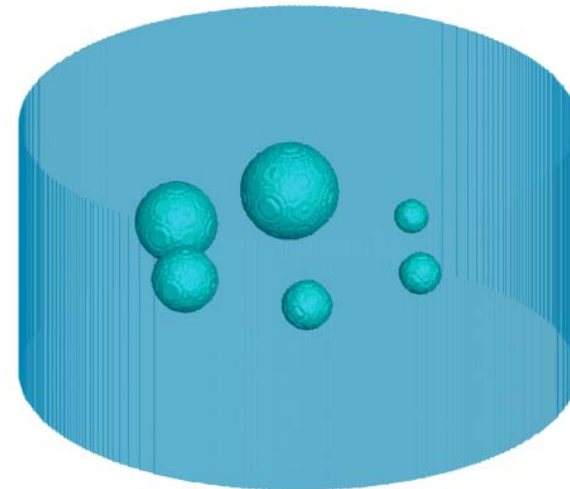
n^* = measured projection data

\hat{n} = estimated projection data

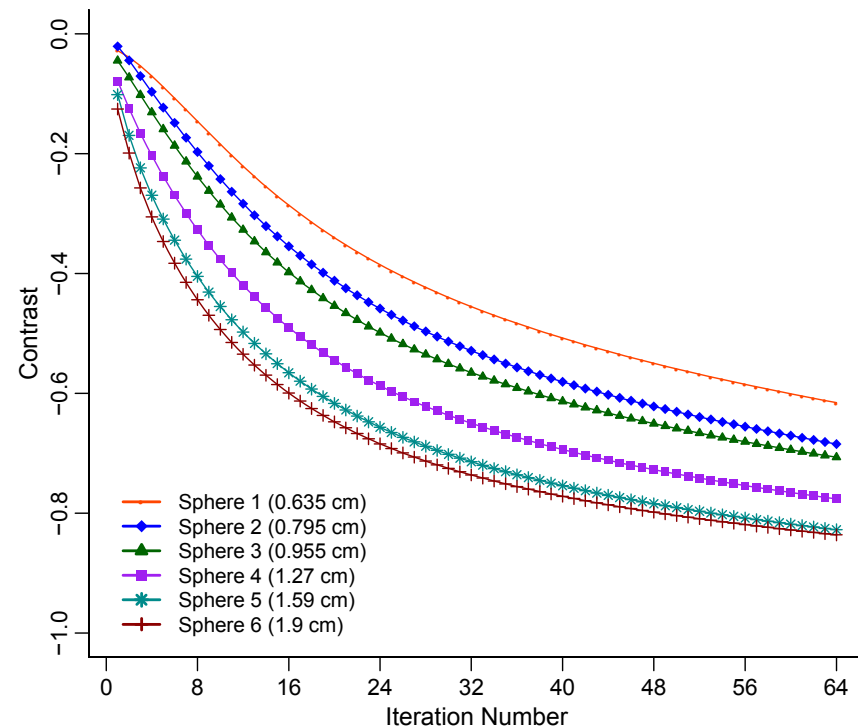
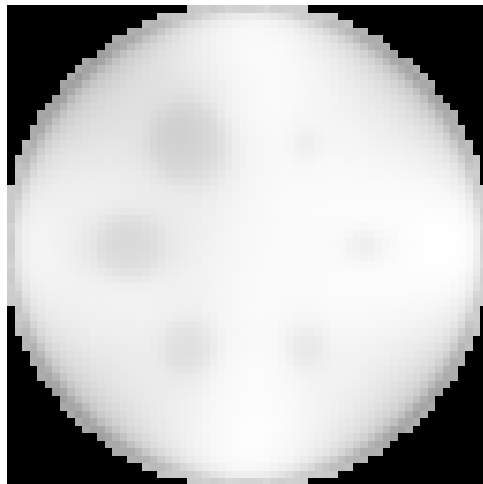


2) Jaszczak Cold Sphere Phantom

- 6 cold spheres with radii of 0.635, 0.795, 0.955, 1.27, 1.59, and 1.9 cm
- 185 MBq Tc-99m source (140 keV)
- Reference projection data obtained at 64 angles over 360° using SIMIND
- System matrix $p(b,d)$
 - Generated by Image Reconstruction Toolbox in MATLAB (models attenuation but not scatter)
 - Dimensions of (64x64x32) by (64x32x64)
- Initial guess is a uniform source distribution
- Three cases of projection data:
 - 1) No noise & no collimator blur
 - 2) Noisy & no collimator blur
 - 3) Noisy collimated data



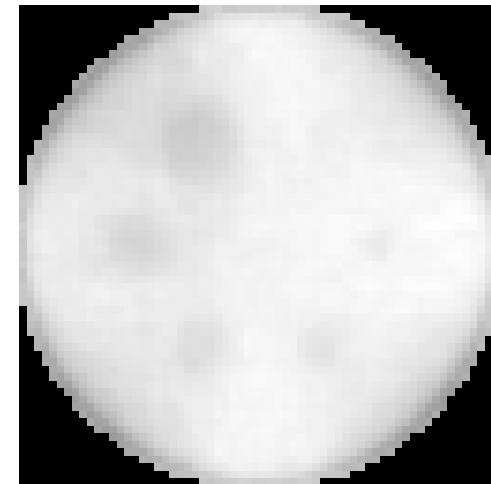
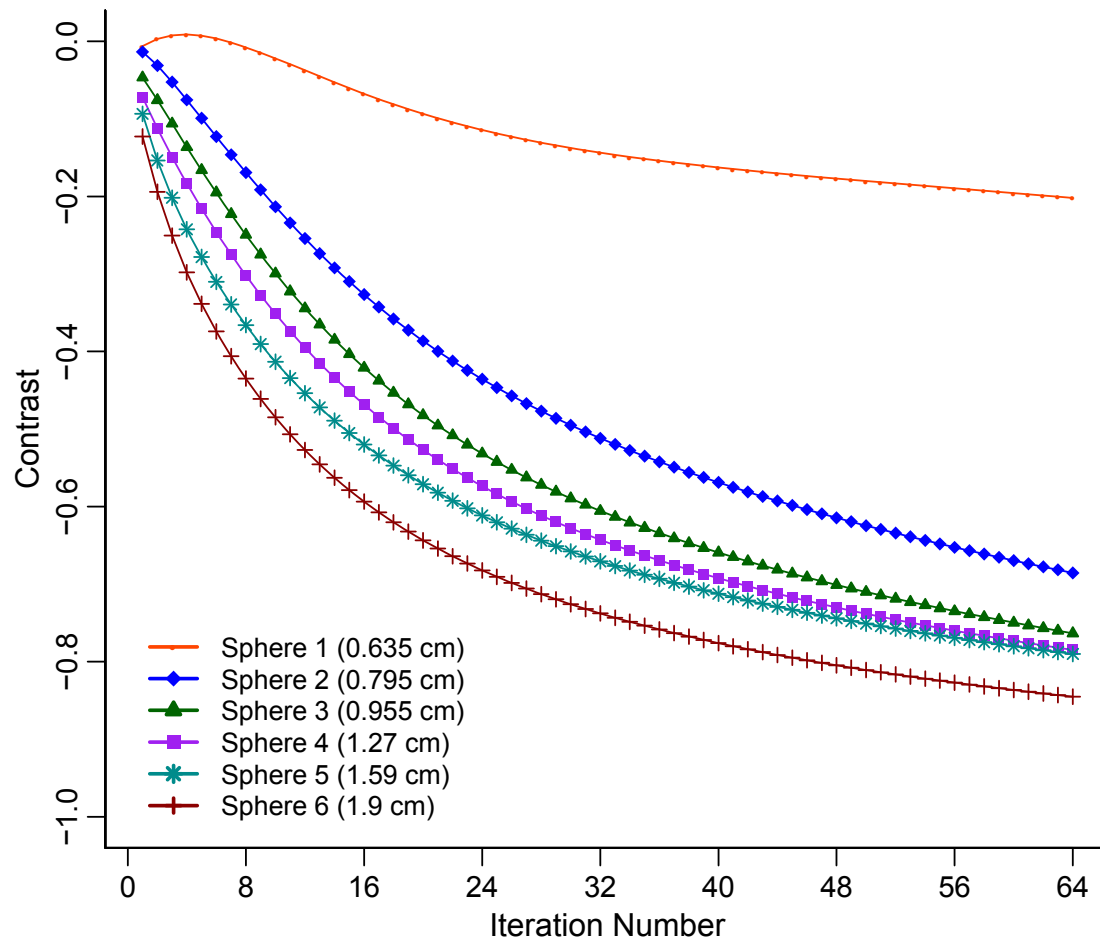
Jaszczak Phantom: Noiseless Projection Data with No Collimator Blur



Contrast in cold spheres in center slice of TITAN-IR (S_6 , coarse mesh) image

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Jaszczak Cold Sphere Phantom: Noisy Projection Data with No Collimator Blur



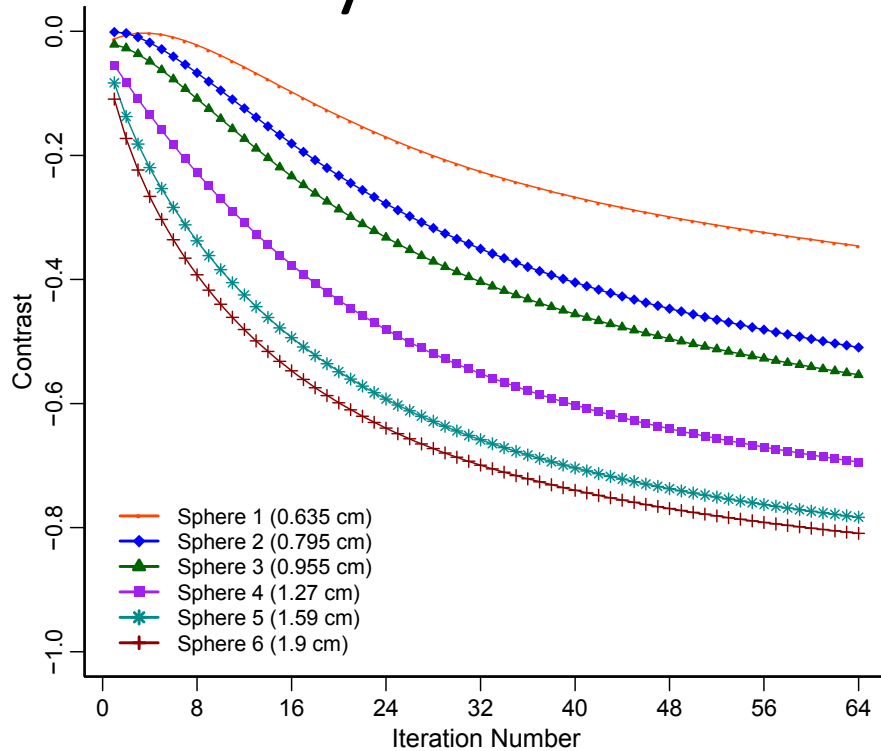
Jaszczak Cold Sphere Phantom: Noisy Collimated Projection Data

Collimator	Hole Diameter	Septa Thickness	Length	Acceptance Angle
GE-LEGP*	0.25 cm	0.03 cm	4.10 cm	1.83°
SE-LEHR†	0.111 cm	0.016 cm	2.405 cm	1.39°

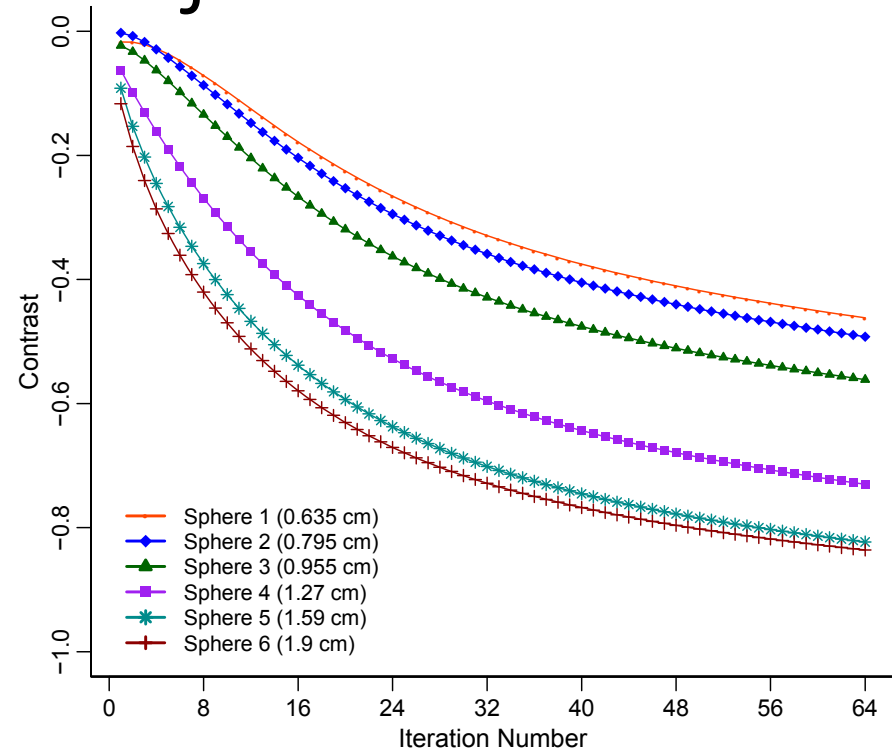
*General Electric – Low energy, general purpose collimator

†Siemens – Low energy, high resolution collimator

Jaszczak Cold Sphere Phantom: Noisy Collimated Projection Data

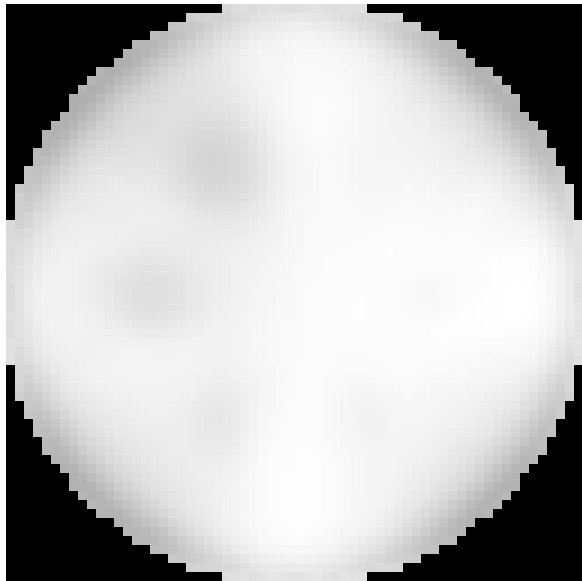


Contrast in each cold sphere (radius) for
noisy GE-LEGP (1.83°) projection data

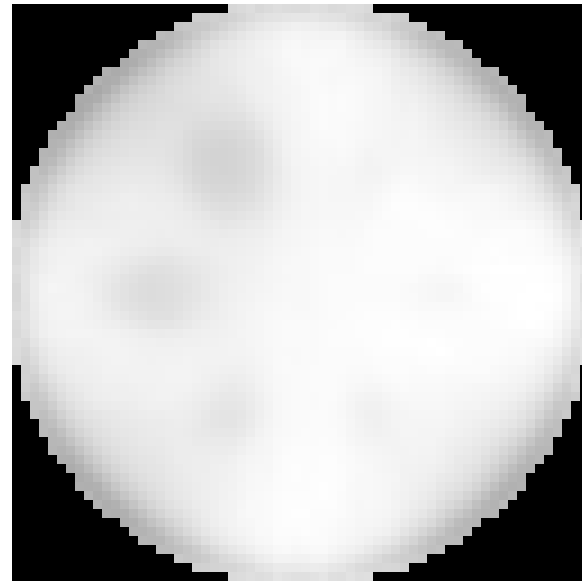


Contrast in each cold sphere (radius) for
noisy SE-LEHR (1.39°) projection data

Jaszczak Cold Sphere Phantom: Noisy Collimated Projection Data



Reconstruction of noisy
GE-LEGP data



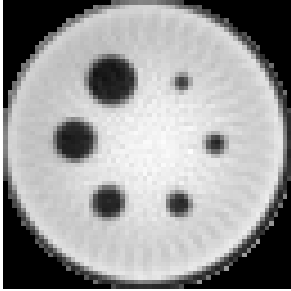
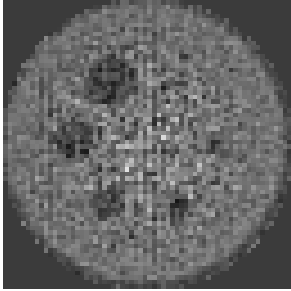
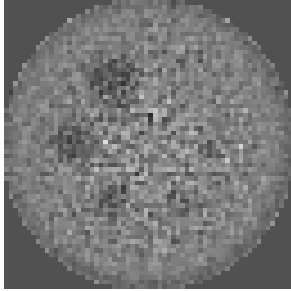
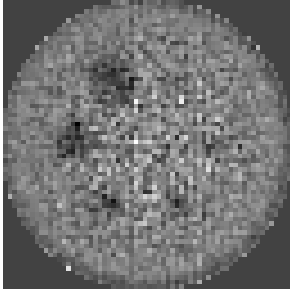
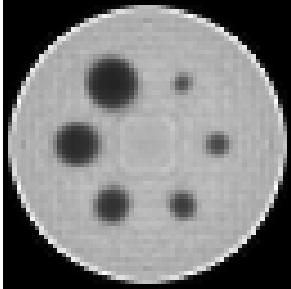
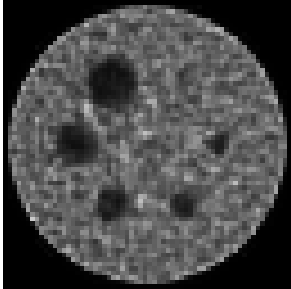
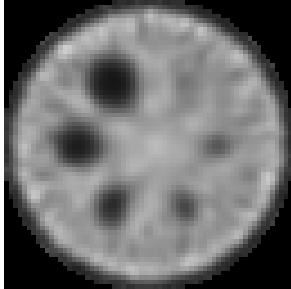
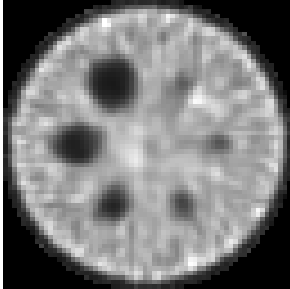
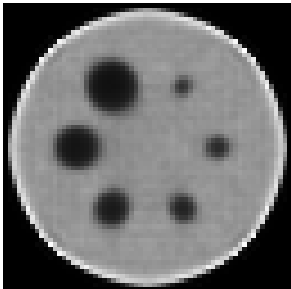
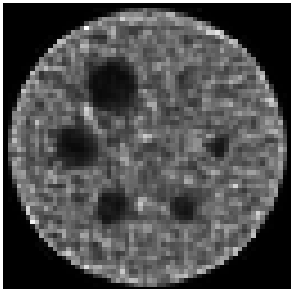
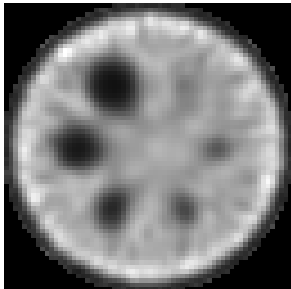
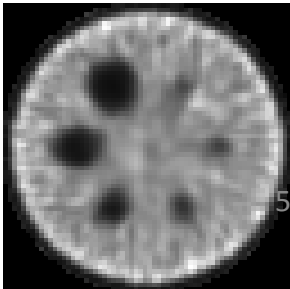
Reconstruction of noisy SE-
LEHR data

Comparison of TITAN-IR with Other Methods Based on Jaszczak Phantom:

- Filtered backprojection (FBP)
 - Traditional standard for image reconstruction
 - Implemented in MATLAB and includes the Chang attenuation correction*
- ML-EM with System Matrix (SM) only
 - Standard ML-EM reconstruction method
 - Algorithm written in Fortran 90
 - Uses the same system matrix that TITAN-IR uses for backprojection

*L.-T.Chang, "A method for attenuation correction in radionuclide computed tomography," *IEEE Trans. Nucl. Sci.*, 1978

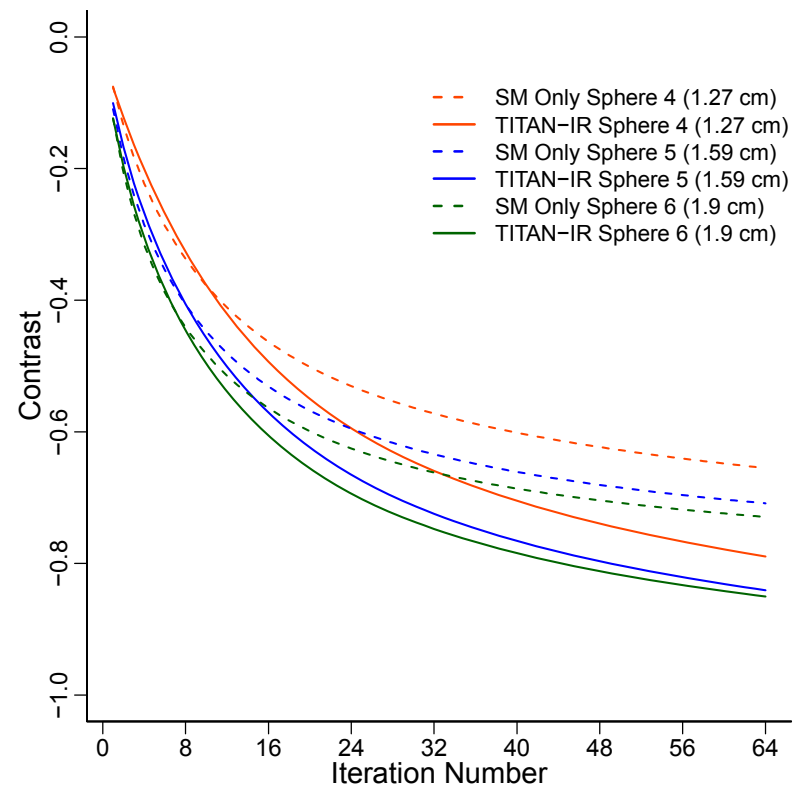
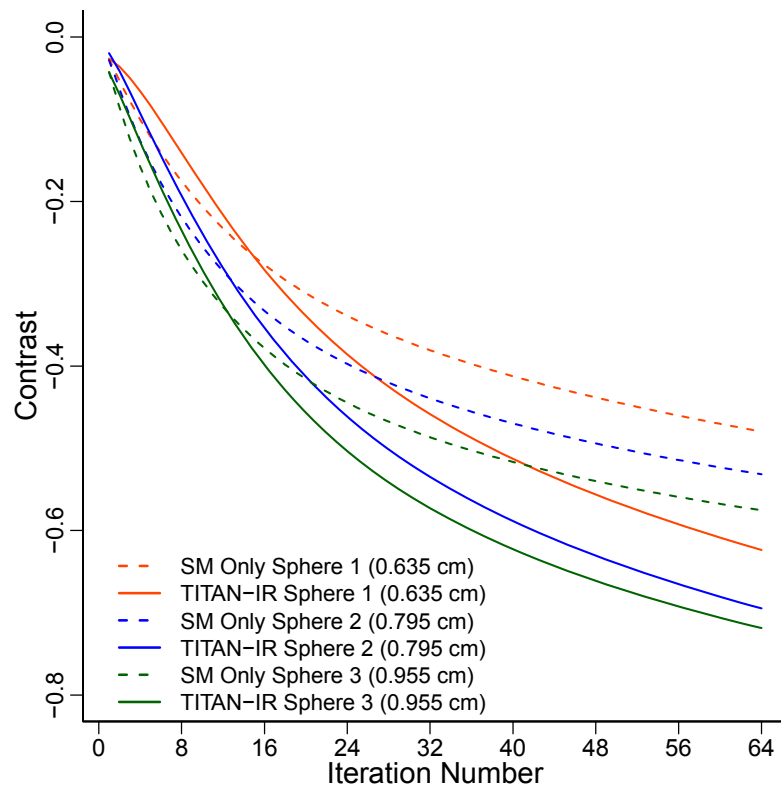
Comparison of Methods with Jaszczak Phantom

Algorithm	Noiseless, no collimator blur	Noisy, no collimator blur	Noisy GE-LEGP	Noisy SE-LEHR
FBP				
ML-EM with SM only				
TITAN-IR				

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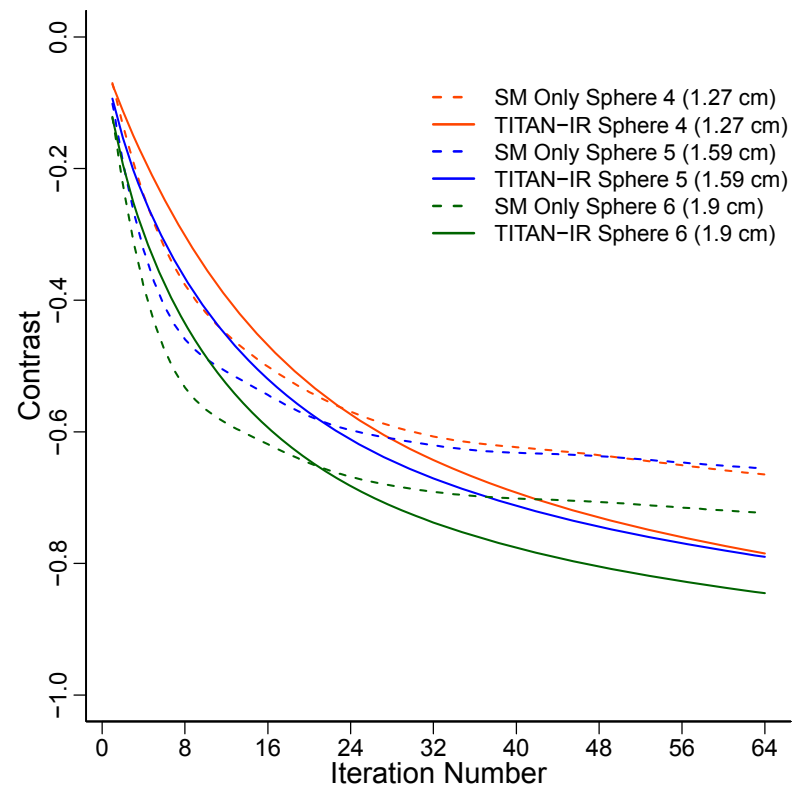
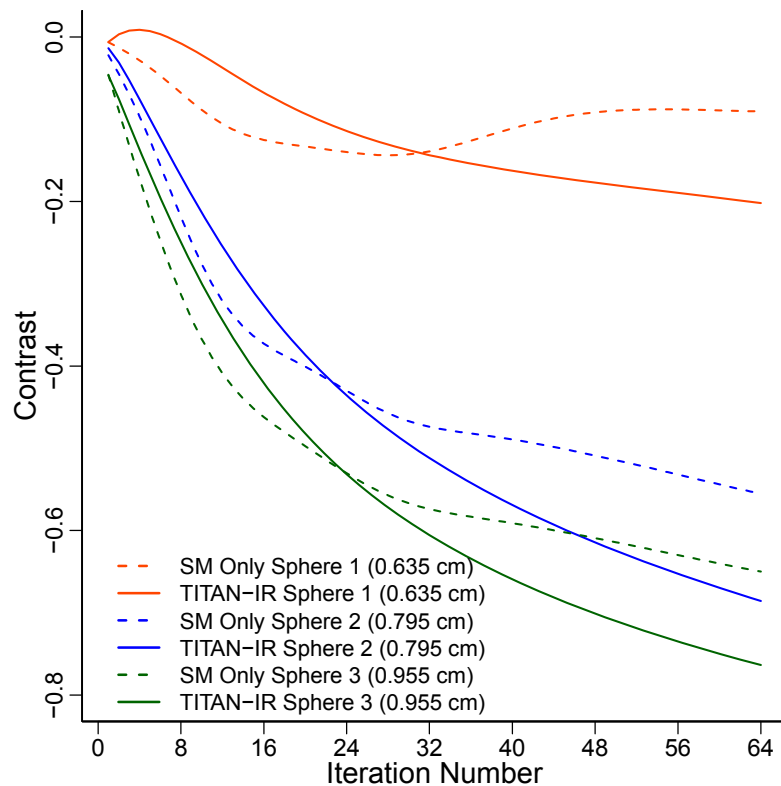
Comparison of Methods with Jaszczak Phantom

- Contrast in reconstruction of noiseless projection data with no collimator blur



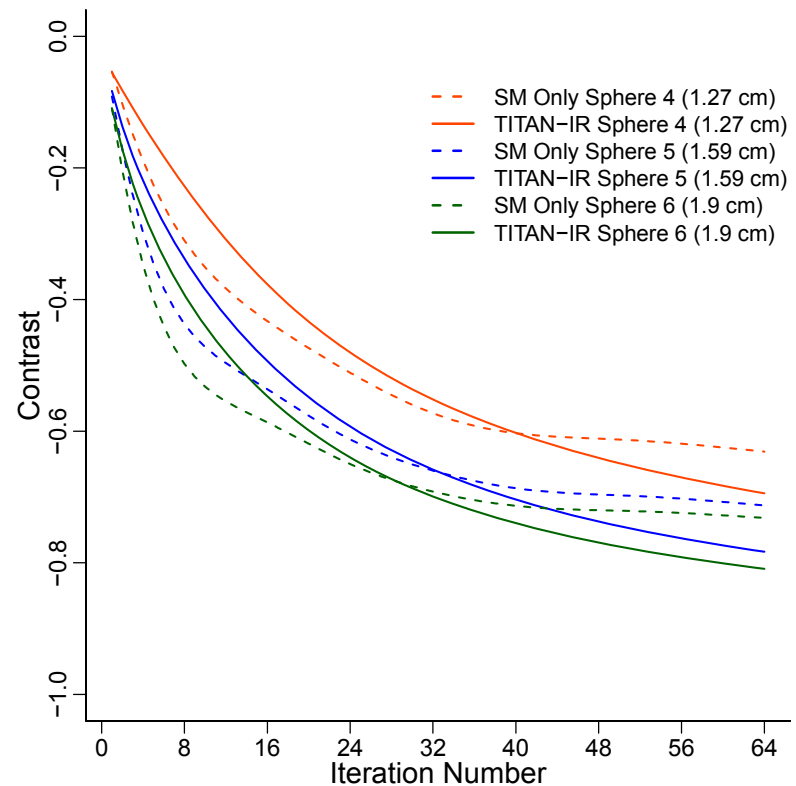
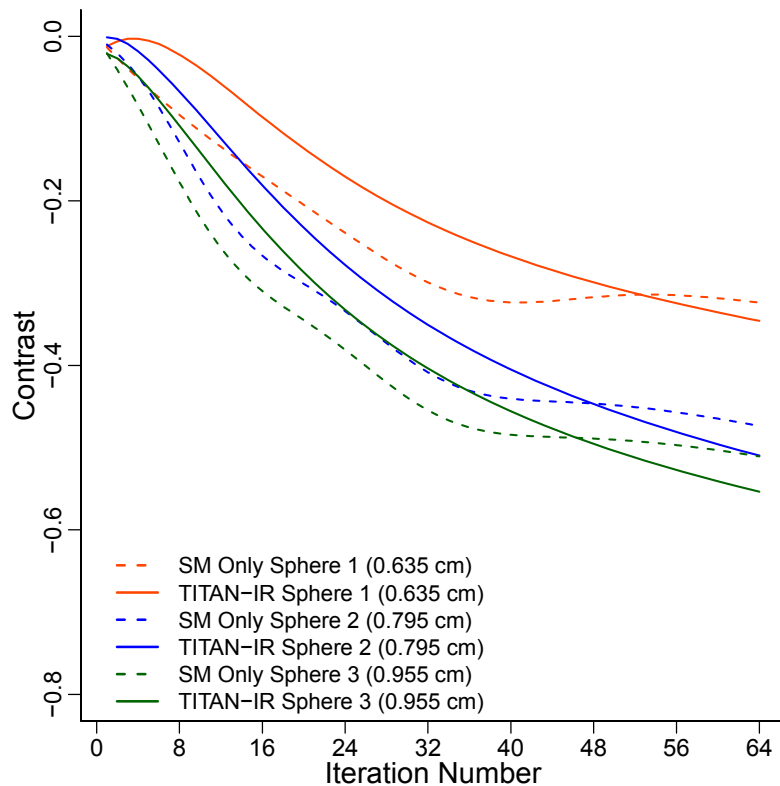
Comparison of Methods with Jaszczak Phantom

- Contrast in reconstruction of noisy projection data with no collimator blur



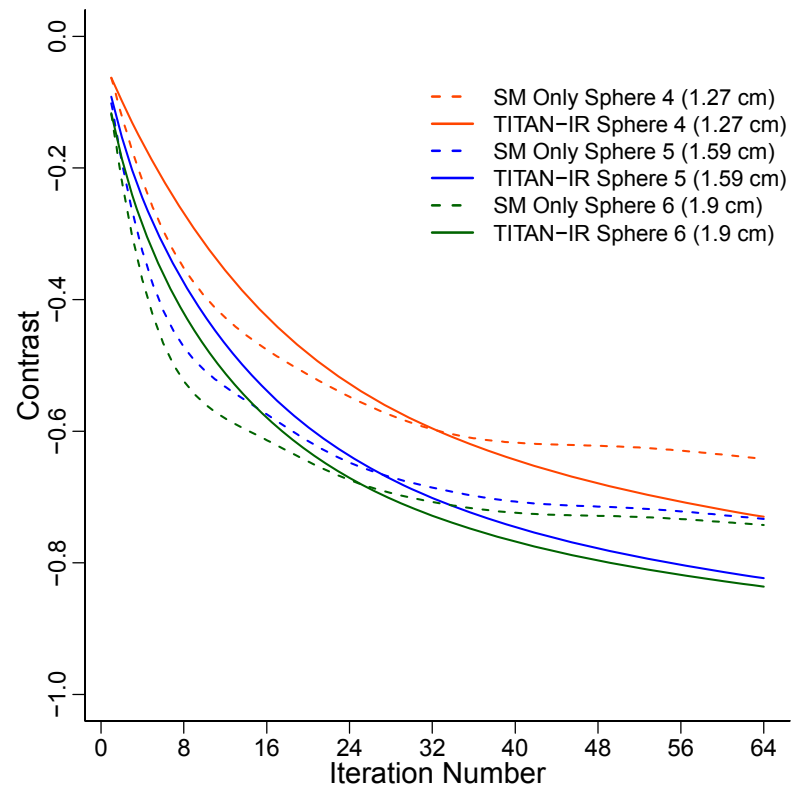
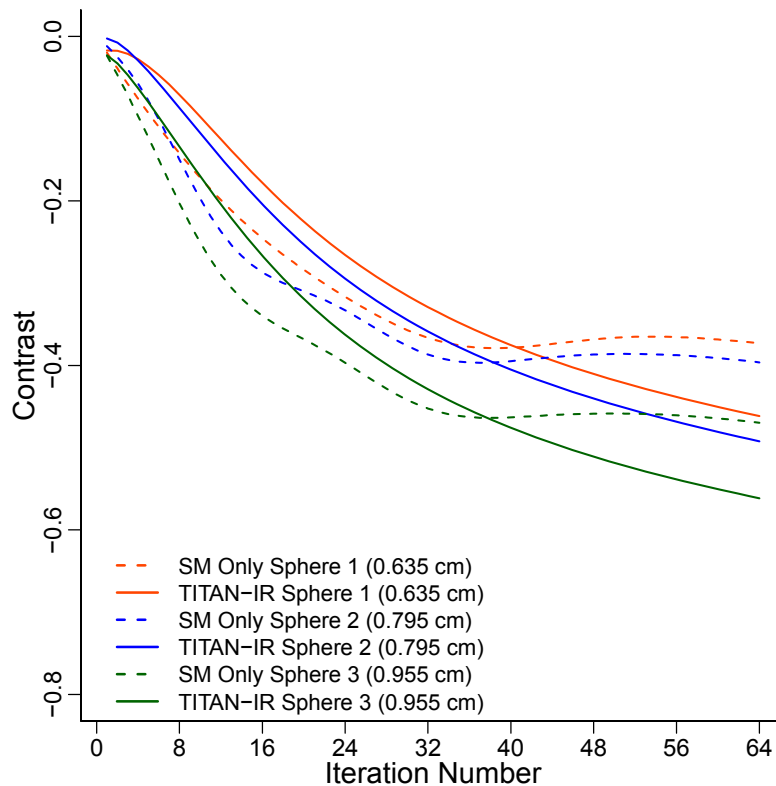
Comparison of Methods with Jaszczak Phantom

- Contrast in reconstruction of noisy GE-LEGP projection data

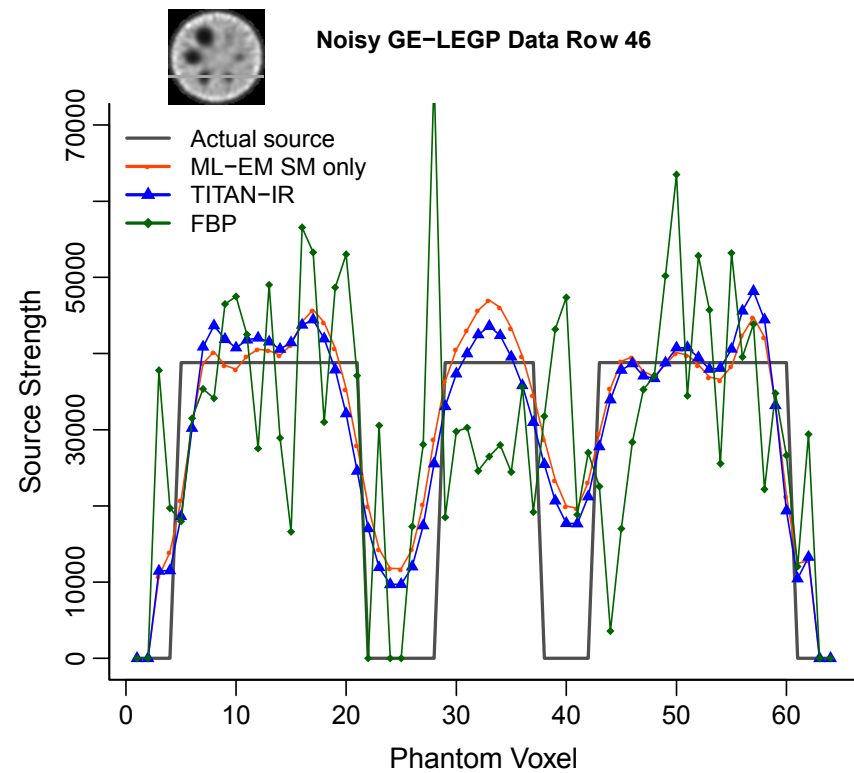
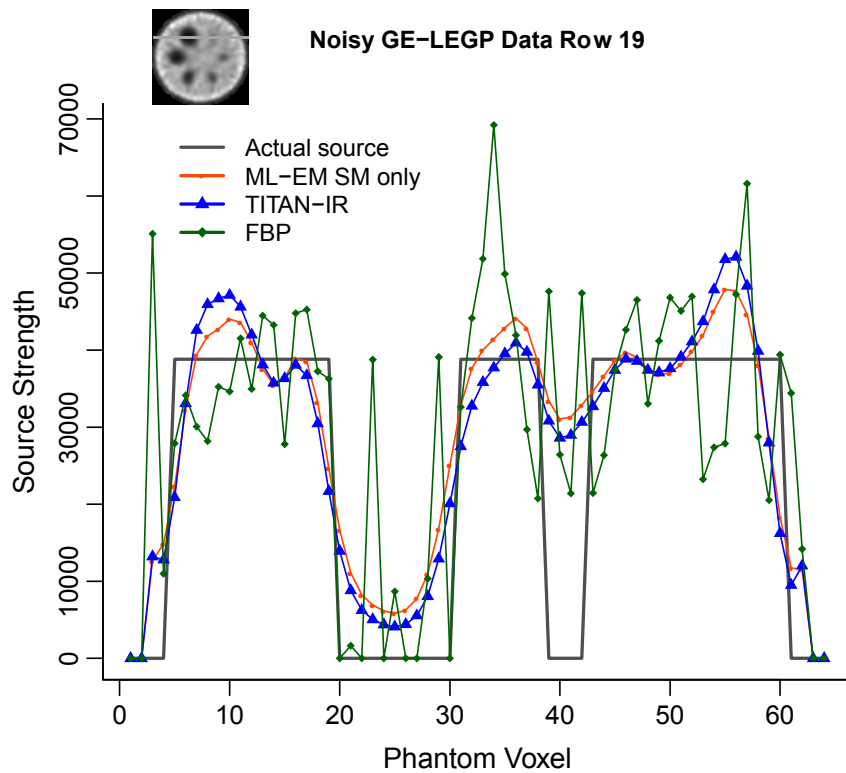


Comparison of Methods with Jaszczak Phantom

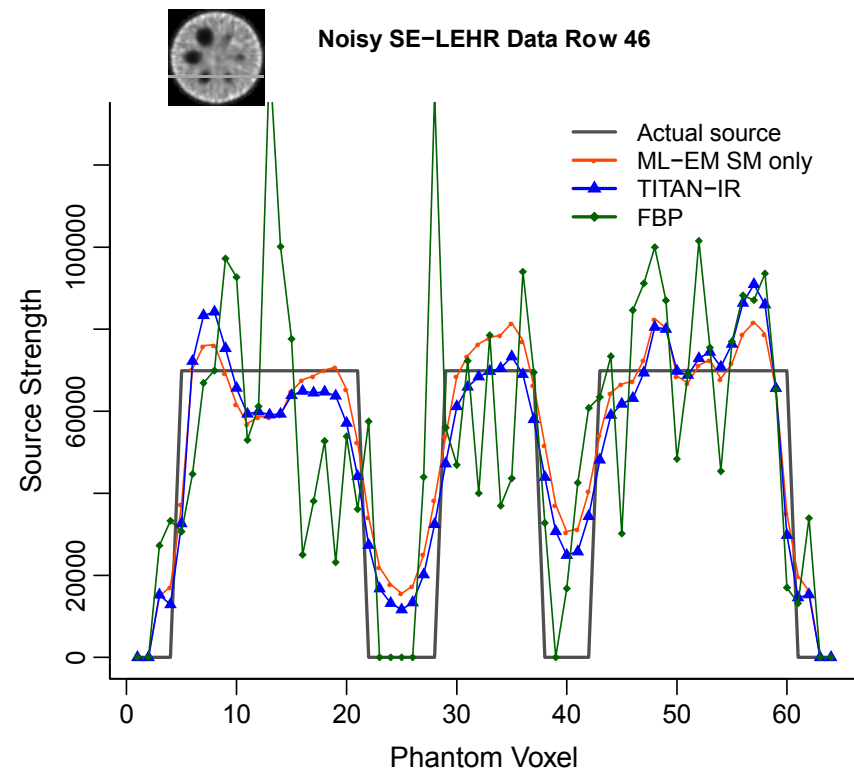
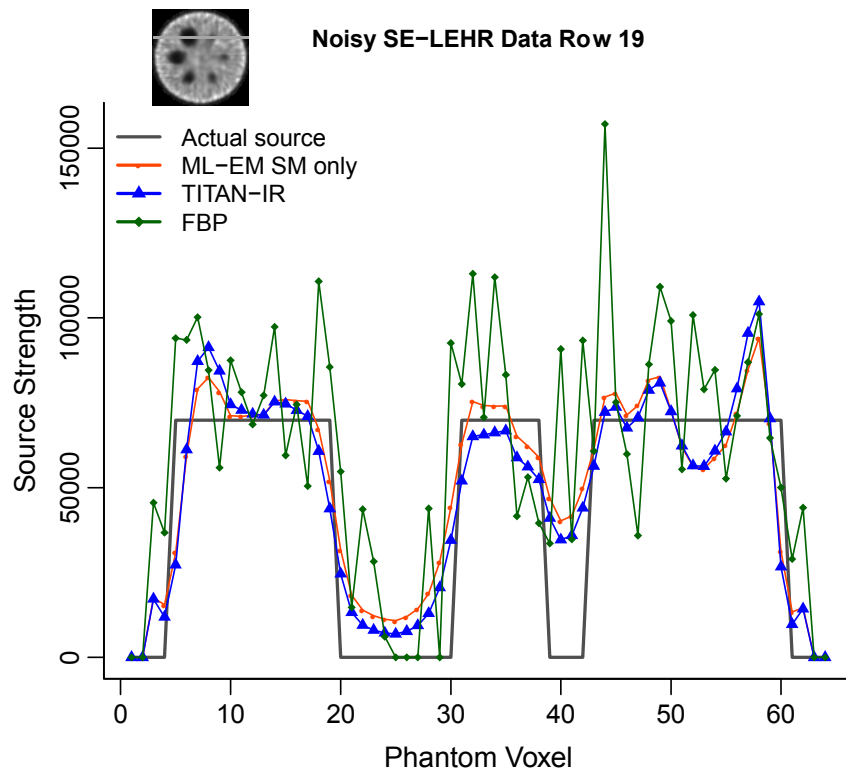
- Contrast in reconstruction of noisy SE-LEHR projection data



Comparison of Methods with Jaszczak Phantom



Comparison of Methods with Jaszczak Phantom



Computation Time

- To be viable for use in a clinical setting, as well as useful to researchers, computation time must be “reasonable”
- All calculations on a dedicated computer cluster:
 - Intel Xeon E5 2.6 GHz processors
 - 16 GB per processor core
 - 16 processor cores per compute node

Computation Time

Jaszczak phantom: TITAN-IR computation time for coarse meshing, S_6 , 64 iterations

Noiseless projection data with no collimator blur

Processor Cores	Wall Clock Time (s)	Speedup
1	575.7	-
2	291.5	2.0
4	149.9	3.8
8	81.4	7.1
16	36.8	15.6

Noisy GE-LEGP projection data

Processor Cores	Wall Clock Time (s)	Speedup
1	1665.7	-
2	905.1	1.8
4	524.3	3.2
8	341.4	4.9
16	172.0	9.7

Conclusion

MRT methodology allows for development of real-time tools for analysis of nuclear systems

Thanks!

Questions?