MRT Methodologies for Real-Time Simulation of Nuclear Systems

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**Objective**

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

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

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

\[
\Omega \cdot \nabla \Psi(\vec{r}, E, \hat{\Omega}) + \sigma(\vec{r}, E)\Psi(\vec{r}, E, \hat{\Omega}) = \\
\int_{0}^{\infty} dE' \int_{0}^{4\pi} d\Omega' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})\Psi(\vec{r}, E', \hat{\Omega}) + \\
\frac{\chi(E)}{4\pi} \int_{0}^{\infty} dE' \int_{0}^{4\pi} d\Omega' \nu \sigma_f(\vec{r}, E')\Psi(\vec{r}, E', \hat{\Omega}) + S(\vec{r}, E, \hat{\Omega})
\]

- Integral form

\[
\psi(\vec{r}, E, \hat{\Omega}) = \int_{0}^{R} d |\vec{r} - \vec{r'}| Q(r') e^{-\tau_E(\vec{r}, \vec{r'})} + \psi(\vec{r'}, E, \hat{\Omega}) e^{-\tau_E(\vec{r}, \vec{r'})}
\]
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, \( \sigma_g \)
**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

Path-length

\[ r = \frac{-\ln \xi}{\Sigma_t} \]

Type of collision

\[ \xi \leq \frac{\Sigma_s}{\Sigma_t} \]

Scattering angle (isotropic scattering)

\[ \mu_0 = 2\xi - 1 \]

Sample

\[ S (r, E, \Omega) \]

Tally (count)

Issue:

Precise expected values; i.e., small relative uncertainty,

\[ R_x = \frac{\sigma_x}{\bar{x}} \]

Variance Reduction techniques are needed for real-world problems!
### Deterministic vs. Monte Carlo

<table>
<thead>
<tr>
<th>Item</th>
<th>Deterministic</th>
<th>MC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Geometry</td>
<td>Discrete/ Exact</td>
<td>Exact</td>
</tr>
<tr>
<td>Energy treatment – cross section</td>
<td>Discrete</td>
<td>Exact</td>
</tr>
<tr>
<td>Direction</td>
<td>Discrete/ Truncated series</td>
<td>Exact</td>
</tr>
<tr>
<td>Input preparation</td>
<td>Difficult</td>
<td>simple</td>
</tr>
<tr>
<td>Computer memory</td>
<td>Large</td>
<td>Small</td>
</tr>
<tr>
<td>Computer time</td>
<td>Small</td>
<td>Large</td>
</tr>
<tr>
<td>Numerical issues</td>
<td>Convergence</td>
<td>Statistical uncertainty</td>
</tr>
<tr>
<td>Amount of information</td>
<td>Large</td>
<td>Limited</td>
</tr>
<tr>
<td>Parallel computing</td>
<td>Complex</td>
<td>Trivial</td>
</tr>
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</table>
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 of use deterministic adjoint) (VT³G has developed CADIS, A³MCNP in 1997; CADIS has become popular recently!)
<table>
<thead>
<tr>
<th>Year</th>
<th>Event</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>1986</td>
<td>Vector computing of 1-D Sn spherical geometry algorithm</td>
<td>Prof. Haghighat</td>
</tr>
<tr>
<td>1989</td>
<td>Development an adjoint methodology for simulation TMI-2 reactor</td>
<td>Prof. R. Mattis, Pitt.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Prof. B. Petrovic, GT</td>
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<tr>
<td>1989</td>
<td>Vector and parallel processing of 2-D Sn algorithms</td>
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<tr>
<td>1992</td>
<td>Simulation of Reactor Pressure Vessel (RPV)</td>
<td></td>
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<tr>
<td>1992</td>
<td>Parallel processing of 2-D Sn algorithms &amp; Acceleration methods</td>
<td>Dr. M. Hunter, W</td>
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<td>1994</td>
<td>Determination of uncertainties in the RPV transport calculations</td>
<td>Prof. B. Petrovic, GT</td>
</tr>
<tr>
<td>1994</td>
<td>3-D parallel Sn Cartesian algorithms</td>
<td>Dr. G. Sjoden, DOD</td>
</tr>
<tr>
<td>1995</td>
<td>Monte Carlo for Reactor Pressure Vessel (RPV) benchmark using Weight-window generator; deterministic benchmarking of power reactors</td>
<td>Dr. J. Wagner, ORNL</td>
</tr>
<tr>
<td>1995</td>
<td>Directional Theta Weight (DTW) differencing formulation</td>
<td>Dr. B. Petrovic</td>
</tr>
<tr>
<td>1997</td>
<td>PENTRAN (Parallel Environment Neutral Particle TRANsport) code system</td>
<td>Dr. G. Sjoden, DOD</td>
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<td>1997</td>
<td>CADIS (Consistent Adjoint Driven Importance Sampling) formulation for Monte Carlo Variance Reduction</td>
<td>Dr. J. Wagner, ORNL</td>
</tr>
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<td>1997</td>
<td>A³MCNP (Automated Adjoint Accelerate MCNP)</td>
<td></td>
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<tr>
<td>2001</td>
<td>Parallel Angular &amp; Spatial Multigrid acceleration methods for Sn transport</td>
<td>Dr. V. Kucukboyaci, W</td>
</tr>
<tr>
<td>2001</td>
<td>Hybrid algorithm for PGNNA device</td>
<td>Dr. B. Petrovic</td>
</tr>
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<td>2001</td>
<td>PENMSH &amp; PENINP for mesh and input generation of PENTRAN</td>
<td>Prof. Haghighat</td>
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<td>2001</td>
<td>Ordinate Splitting (OS) technique for modeling a x-ray CT machine</td>
<td>Prof. Haghighat</td>
</tr>
<tr>
<td>2001</td>
<td>Simplified Sn Even Parity (SSn-EP) algorithm for acceleration of the Sn method</td>
<td>Dr. G. Longonil, PNNL</td>
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<tr>
<td>2004</td>
<td>RAR (Regional Angular Refinement) formulation</td>
<td>Dr. A. Patchimpattapong, IAEA</td>
</tr>
<tr>
<td>2004</td>
<td>Pn-Tn angular quadrature set</td>
<td>Dr. A. Alpan, W</td>
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<td>2004</td>
<td>FAST (Flux Acceleration Simplified Transport)</td>
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<td>2004</td>
<td>PENXMSH, An AutoCad driven PENMSH with automated meshing and parallel decomposition</td>
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<td>2004</td>
<td>CPXSD (Contributon Point-wise cross-section Driven) for generation of multigroup libraries</td>
<td></td>
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<tr>
<td>2007</td>
<td>TITAN hybrid parallel transport code system &amp; a new version of PENMSH called PENMSHXF</td>
<td>Dr. C. Yi, GT</td>
</tr>
<tr>
<td>2007</td>
<td>ADIES (Angular-dependent Adjoint Driven Electron-photon Importance Sampling) code system</td>
<td>Dr. B. Dionne, ANL</td>
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<tr>
<td>2011</td>
<td>TITAN fictitious quadrature set and ray-tracing for SPECT (Single Photon Emission Computed Tomography)</td>
<td>Dr. C. Yi, GT</td>
</tr>
<tr>
<td>2011</td>
<td>FMBMC-ICEU (Fission Matrix Based Monte Carlo with Initial source and Controlled Elements and Uncertainties)</td>
<td>Dr. M. Wenner, W</td>
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<tr>
<td>2011</td>
<td>New WCOS (Weighted Circular Ordinated Splitting) Technique for the TITAN SPECT Formulation</td>
<td></td>
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<tr>
<td>2013</td>
<td>Adaptive Collision Source (ACS) for Sn transport</td>
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<tr>
<td>2013</td>
<td>AIMS (Active Interrogation for Monitoring Special-nuclear-materials), a MRT algorithm</td>
<td></td>
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<tr>
<td>2014</td>
<td>TITAN-SDM - includes Subgroup Decomposition Method for multigroup transport calculation</td>
<td>N. Roskoff, PhD Stud.</td>
</tr>
<tr>
<td>2014</td>
<td>TITAN-IR - TITAN with iterative image Reconstruction for SPECT</td>
<td>K. Royston, PhD Cand.</td>
</tr>
</tbody>
</table>
Remarks

• Particle transport-based methodologies are needed for real-time simulation

• Particle transport codes, even those parallel with hybrid algorithms, are slow because of a 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 Conversation 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

\[ H\psi(\vec{p}) = \frac{1}{k} F\psi(\vec{p}) \]

Where,

\[ \vec{p} = (\vec{r}, E, \Omega) \]

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

\[ F = \frac{\chi(E)}{4\pi} \int_0^{\infty} dE' \int_{4\pi} d\Omega' \nu \sigma_f(\vec{r}, E') \]
FM Derivation (cont)

• We may rewrite above equation as

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

Where,

\[ S = F\psi , \quad A = \bar{F} H^{-1} \chi , \quad \& \]

\[ F = \frac{1}{4\pi} \int_{0}^{\infty} dE' \int_{4\pi} d\Omega' v\sigma_f(\bar{r},E') \]
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**

\[ F_i = \sum_{j=1}^{N} \left( a_{i,j} F_j + b_{i,j} S_j^{\text{intrinsic}} \right) \]

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

- \( b_{i,j} \) 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)
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

<table>
<thead>
<tr>
<th>Case #</th>
<th>Number of Assemblies</th>
<th>Fuel Type</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>1x1</td>
<td>4.95%</td>
</tr>
<tr>
<td>2</td>
<td>6x1</td>
<td>4.95%</td>
</tr>
<tr>
<td>3</td>
<td>3x3</td>
<td>4.95%</td>
</tr>
<tr>
<td>4</td>
<td>9x9</td>
<td>4.95%</td>
</tr>
<tr>
<td>5</td>
<td>1x1</td>
<td>4.45%</td>
</tr>
<tr>
<td>6</td>
<td>6x1</td>
<td>4.45%</td>
</tr>
<tr>
<td>7</td>
<td>3x3</td>
<td>4.45%</td>
</tr>
<tr>
<td>8</td>
<td>9x9</td>
<td>4.45%</td>
</tr>
<tr>
<td>9</td>
<td>2x1</td>
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<tr>
<td>10</td>
<td>6x1</td>
<td>Mixed</td>
</tr>
<tr>
<td>11</td>
<td>3x3</td>
<td>Mixed</td>
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</tbody>
</table>
Case 3 Eigenfunction

Comparison of RAPID with MC
Case 11 Eigenfunction

Comparison with RAPID with MC

Reference Solution

Fission Source

Assembly number

Nuclear Science and Engineering Lab (NSEL) at Arlington
Case 4 Eigenfunction distribution

Comparison with RAPID with MC

Reference Solution

Nuclear Science and Engineering Lab (NSEL) at Arlington
# Comparison of calculated M - RAPID vs. MCNP

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

*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 \(\sim 0.18\) cm
  • Septa thickness \(\sim 0.02\) cm
  • Length \(\sim 3.3\) cm
  • Acceptance Angle \(\sim 1.6^\circ\)

\(S_{20}\) Quadrature Set (440 directions)
\(S_{86}\) Quadrature Set (7568 directions)
4-Stage TITAN Hybrid formulation for SPECT simulation

Stage 1 - Sn calculation in phantom

Stage 2 – Selection of fictitious angular quadrature & Circular OS (COS) directions

Stage 3 – Sn 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)

<table>
<thead>
<tr>
<th>Number of Projection Images</th>
<th>1</th>
<th>4</th>
<th>8</th>
<th>45</th>
<th>90</th>
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</thead>
<tbody>
<tr>
<td>SIMIND Time (sec)</td>
<td>17</td>
<td>67</td>
<td>140</td>
<td>754</td>
<td>1508</td>
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<tr>
<td>TITAN Time (sec)</td>
<td>200</td>
<td>202</td>
<td>212</td>
<td>274</td>
<td>352</td>
</tr>
</tbody>
</table>

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
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:

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

Log-likelihood will have the same maximum location:

\[
\ln(L(\hat{\lambda})) = \sum_{d=1}^{D} (-\bar{n}_d + n_d^* \ln(\bar{n}_d) - \ln(n_d^*))
\]

\[
= \sum_{d=1}^{D} \left[ -\sum_{b=1}^{B} p_{b,d} \hat{\lambda}_b + n_d^* \ln(\sum_{b=1}^{B} p_{b,d} \hat{\lambda}_b) - \ln(n_d^*) \right]
\]

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:

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

\[
\hat{\lambda}_b^{(i+1)} = \frac{\hat{\lambda}_b^{(i)}}{\sum_{d=1}^{D} p_{b,d}} \sum_{d=1}^{D} \hat{n}_d^{(i)} p_{b,d}, \quad b = 1, \ldots, B
\]

- 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)

Initialize problem

Particle transport in patient

\[ H \psi = \lambda^{(i)} \]

For each angle \( \alpha \):
- Generate projection
- Backproject

\[ x_b = x_b + \sum_{d \in \alpha} n_d^* p_{b,d} \]

Modify source & normalize

\[ \lambda_b^{(i+1)} = \frac{\lambda_b^{(i)}}{\sum_d p_{b,d}} x_b \]

Are tolerances met?

Yes

Reconstructed image

No

\[ i = i + 1 \]
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
Reconstruction Analysis

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

  • Mean relative error (MRE)
  \[
  \text{MRE} = \frac{1}{N_d} \sum_{d=1}^{N_d} \left| \frac{\hat{n}_d^{(i)} - n_d^*}{n_d^*} \right|
  \]

  • Mean squared error (MSE)
  \[
  \text{MSE} = \frac{1}{N_d} \sum_{d=1}^{N_d} \left( \frac{\hat{n}_d^{(i)} - n_d^*}{n_d^*} \right)^2
  \]

  • Contrast
  \[
  C_l = \frac{\bar{I}_l - \bar{I}_0}{\bar{I}_0}
  \]

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

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

  \( n_d^* \) = measured counts in detector bin \( d \)

  \( \bar{I}_l \) = 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

*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

2-D Phantom Image Reconstruction with TITAN

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

<table>
<thead>
<tr>
<th>5 Iterations</th>
<th>10 Iterations</th>
<th>20 Iterations</th>
<th>40 Iterations</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="555x687" alt="Image" /></td>
<td><img src="555x687" alt="Image" /></td>
<td><img src="555x687" alt="Image" /></td>
<td><img src="555x687" alt="Image" /></td>
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</tr>
<tr>
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<td><img src="555x687" alt="Image" /></td>
<td><img src="555x687" alt="Image" /></td>
<td><img src="555x687" alt="Image" /></td>
</tr>
</tbody>
</table>

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
2D Phantom: Comparing Reconstructed Images

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

\[
C_l = \frac{\overline{T}_l - \overline{T}_0}{\overline{T}_0}
\]

$\overline{T}_l$ = average source intensity in large circle
$\overline{T}_0$ = average reference background intensity

\[
\text{Likelihood} = L(\hat{\lambda}) = \prod_{d=1}^{D} \frac{e^{-\overline{n}_d} \overline{n}_d^{n_d}}{n_d^{n_d^*}}
\]

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

$n^*$ = 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
Jaszczak Cold Sphere Phantom: Noisy Projection Data with No Collimator Blur

![Graph showing the contrast of spheres with different diameters over iteration number.](image)
Jaszczak Cold Sphere Phantom: Noisy Collimated Projection Data

<table>
<thead>
<tr>
<th>Collimator</th>
<th>Hole Diameter</th>
<th>Septa Thickness</th>
<th>Length</th>
<th>Acceptance Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>GE-LEGPM</td>
<td>0.25 cm</td>
<td>0.03 cm</td>
<td>4.10 cm</td>
<td>1.83°</td>
</tr>
<tr>
<td>SE-LEHR†</td>
<td>0.111 cm</td>
<td>0.016 cm</td>
<td>2.405 cm</td>
<td>1.39°</td>
</tr>
</tbody>
</table>

*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

Comparison of Methods with Jaszczak Phantom

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Noiseless, no collimator blur</th>
<th>Noisy, no collimator blur</th>
<th>Noisy GE-LEGP</th>
<th>Noisy SE-LEHR</th>
</tr>
</thead>
<tbody>
<tr>
<td>FBP</td>
<td><img src="image1" alt="FBP Noisy, no collimator blur" /></td>
<td><img src="image2" alt="FBP Noisy, no collimator blur" /></td>
<td><img src="image3" alt="FBP Noisy GE-LEGP" /></td>
<td><img src="image4" alt="FBP Noisy SE-LEHR" /></td>
</tr>
<tr>
<td>ML-EM with SM only</td>
<td><img src="image5" alt="ML-EM Noisy, no collimator blur" /></td>
<td><img src="image6" alt="ML-EM Noisy, no collimator blur" /></td>
<td><img src="image7" alt="ML-EM Noisy GE-LEGP" /></td>
<td><img src="image8" alt="ML-EM Noisy SE-LEHR" /></td>
</tr>
<tr>
<td>TITAN-IR</td>
<td><img src="image9" alt="TITAN-IR Noisy, no collimator blur" /></td>
<td><img src="image10" alt="TITAN-IR Noisy, no collimator blur" /></td>
<td><img src="image11" alt="TITAN-IR Noisy GE-LEGP" /></td>
<td><img src="image12" alt="TITAN-IR Noisy SE-LEHR" /></td>
</tr>
</tbody>
</table>
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

---

![Graph showing contrast in reconstruction of noisy SE-LEHR projection data for different sphere sizes and methods.](image-url)
Comparison of Methods with Jaszczak Phantom

Noisy GE–LEGp Data Row 19

Noisy GE–LEGp Data Row 46

Source Strength vs. Phantom Voxel
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

<table>
<thead>
<tr>
<th>Processor Cores</th>
<th>Wall Clock Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>575.7</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>291.5</td>
<td>2.0</td>
</tr>
<tr>
<td>4</td>
<td>149.9</td>
<td>3.8</td>
</tr>
<tr>
<td>8</td>
<td>81.4</td>
<td>7.1</td>
</tr>
<tr>
<td>16</td>
<td>36.8</td>
<td>15.6</td>
</tr>
</tbody>
</table>

Noiseless projection data with no collimator blur

<table>
<thead>
<tr>
<th>Processor Cores</th>
<th>Wall Clock Time (s)</th>
<th>Speedup</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1665.7</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>905.1</td>
<td>1.8</td>
</tr>
<tr>
<td>4</td>
<td>524.3</td>
<td>3.2</td>
</tr>
<tr>
<td>8</td>
<td>341.4</td>
<td>4.9</td>
</tr>
<tr>
<td>16</td>
<td>172.0</td>
<td>9.7</td>
</tr>
</tbody>
</table>

Noisy GE-LEGP projection data
Conclusion

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

Questions?