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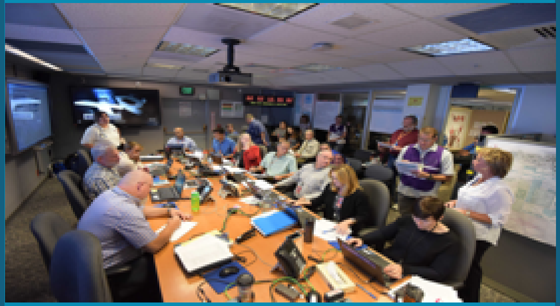
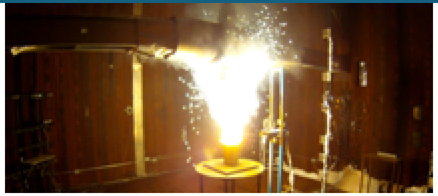
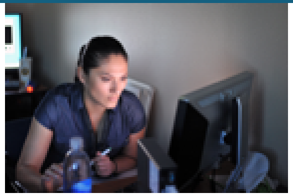
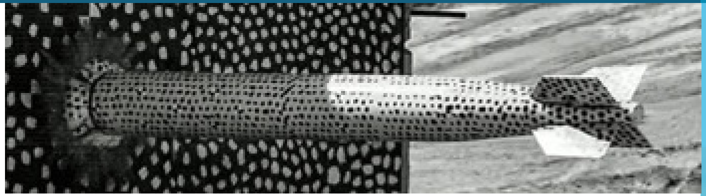
Sandia National Laboratories

Virtual Testbed for Simulating Polychromatic Imaging Systems via PHITS









PRESENTED BY

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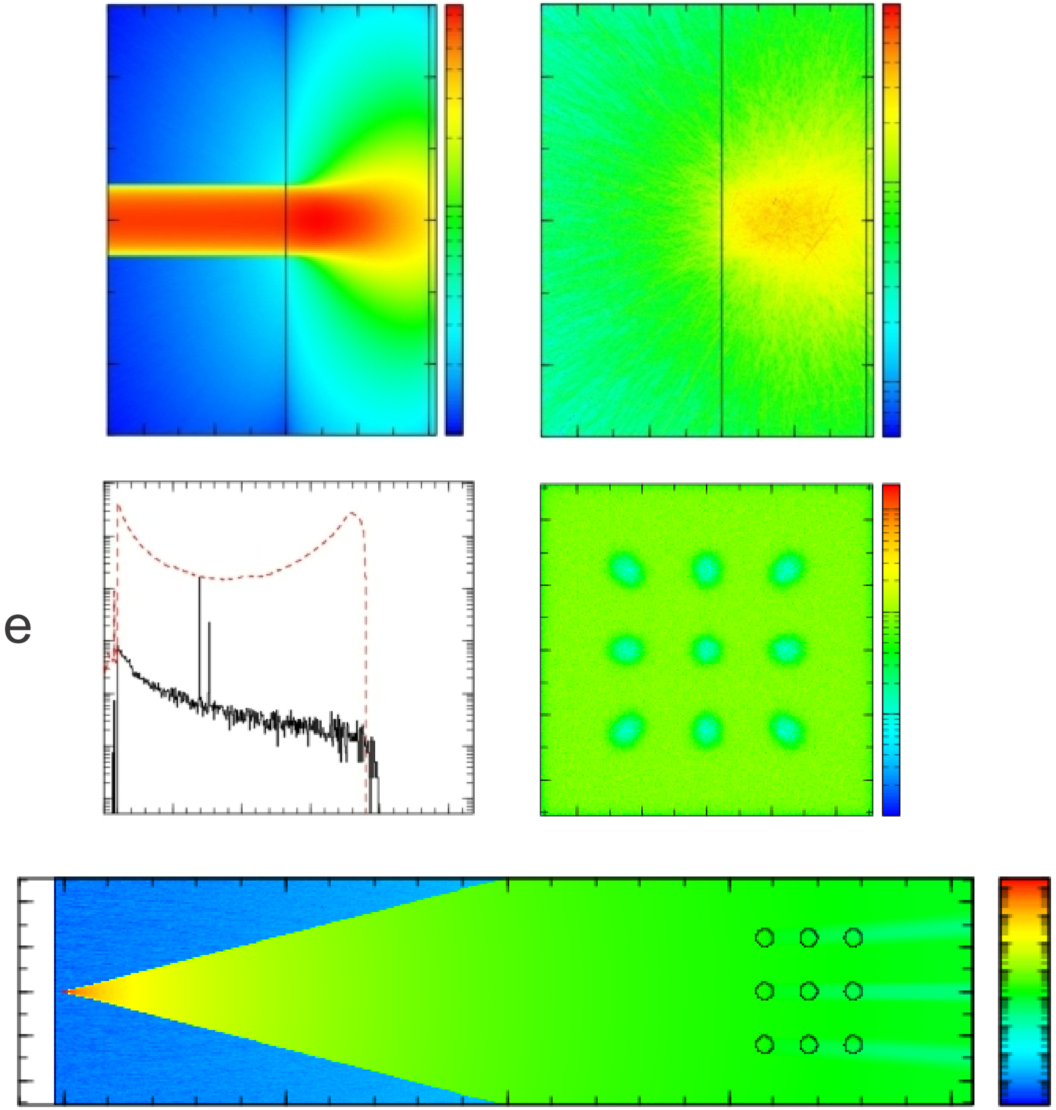
Outline

- Overview of the virtual testbed
- Imaging systems and the integration of Monte Carlo methods in transmission imaging
- X-ray Computed Tomography X-ray CT
- Main features of the radiation and transport particle simulator, PHITS
- Implementation of the prototype
- Applications used to test the performance of the particle simulator
- Results and Discussion
- Conclusion and Future Work

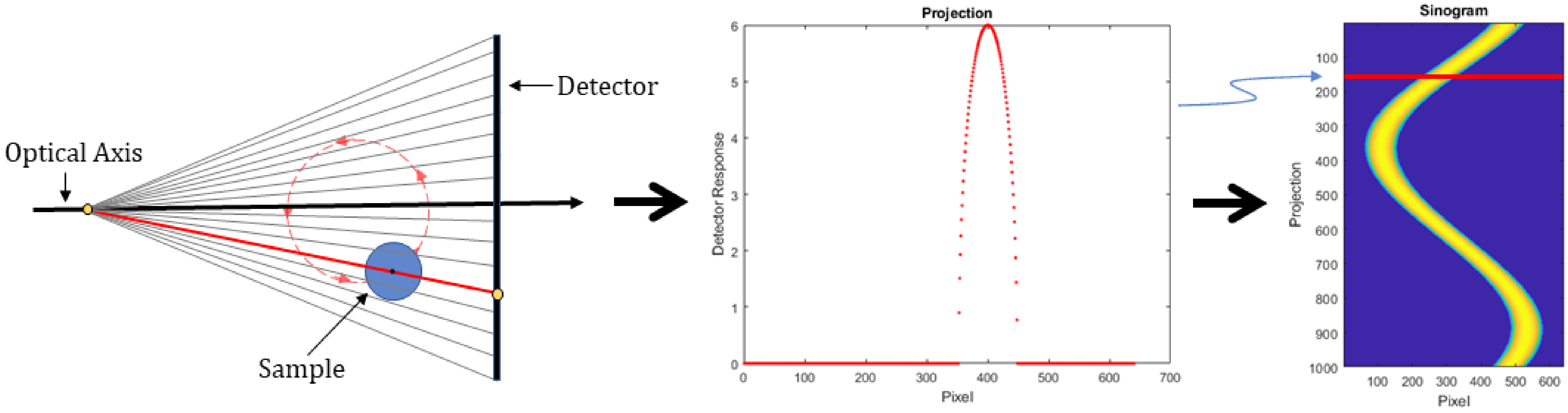


Overview of the Virtual Testbed

- Ability to generate synthetic data
- Allows for the mass generation of imaged data in fields such as national security, industry, and medicine
- Simplifies access to a multifaceted Monte Carlo (MC) based library
- Applications?
  - Anomaly detection
  - Machine Learning
    - Physics informed machine learning (PI-ML) → Material classification and identification

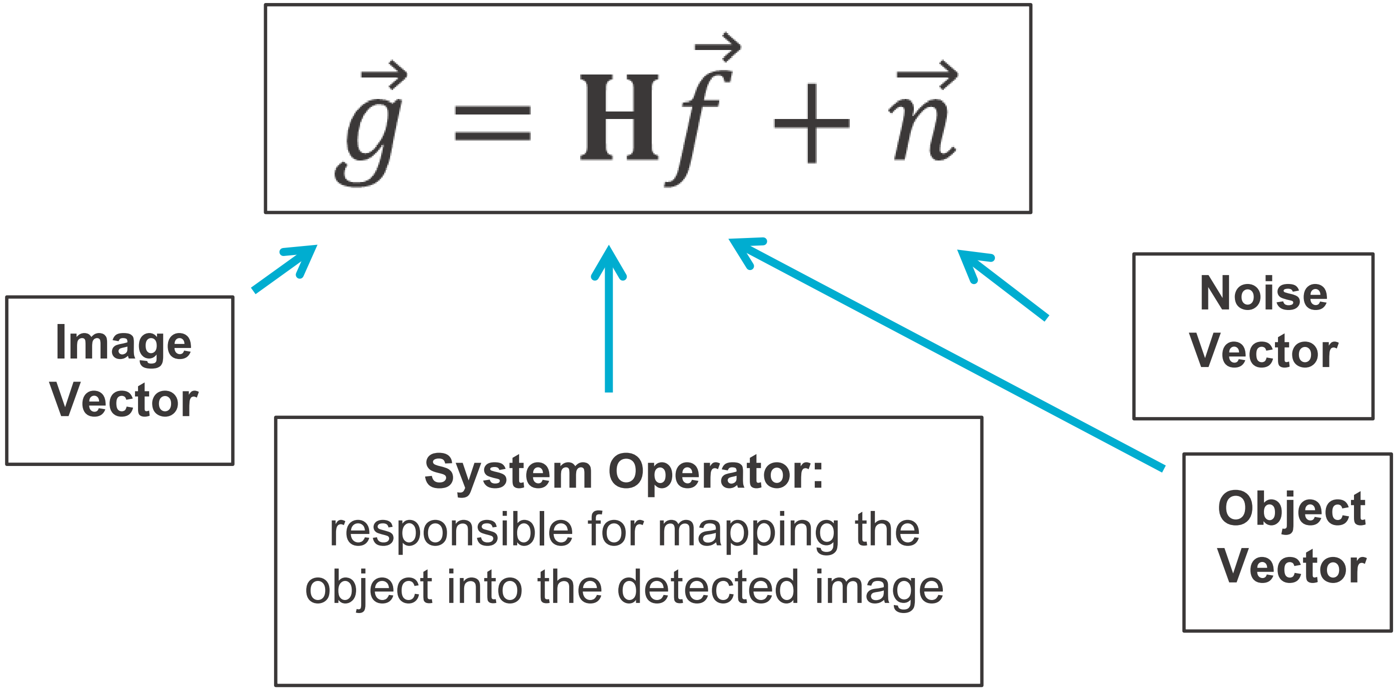
Overview of Imaging System

- This work focuses on a particular type of indirect imaging, namely X-ray Computed Tomography (CT)
  - X-ray CT is a 3D imaging technique where an x-ray source and a detector are diametrically rotated around an object to generate projection data
  - Once the projection data is generated, image data is post-processed with a reconstruction algorithm which produces cross-sectional slices of internal and external structure of imaged object



Overview of Imaging System: Continued

- Image formation process is a mapping from one Hilbert space to another
- For our imaging system, we will consider a Hilbert-space operator
- Traditional vs X-ray CT System Operator:
  - Traditional System Operator → Highly nonlinear due to the nonlinear relationship between material, geometry, thickness, and energy
  - X-ray CT System Operator→ Linear!

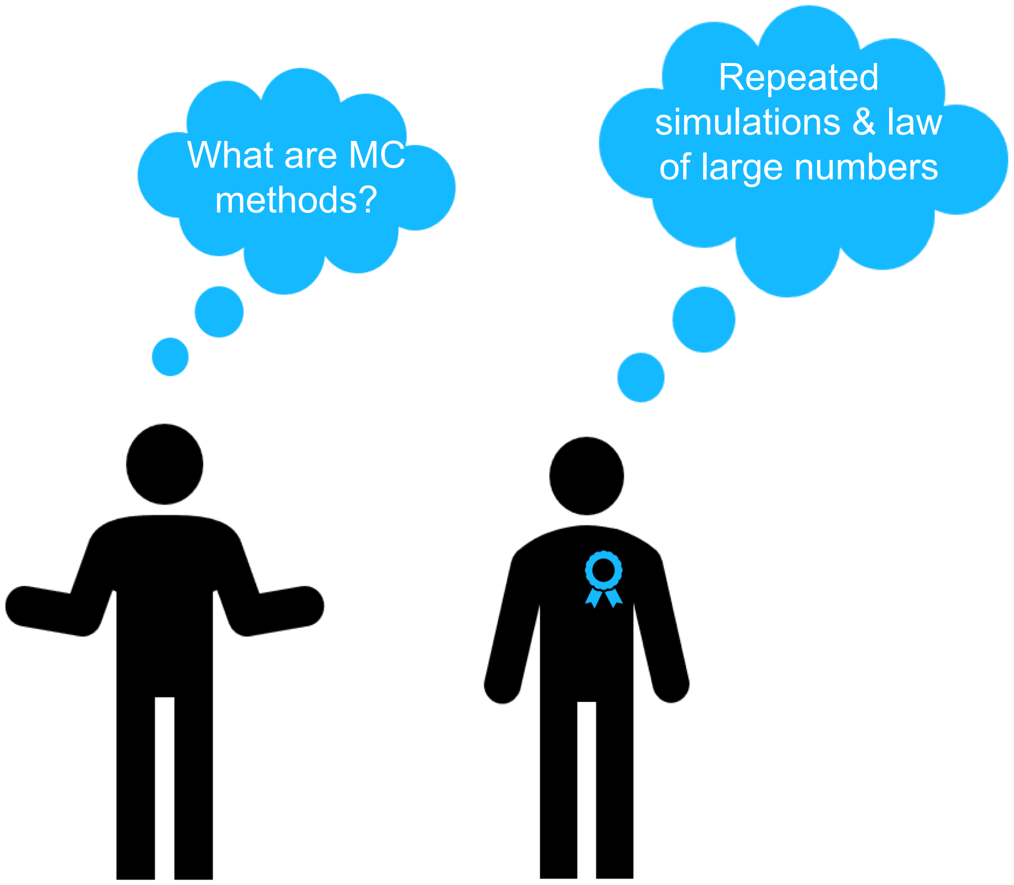


Hyperspectral X-ray Computed Tomography Imaging System

SNL has developed the ***world's only hyperspectral x-ray computed tomography (H-CT) imaging system*** specifically engineered and designed for industrial and security applications.

- 500 mm field-of-view
- 300keV maximum energy (detector limited)
- 640×640 voxel slices with submillimeter resolution
- Successfully demonstrated material identification across multiple materials
- For a majority of NDE applications, low energy is not feasible due to lack of penetrating power
- Imaging system operator is a sequence of linear operators

Monte Carlo Methods: Overview of Monte Carlo Methods

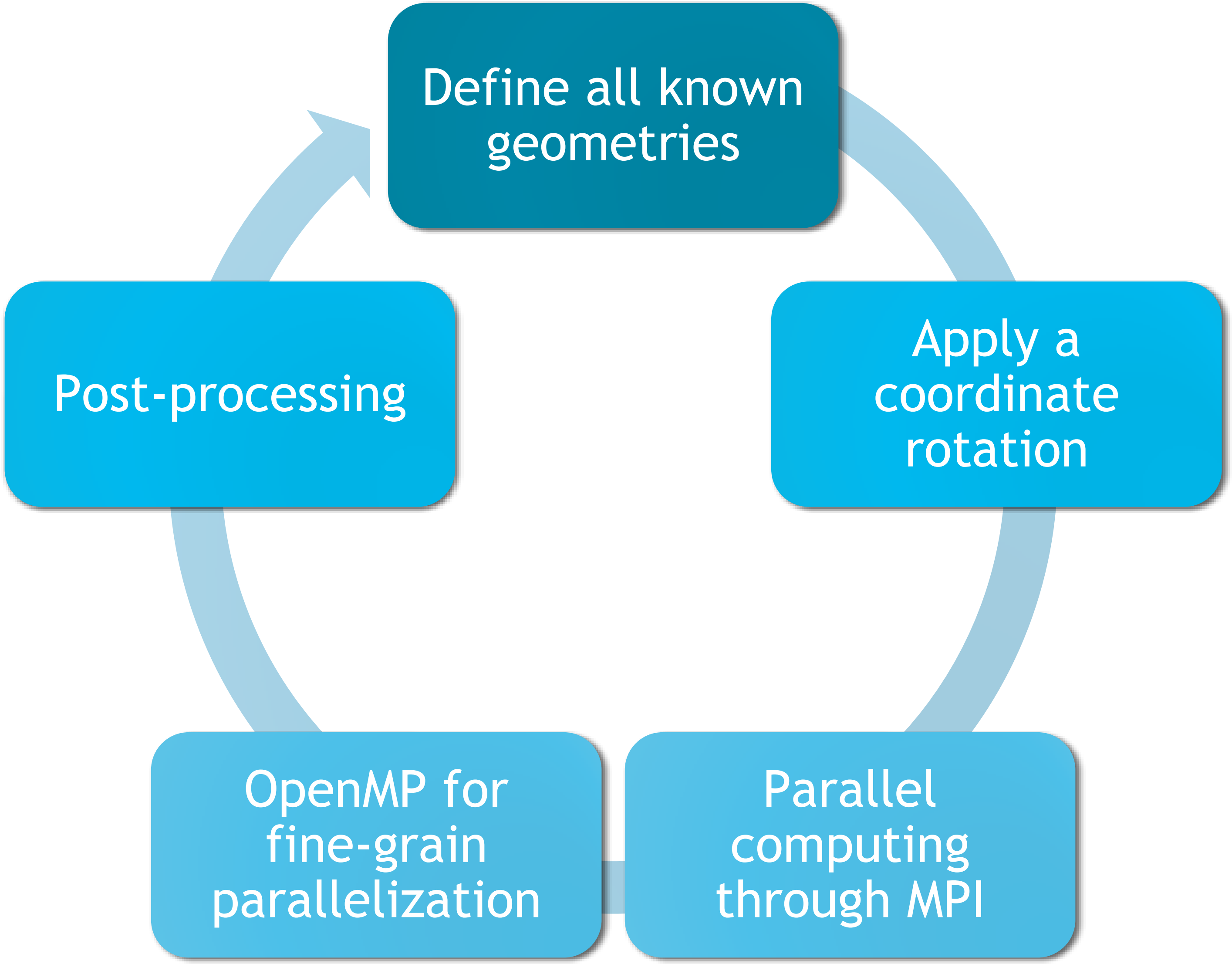


- MC methods are used to model the outcome of complex environments where random variables are present
- MC method simulates expected behavior of a particle and determines the probability of a particle interacting with the object in the field-of-view (FOV)
  - Pivotal in analyzing particle transport over broad energy ranges
  - Investigating the integrity of an imaging system
  - Assisting in detector design
  - In-depth analysis of radiation transport and optimization of computer algorithms
- Essential tools for investigating outcome of mathematical or physical experiments that are often difficult or impossible to determine otherwise
  - Physical data acquisition → long time
  - Simulations → access to parallelization techniques

Particle and Heavy Ion Transport code System (PHITS)

- General-purpose MC particle transport code system developed by the Japanese Atomic Energy Agency (JAEA)
  - Capable of tracking the transport of particles over wide energy ranges
  - Compatible with Linux, Macintosh, and Windows platforms
  - All contents of the system are fully integrated into one package
- PHITS offers features to perform parallelization techniques
  - Message Passing Interface (MPI) or open multiprocessing (OpenMP) conventions
  - Hybrid MPI and OpenMP features are also attainable
- Novelty of work:
  - Using PHITS to simulate environment of a polychromatic imaging system while employing distributive and shared memory parallelization techniques through available MPI and OpenMP features

Approach


Define all known geometries
Apply a coordinate rotation
Parallel computing through MPI
OpenMP for fine-grain parallelization
Post-processing

Implementation

Software:
- MATLAB 2018a
- PHITS Version 3.02
- FORTRAN
- Intel Visual Fortran Compiler 19.0 Update 3
- Windows HPC package

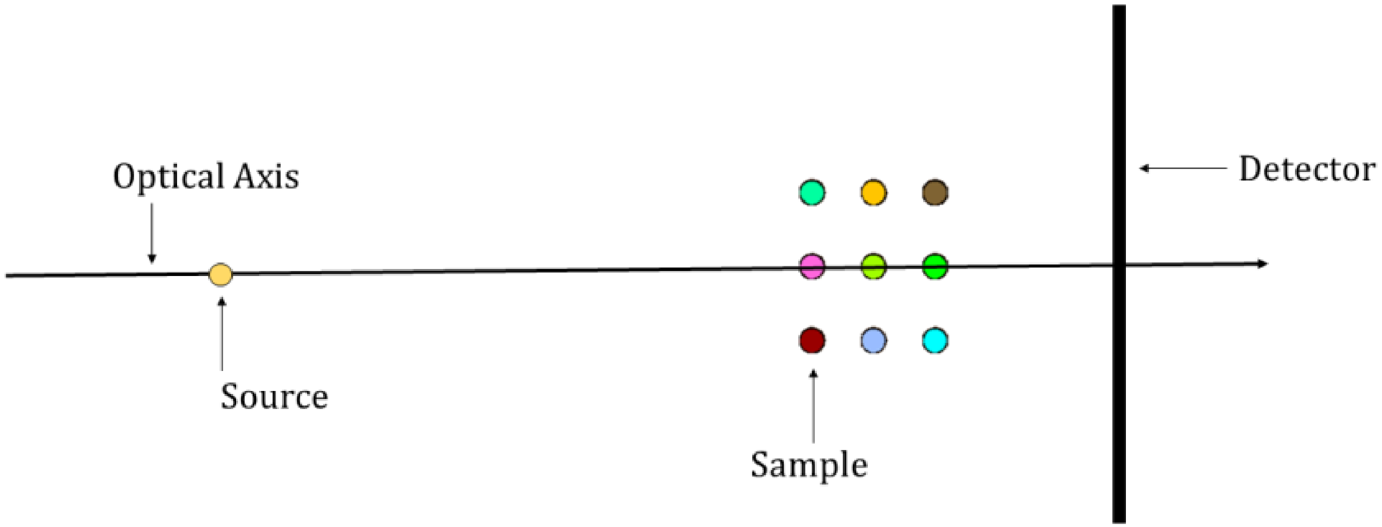
Hardware:
- Microsoft Windows Server 2012 R2
- OpenMP
- MPI

Simulation:
- Shared memory parallel computing schemes were implemented by defining the number of available CPU cores
- Number of jobs distributed across each node is exactly equal to the total number of simulated projections
- Once each task is submitted and the simulated image dataset is complete, a MATLAB script is ran to create sinogram data from the MC output
  - A CT reconstruction algorithm, RECON, is used to create sinogram data for each energy-channel to generate cross-sectional slices of the imaged object

Experimental Design

- Material classification and identification purposes using various neural network architectures
  - Neural network application

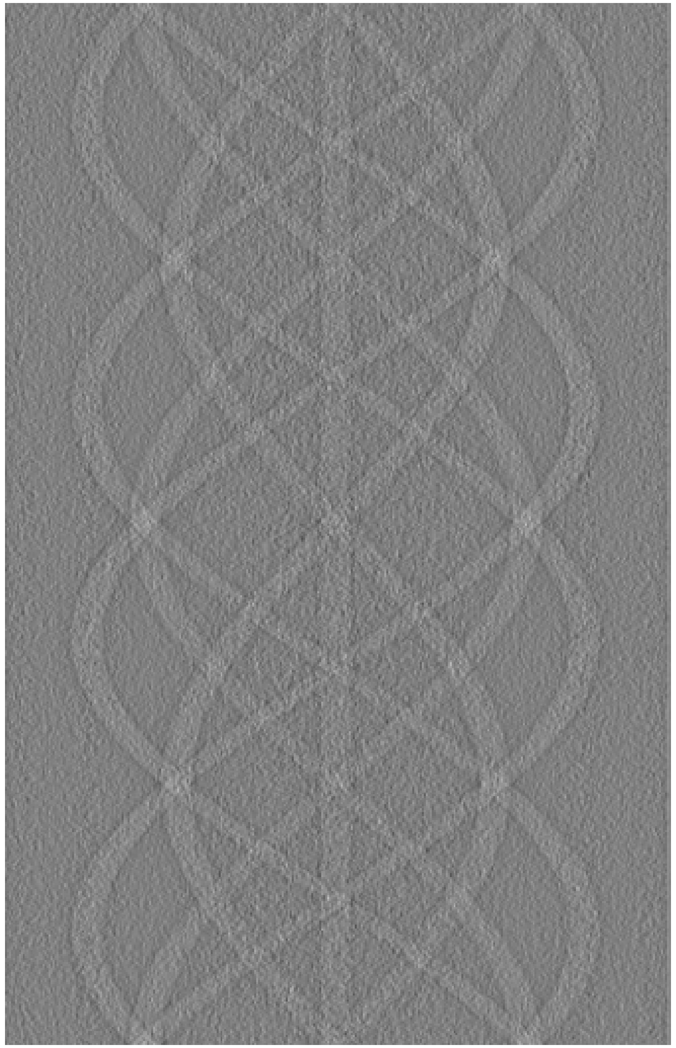
- Testbed was used to generate simulated datasets with nine samples of water, hydrogen perc



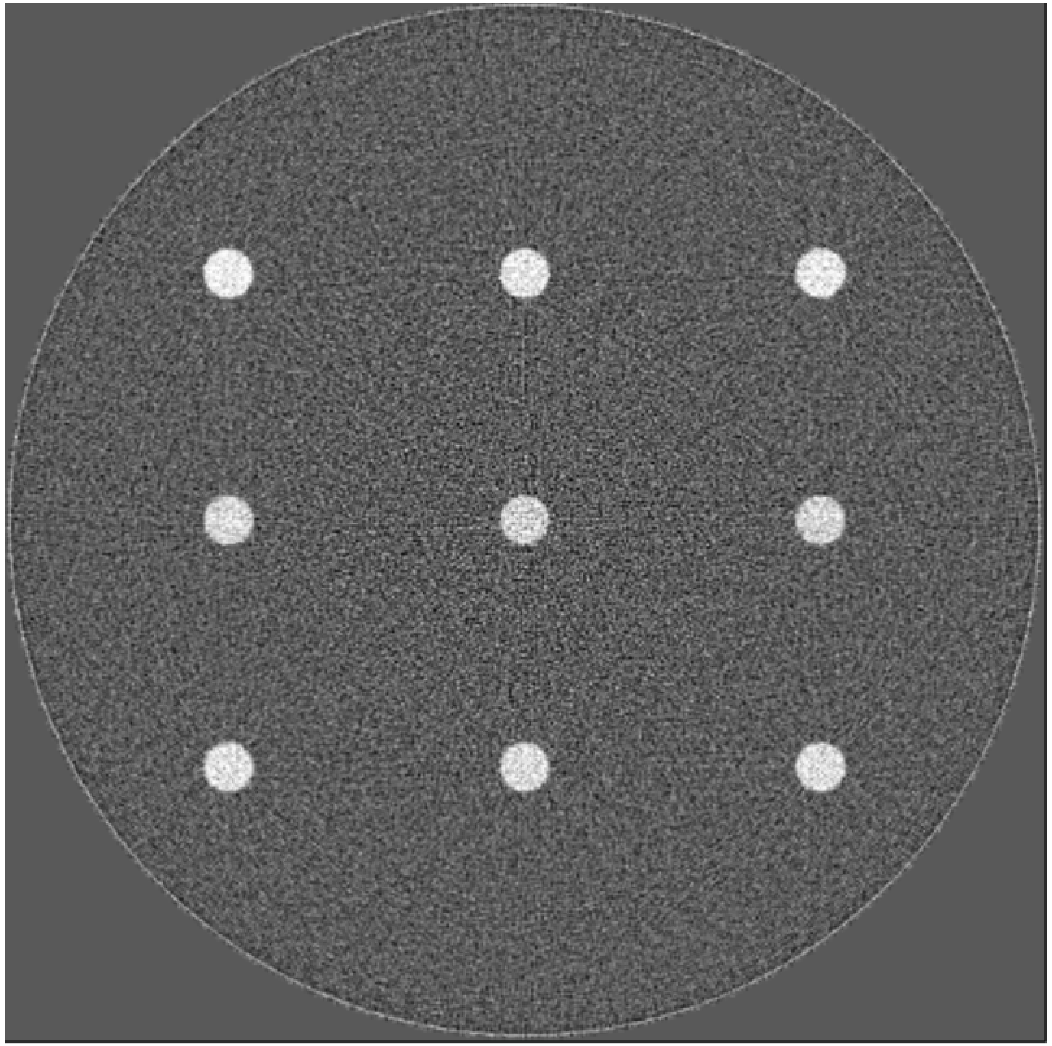
Experimental Design: Continued

- Classifiers were trained using Water, HP, and RDX
- Each material was simulated in different shielding conditions: no shielding, aluminum shielding (30 mm), and polyethylene shielding (1, 2, and 30 mm)
- Each scan was manually segmented to identify the material, shielding if applicable, and valid region of the scan
- From segmentation, a label corresponding to a given material and shielding type was then applied to each voxel
- In total, the data set consists of 84 images, where each image contains 640x640 voxels and each voxel consists of 128 channels

Experimental Design: Continued



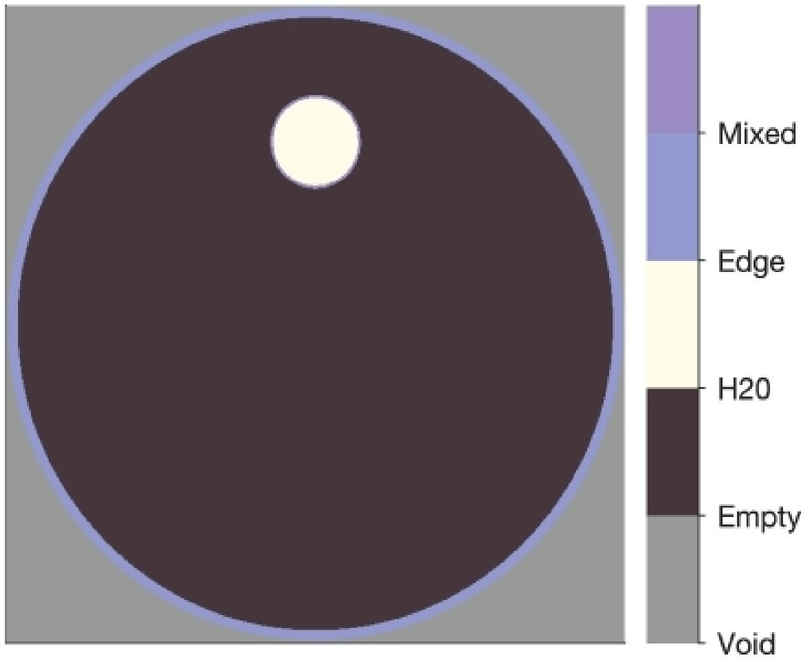
Sinogram Data of Nine H202 Samples (Channel 60)



Reconstruction of Nine H202 Samples (Channel 60)

Experimental Design: Continued

- Void labels denotes pixels that are outside of the scanning region
- Empty label denotes voxels inside the scanning valid containing air
- Water label denotes the voxels that contain the water sample
- Edge label denotes the voxels that are adjacent to the valid and non-valid scanning regions
- Mixed label denotes the voxels that are adjacent to the water and empty voxels



Results and Discussion

- Although we have obtained very high classification accuracy for each material type with this data it is expected that the classifier performance will be degraded with scans collected from real instrumentation
- From the results below, the U-Net model outperformed both the DNN and CNN models, where the DNN had the worst performance
- All three models perform the worst on classifying voxels labeled as mixed, which is expected since a single voxel contains different fractions of adjacent materials.

Material	DNN			CNN			U-Net		
	PREC	RCL	F1	PREC	RCL	F1	PREC	RCL	F1
Void	N/A	N/A	N/A	N/A	N/A	N/A	100.0	99.8	99.9
Empty	67.2	89.9	76.9	90.1	77.2	83.1	100.0	99.7	99.8
H_2O	34.6	28.7	31.4	70.8	66.9	68.8	98.7	97.6	98.2
H_2O_2 [100%]	91.3	31.0	46.2	94.3	87.9	91.0	99.8	99.8	99.8
H_2O_2 [90%]	40.2	73.0	51.8	77.8	94.8	85.5	99.4	98.4	98.9
H_2O_2 [80%]	58.3	77.8	66.7	90.6	98.2	94.2	99.6	96.5	98.0
H_2O_2 [70%]	62.3	68.7	65.3	84.2	87.9	86.0	99.9	95.0	97.4
H_2O_2 [60%]	47.2	80.8	59.6	93.8	94.8	94.3	99.8	95.4	97.5
H_2O_2 [50%]	68.7	94.1	79.4	90.9	93.1	92.0	99.5	97.8	98.6
H_2O_2 [40%]	63.5	75.4	68.9	84.4	86.7	85.5	100.0	91.7	95.7
H_2O_2 [30%]	42.6	14.5	21.7	81.9	93.8	87.5	98.9	96.8	97.8
H_2O_2 [20%]	61.8	34.3	44.1	90.1	91.1	90.6	100.0	95.3	97.6
H_2O_2 [10%]	55.0	51.2	53.1	96.6	99.8	98.2	99.5	96.6	98.0
RDX	89.3	100.0	94.4	94.4	99.9	97.1	98.0	99.6	98.8
Al [30 mm]	89.4	100.0	94.4	95.1	99.4	97.2	99.2	97.9	98.6
Poly [30 mm]	42.7	44.1	43.4	70.2	65.4	67.7	97.7	94.9	96.3
Poly [1mm]	40.9	13.5	20.3	64.8	72.5	68.4	86.5	99.2	92.4
Edge	96.5	100.0	98.2	99.3	100.0	99.6	95.9	100.0	97.9
Mixed	51.4	19.1	27.9	91.8	34.0	49.7	77.0	94.5	84.9

Conclusion and Future Work

- Testbed can be used to simulate nonlinear and linear polychromatic imaging systems with high fidelity as demonstrated by Gallegos et al. [12] for the characterization of the system operator and the PI-ML application for deep learning methods
- Ability to simulate such imaging systems using MC methods allows for the generation of large amounts of synthetic data, creating new frontiers for applications in machine learning and material identification, classification, and quantification
- Demonstrated the feasibility of using MC methods for the creation of synthetic data from a stochastic standpoint
- More work must be done to capture other sources of stochastic noise, such as temporal noise for a real-world H-CT imaging system
- Additional future work lies in leveraging MC techniques to aid in the optimization of iterative reconstruction algorithms and detector design for imaging systems