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EASTERN TIME [GMT-4]

Design and validation of X-ray Diffraction in MCGPU

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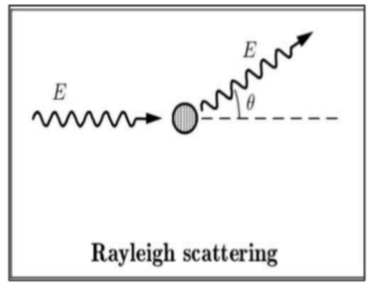
INTRODUCTION

- Monte Carlo simulations are ubiquitously considered the gold standard in radiation transport simulations because of its statistics- based approach of tracking each particle interaction rather than relying on analytical physics models.
- MCGPU distinguishes itself from other Monte Carlo simulation packages because it runs on a GPU leading to demonstrably faster computation times (40x faster than a CPU).
- While traditional x-ray transmission imaging is based mostly on material density, XRD (x-ray diffraction) has shown promise in material characterization and identification because of its ability to obtain material specific information based on chemical and structural information.
- The XRD scatter signal is collected from photons that have undergone rayleigh scattering – a photon-atomic interaction event that occurs at low energy.
- MCGPU is verified against theoretical data by comparing detected scatter intensity and distribution and is validated against experimental data by again comparing detected scatter intensity and distribution.
- Once MCGPU is validated against the pencil and fan beam systems, a rapid simulation toolkit can be designed for cancer detection in the medical realm or opioid/explosives/threat detection in the aviation security realm.

Rayleigh interaction probability

$$\frac{d\sigma_{Ra}}{d\Omega} = \frac{d\sigma_T}{d\Omega}[F(q,z)]^2$$

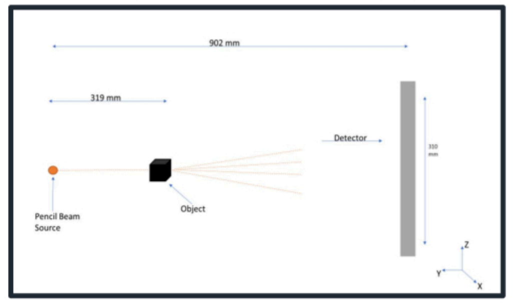
$$\frac{d\sigma_T}{d\Omega} = r_e^2\,\frac{1+\cos^2\theta}{2}$$



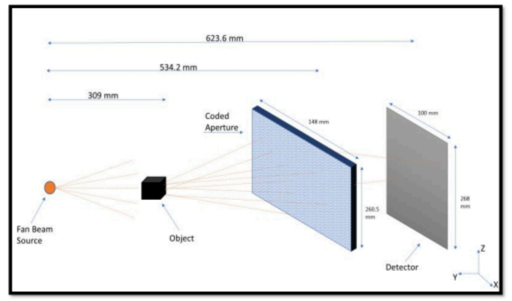
METHOD

- MCGPU requires an input file containing molecular and chemical information about the material being scanned: this is typically in the form of an F(q) (Form factor) curve.
- The geometry, source, MCGPU material file, and number of histories(photons) are specified in an input file then the simulation is run.
- A data file containing the 2D Rayleigh scatter data is extracted and processed in MATLAB for analysis.

Pencil Beam (ED LAUE) Scanner

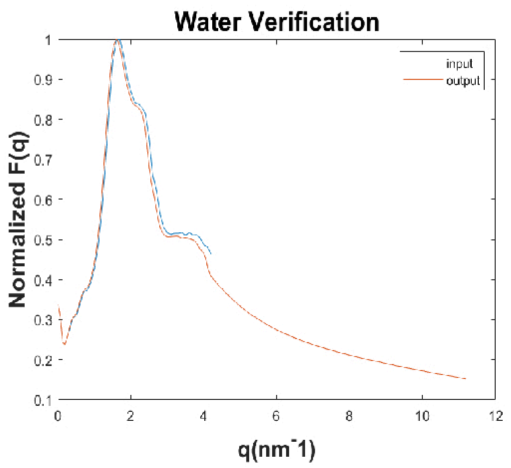


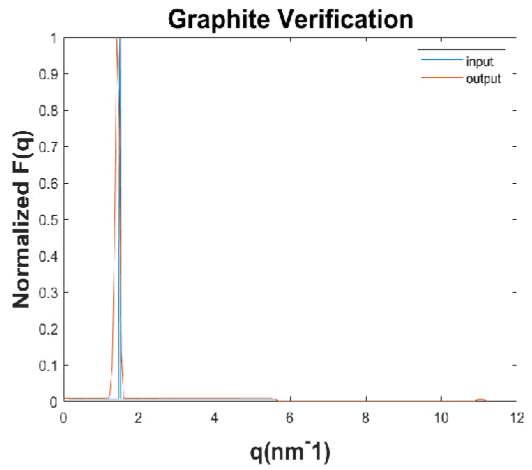
Fan Beam Scanner

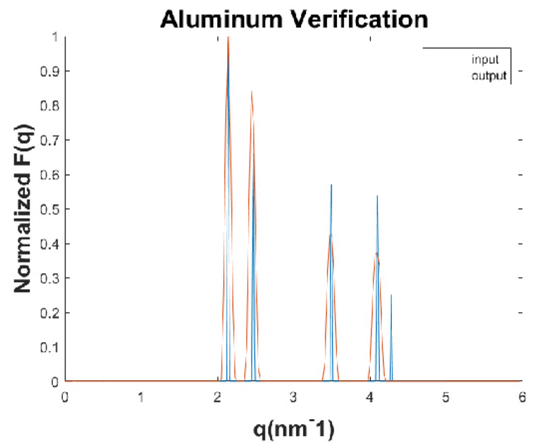


- Form Factor (F(q)) plots can be used to discern the relative scatter intensity on a 2D detector. For an isotropic signal, the scatter intensity can be integrated for a given radius and normalized to the maximum intensity to procure spectral information.

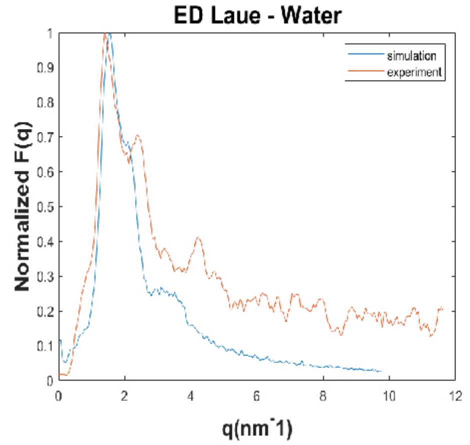
Verification

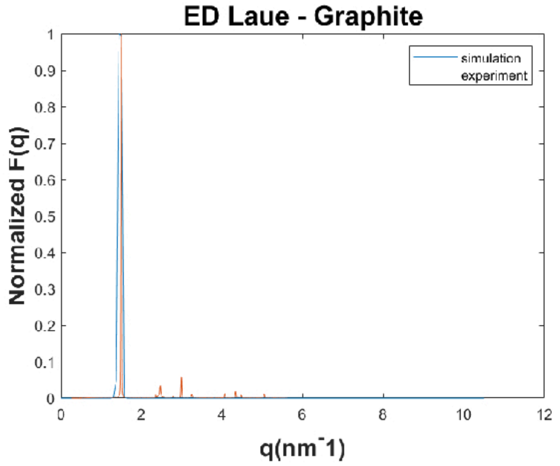






Validation – Pencil Beam System





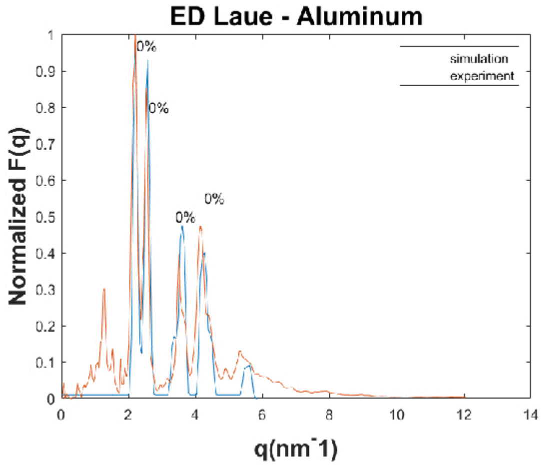


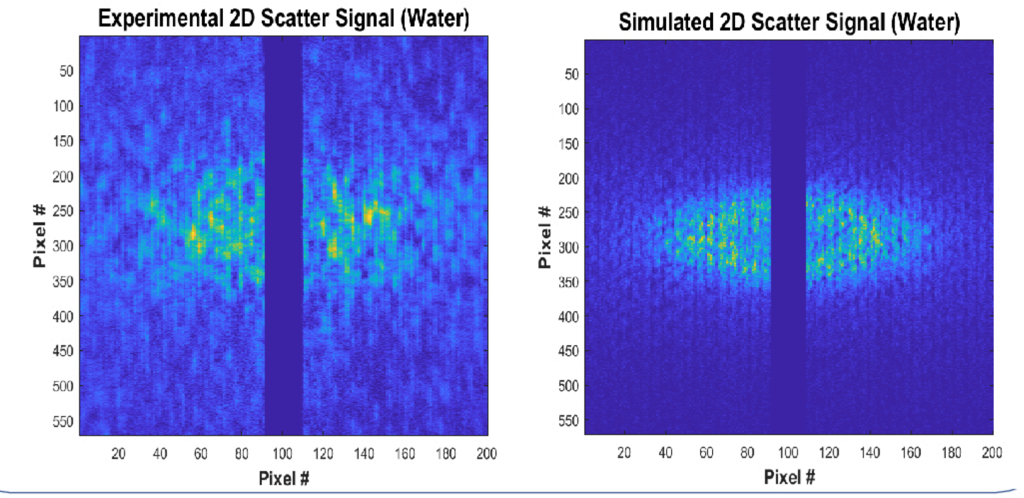
Table 1: Simulated vs Theoretical Attenuation Coefficients

Material	NIST (cm^-1)	Simulation (cm^-1)	%Difference	Absolute Difference
Graphite	0.02	0.021	4.60%	0.001
Aluminum	0.091	0.086	3.90%	0.005
Water	0.014	0.014	0.30%	0

Table 2: Simulated vs Experimental Peak Locations

Material	Exp. Peak Location(nm^-1)	Sim. Peak Location(nm^-1)	%Difference
Graphite	1.49	1.43	4.10%
Water	1.57	1.51	3.89%
Aluminum - 1	2.22	2.22	0%
Aluminum - 2	2.54	2.54	0%
Aluminum - 3	3.51	3.51	0%
Aluminum - 4	4.16	4.16	0%

Validation – Fan Beam System – 2D Scatter Comparison



CONCLUSIONS

- **The comparison metrics (peak location and attenuation coefficient percent differences) verify MCGPU simulations against theoretical data; all peak location and attenuation coefficients have percent differences < 5%.**
- **The peak location percent difference and the relative scatter intensity and 2D scatter distribution validate MCGPU against the pencil beam test bed. (again, all peak location percent differences < 5%).**
- **The fan beam system is still in the early validation stage: the 2D scatter signal from water shown above features the coded aperture that was added in the MCGPU model.**
- **Moving forward, the validated MCGPU simulator will be used to model complex geometries and scanners for a diverse set of materials and system configurations.**

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