

Abstract

Pencil beam algorithms^{1,2,3} are fast but inaccurate in heterogeneous media, while Monte Carlo (MC) simulation is accurate but too slow for routine use. Conceptually, primary protons propagate nearly rectilinearly, but are subject to continuous energy loss and angular changes; we use this behavior to classify particles into primary protons and secondary particles — analogous to the primary/secondary decomposition used for photons.

Rather than classifying primary protons by interaction type, we use statistics: a per-step energy-loss threshold, $\Delta E_{\text{thresh}} = 1.2(2P_{99} - P_{98})$, where P_{98} and P_{99} are the 98th and 99th percentiles of the per-step energy-loss distribution at a given incident energy — i.e., the threshold linearly extrapolates one step past the 99th-percentile energy loss into the distribution's tail, with a $1.2\times$ safety margin. This threshold is derived from a voxelized Geant4 simulation of a 250 MeV pencil beam in a water phantom with 1 mm^3 voxels. Using the resulting per-step angular and range-resolved energy statistics, we implement a custom Monte Carlo simulation of primary proton fluence. Validated against Geant4 ground truth via a gamma index computed on $\log_{10}$ -fluence maps, the custom MC achieves a 73.5% passing rate at a 1%/1mm criterion, while running $18.36\times$ faster (14 s vs. 257 s for 10^8 particles on 120 threads).

Introduction

- Proton therapy's Bragg peak gives a sharp dosimetric advantage over photons, but pencil beam scanning (PBS) plans require the dose from thousands of individual spots to be computed separately during optimization — a heavy computational burden.
- Two existing approaches, each with a fundamental trade-off:
 - Pencil beam (PB) algorithms:** fast (convolution of an analytical dose kernel with fluence), but the lateral/central-axis decomposition breaks down under oblique incidence and at lateral heterogeneity^{4,5}, causing dose errors of 30%+ in heterogeneous sites such as lung.
 - Monte Carlo (MC) simulation:** the gold standard for accuracy, but particle-by-particle transport imposes an irreducible computational cost (~1 hour on a 100-core cluster for a full treatment plan), too slow for iterative optimization or online adaptive replanning.
- Long-term goal:** develop an analytical proton dose calculation framework, in which the primary proton fluence serves as the source term from which the secondary particle fluence — and ultimately dose — is derived, analogous to the collapsed-cone convolution/superposition (CCCS) approach used for photons (e.g., Acuros XB).
- This work:** as a first step toward that goal, we focus on characterizing and modeling primary proton fluence. Unlike photons, protons interact continuously with matter (no clean "first interaction" boundary), so the primary/secondary split must be defined operationally from simulation data rather than by interaction type.

Methods and Materials

1. Primary proton definition

Simulated a monochromatic 250 MeV pencil beam in a $255 \times 255 \times 512$, 1 mm^3 -voxel water phantom in Geant4⁶ (10^7 particles), classifying each simulation step as primary or secondary by its energy loss. No angular threshold is imposed, which limits the per-step attenuation rate — the fraction of primary protons reclassified as secondary at each step — keeping the primary population dominant throughout the phantom.

2. Single-voxel angular scattering statistics

Fired monochromatic beams (1–250 MeV, 1 MeV steps, 10^6 particles/energy) through an isolated 1 mm^3 voxel and recorded the net angular deflection of protons that stayed primary through exit. Angular deflection is empirically independent of concurrent energy loss.

3. Range-resolved energy spectrum

Full-phantom Geant4 simulation (10^7 particles), applying the Step 1 threshold, tallying energy, direction, and position at each cumulative-range checkpoint. The energy spectrum at a given range is empirically independent of both lateral radius and cumulative deflection angle, so range alone characterizes a primary proton's energy state, $p(E | r)$. The cumulative angular distribution is heavier-tailed than a Rayleigh/Gaussian model at every checkpoint, motivating a directly measured kernel over a Gaussian approximation.

4. Custom Monte Carlo simulation & validation

Combined $p(\alpha | E_{\text{in}})$, $p(E | r)$, and the attenuation curve $p_{\text{SURV}}(r)$ into a table-driven simulator that advances particles step by step in range, sampling a deflection and depositing fluence weighted by $p_{\text{SURV}}(r)$ at each step. Validated against Geant4 via 2D/1D fluence comparisons, a $\log_{10}$ -fluence gamma index, and runtime (both configured for dense-grid accumulation, same thread count).

Results

- Primary proton fluence is highly collimated along the beam axis** and back-projected fluence shows near-axis targets are reached by compact, near-parallel trajectories, while off-axis targets are reached by more dispersed trajectories. (**Figure 1**)
- Single-voxel statistics:** angular scattering distributions are nearly indistinguishable across energy-loss bins at each incident energy, confirming energy/angle independence within a voxel; mean energy loss per voxel decreases from ~2.74 MeV at 20 MeV incident to ~0.41 MeV at 230 MeV. (**Figure 2**)
- Custom MC vs. Geant4 validation:** 2D fluence maps nearly identical. (Figure 3)

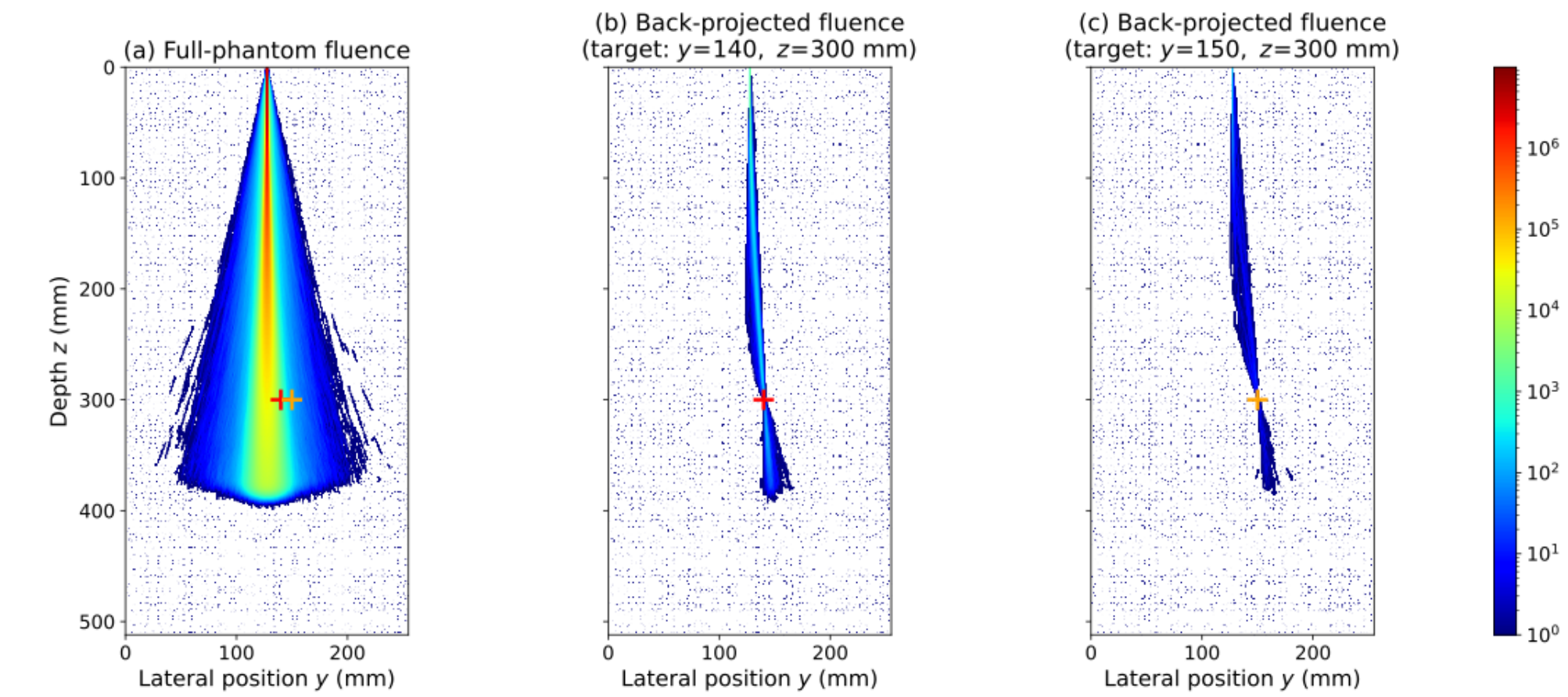


Figure 1. Central yz slice of primary proton fluence (log scale, 250 MeV beam): (a) full-phantom fluence; (b–c) back-projected fluence for a near-axis vs. an off-axis target

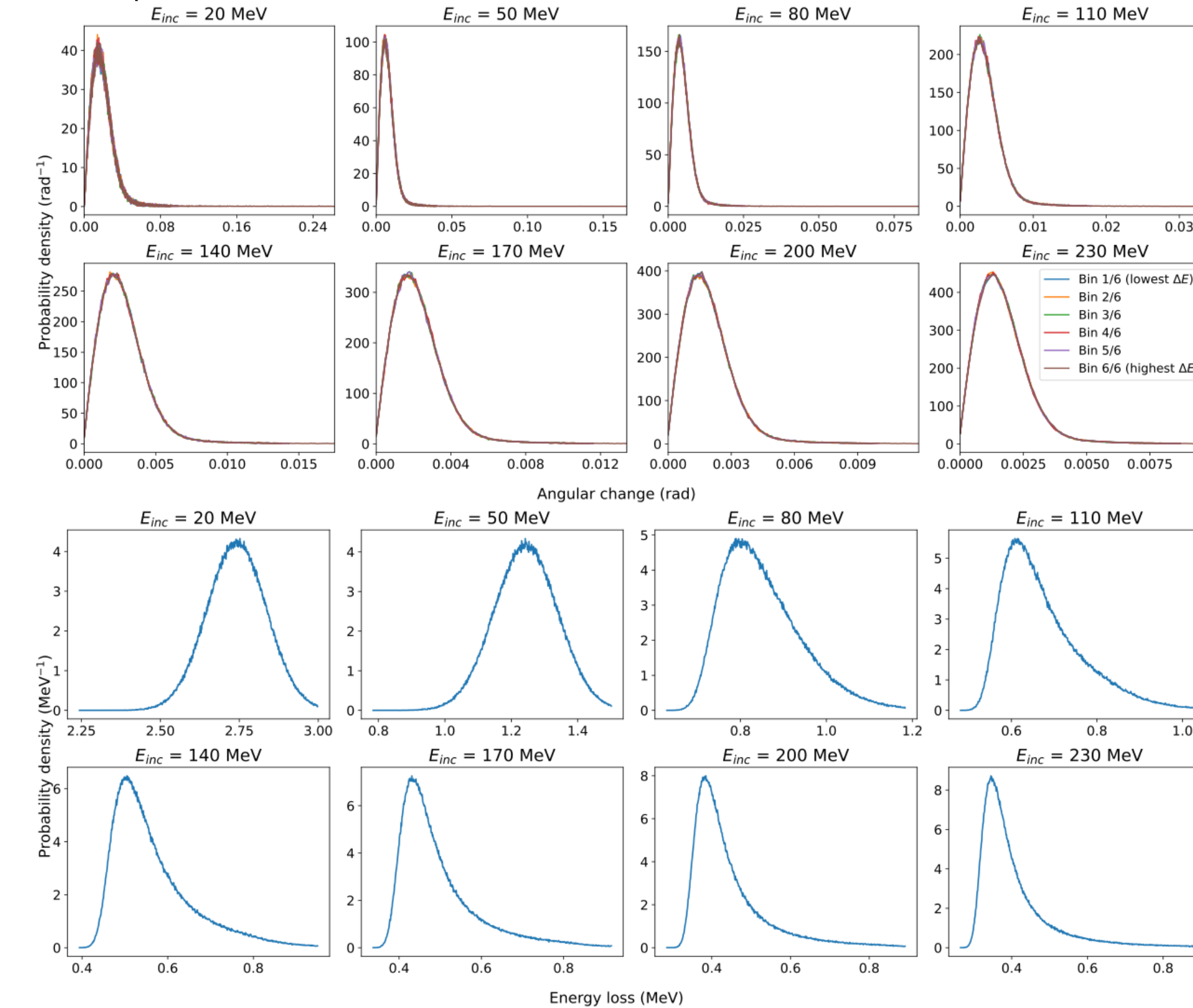


Figure 2. Statistics for primary protons traversing a single 1 mm^3 water voxel at eight incident kinetic energies (10^6 particles/energy). Upper: angular scattering distributions, stratified into six equal-probability energy-loss bins. Lower: Energy loss distributions.

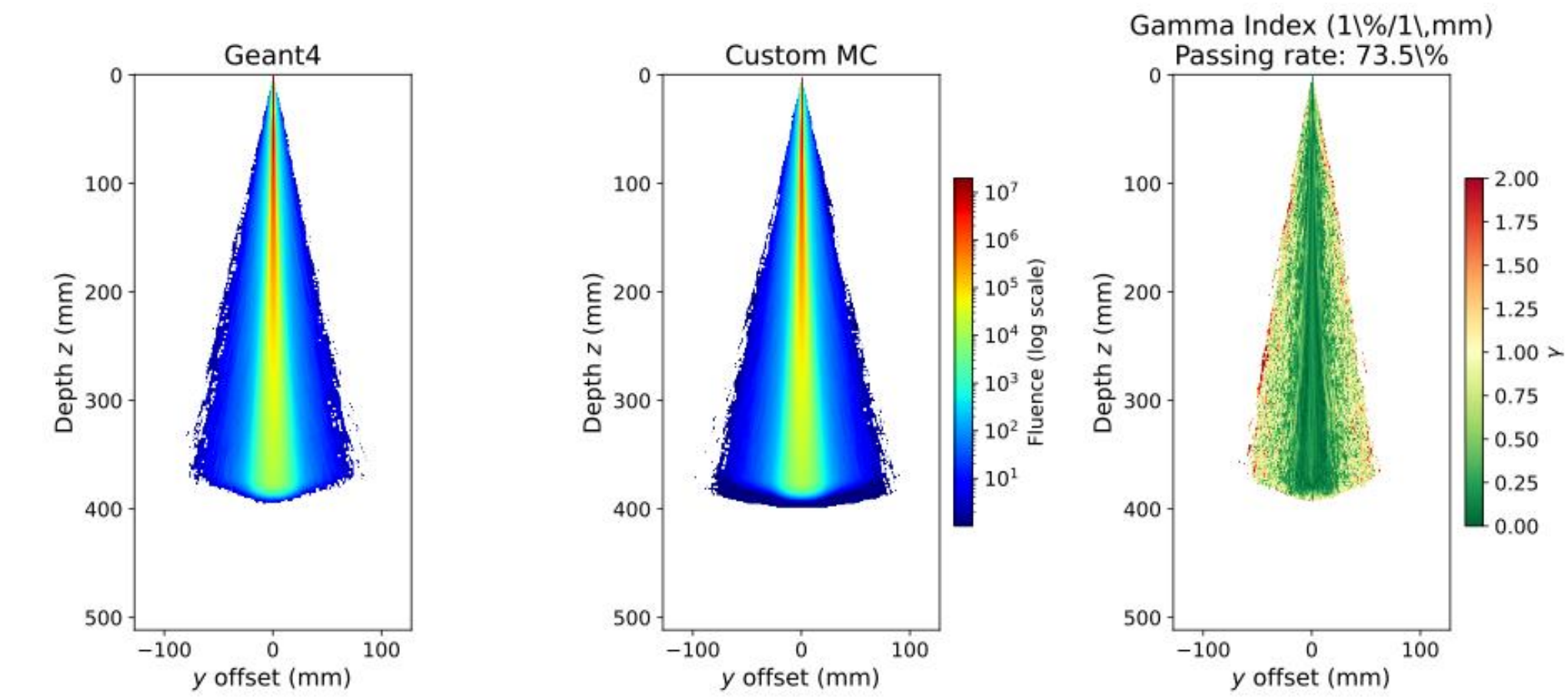


Figure 3. Central yz slice of primary proton fluence for a 250 MeV pencil beam (log scale): (a) Geant4, (b) Custom MC, (c) gamma index map (1%/1mm criterion, computed on $\log_{10}$ -fluence).

Discussion & Conclusions

Two empirical independence properties (angle $\perp$ energy loss per voxel; energy spectrum $\perp$ radius/angle at fixed range) justify a compact three-table statistical representation of primary proton transport — a per-step angular kernel, a range-resolved energy spectrum, and an attenuation curve — which together fully and accurately describe primary proton transport in a homogeneous phantom, validated against Geant4.

Future steps:

- Path to heterogeneous media:** extending to heterogeneous phantoms is conceptually straightforward — step size fixed in water-equivalent terms, physical step length derived per voxel from local stopping power relative to water.
- Path to dose:** computing dose (not just fluence) requires the secondary-particle contribution at each voxel, which in a CCCS-style framework depends on the local primary energy spectrum — straightforward in a homogeneous medium (protons reaching a voxel occupy a thin, near-common-range arc) but more involved in heterogeneous media, where arriving protons may have traversed very different paths.
- Path to analytical solution:** the step-by-step angular structure maps naturally onto the Linear Boltzmann Transport Equation (LBTE), but the strongly forward-peaked kernel will require careful angular discretization.

The table-lookup structure (vs. Geant4's branching physics logic) is also well suited to GPU acceleration, offering a complementary speedup path even before an analytical solution is reached.

Contact

Qifan Xu
University of California, San Francisco
Email: Qifan.Xu@ucsf.edu

References

- Hong L, et al. A pencil beam algorithm for proton dose calculations. *Phys Med Biol.* 1996
- Szymanowski H, Oelfke U. Two-dimensional pencil beam scaling: an improved proton dose algorithm for heterogeneous media. *Phys Med Biol.* 2002.
- Westerly DC, et al. Generalization and validation of the 2D analytic proton dose algorithm for heterogeneous media. *Med Phys.* 2013.
- Saini J, et al. Advanced proton beam dosimetry part I/II: review and current status. *Transl Lung Cancer Res.* 2018.
- Maes D, et al. Advanced proton beam dosimetry part II: Monte Carlo vs. pencil beam-based planning for lung cancer. *Transl Lung Cancer Res.* 2018.
- Agostinelli S, et al. Geant4 — a simulation toolkit. *Nucl Instrum Methods Phys Res A.* 2003.