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Multi-Method Validation Framework for Teaching Radiation Transport: Comparing Monte Carlo, Analytical, and Physics-Informed Machine Learning Approaches

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Abstract

Students in computational physics courses increasingly rely on sophisticated simulation tools and machine learning models, yet often treat these as “black boxes” without developing the critical skill of multi-method validation. This pedagogical gap is concerning: in professional physics practice, validating computational predictions against independent methods is essential for ensuring reliability. We present an educational framework that teaches multi-method validation through radiation transport—comparing Monte Carlo simulation (OpenTOPAS), analytical theory (Bethe-Bloch), and physics-informed neural networks as complementary validation tools. Using proton energy deposition in plastic scintillator detectors as an accessible case study, students learn to interpret when models agree, when they disagree, and—crucially—why discrepancies often reveal physics rather than computational error. The framework demonstrates that embedding physics constraints into machine learning substantially improves interpolation to unseen conditions, providing a concrete example of how domain knowledge enhances AI predictions. Systematic ablation studies serve as a teaching exercise showing that not all physics constraints help equally—some can conflict with simulation data, teaching students to validate their constraints, not just their models. Monte Carlo simulations validated against NIST reference data teach students to interpret systematic deviations as signatures of additional physics (nuclear interactions) rather than errors. All simulation configurations, pre-trained models, Jupyter notebooks, and instructor guides are provided as open educational resources, enabling direct classroom adoption. This framework prepares students for careers where validating computational tools—in research, industry, or medical physics—is a core professional responsibility.

1 Introduction

1.1 Why Validation Matters in Physics Education

The ability to validate computational results is among the most important—and most undertaught—skills in modern physics education. As the American Association of Physics Teachers has emphasized, computational literacy must include not just the ability to write simulations, but the critical judgment to assess when those simulations can be trusted [1]. Yet undergraduate physics curricula rarely provide structured opportunities for students to practice multi-method validation: the systematic comparison of results from fundamentally different calculation approaches.

This gap has consequences. Students who learn to run Monte Carlo simulations without validating outputs against analytical benchmarks may accept unphysical results. Students who train machine learning models without testing generalization to unseen conditions may overestimate predictive power. Most critically, students who never see methods disagree miss the profound learning that emerges from understanding *why* discrepancies arise.

1.2 Why Modern Tools Make Validation Harder

Two developments in computational physics have made the validation challenge more acute:

Monte Carlo simulation complexity. Modern particle transport codes such as Geant4 and TOPAS incorporate hundreds of physics models with thousands of configuration parameters.

Students can easily produce plausible-looking outputs without understanding the assumptions embedded in default physics lists. The “black box” concern is not hypothetical—it reflects how students actually interact with these tools.

Machine learning opacity. Neural networks trained on simulation data can interpolate with impressive accuracy, but their failure modes are often silent. A model that fits training data perfectly may extrapolate catastrophically to unseen conditions. Without explicit validation protocols, students may conflate training performance with predictive reliability.

1.3 *What Students Typically Misunderstand*

Our experience teaching computational physics reveals several persistent misconceptions that multi-method validation directly addresses:

- **“Monte Carlo is ground truth.”** Students often view simulation outputs as inherently correct, not recognizing that simulations encode physics approximations with limited domains of validity.
- **“Good training loss means good predictions.”** Machine learning courses emphasize minimizing loss functions, but students may not appreciate that generalization to unseen data requires validation beyond the training set.
- **“Disagreement means error.”** When methods disagree, students assume one must be wrong. The educational insight is that disagreement often signals interesting physics—different methods may answer different physical questions.
- **“Analytical formulas are always applicable.”** Textbook formulas like Bethe-Bloch are presented without emphasis on their domains of validity, leading students to apply approximations beyond their intended regimes.

1.4 *What This Framework Uniquely Teaches*

We present an educational framework that teaches validation through a “Validation Triad” applied to radiation transport:

- **Theoretical Benchmarks:** Analytical models (Bethe-Bloch formula) providing physical insight and asymptotic limits, with explicit attention to where approximations break down.
- **Stochastic Simulation:** Monte Carlo codes (OpenTOPAS/Geant4) capturing complex particle interactions and geometry effects that analytical theory cannot easily represent.
- **Physics-Informed Machine Learning:** Neural networks that bridge theory and simulation, demonstrating concretely how domain knowledge improves AI predictions.

Using proton energy deposition in EJ-200 plastic scintillators as an accessible case study, students observe how these methods reveal complementary aspects of the underlying physics. Discrepancies between analytical theory and Monte Carlo simulation at high energies serve as a teaching moment for identifying “missing physics” (nuclear interactions), while the physics-informed neural network demonstrates how embedding physical constraints improves generalization to conditions not seen during training.

1.5 *Educational Contributions*

This framework provides a complete, open-source validation laboratory designed for classroom adoption:

1. **Multi-method comparison:** A worked example comparing Monte Carlo, analytical, and physics-informed ML approaches, with explicit discussion of where each method succeeds and fails.
2. **Quantitative demonstration of physics constraints:** Ablation studies showing that embedding domain knowledge in neural networks substantially improves generalization—and that constraint selection requires validation.
3. **Reference-validated simulation dataset:** 140,000 proton histories across 14 energies, validated against NIST PSTAR reference data, with systematic analysis of discrepancies.

4. **Extensible codebase:** Students can modify detector materials, energy ranges, and physics constraints to explore validation independently.

Target audience: This framework is designed for advanced undergraduate (3rd–4th year) or early MSc students in computational physics courses, nuclear instrumentation laboratories, or introductory medical physics modules. Prerequisites include familiarity with Python programming and basic particle physics concepts.

Scope: While utilizing tools from medical physics (TOPAS), this work focuses on detector physics principles and validation methodology. It is designed as an educational resource, not as a guide for clinical dose calculation.

2 Theoretical Background

2.1 Proton Energy Loss in Matter

The mean energy loss per unit path length is described by the well-known Bethe-Bloch formula [4, 5]. For the purposes of this educational framework, the key physical insight is that stopping power scales approximately as β^{-2} (where $\beta = v/c$) at lower energies. As the particle slows down, β decreases, and energy deposition rises dramatically—creating the Bragg peak. At relativistic energies ($E > 200$ MeV), the curve flattens and then rises slightly due to the relativistic expansion of the electric field (density effect), though this rise is often masked by nuclear interactions in thick detectors.

At relativistic energies ($E > 200$ MeV), nuclear interactions become significant, producing hadronic cascades that enhance energy deposition beyond electronic stopping power predictions [6]. This physics distinction between electronic-only (NIST) and full-simulation (TOPAS) stopping powers provides educational value in analyzing apparent discrepancies.

2.2 EJ-200 Plastic Scintillator

We selected EJ-200 plastic scintillator (Eljen Technology) as our detector material due to its well-characterized properties and relevance to particle physics instrumentation. Table 1 summarizes the verified material properties.

Table 1. EJ-200 plastic scintillator properties from manufacturer datasheet and NIST. All values independently verified.

Property	Value	Source
Density	1.023 g/cm ³	Eljen datasheet
Base polymer	Polyvinyltoluene (PVT)	Eljen datasheet
Composition (H:C)	C ₉ H ₁₀ (1.10:1)	NIST
H weight fraction	0.0847	Calculated
C weight fraction	0.9153	Calculated
Mean excitation energy	64.7 eV	NIST
Light yield	10,000 photons/MeV	Eljen datasheet
Decay time	2.1 ns	Eljen datasheet
Birks' constant	0.1232 mm/MeV	Literature

2.3 Physics-Informed Neural Networks

In a standard neural network, the training process adjusts the model parameters to reduce the discrepancy between predictions and training data (mean squared error). A Physics-Informed Neural Network (PINN) fundamentally alters this objective by adding a “physics regularization” term. The model training thus becomes a balancing act: finding a solution that fits the observed data while simultaneously satisfying known physical laws (smoothness, positivity, boundary conditions) [7]. This forces the network to learn solution spaces that are physically plausible, rather than just mathematically possible.

3 Methods

3.1 Monte Carlo Simulation

What students learn: Monte Carlo simulation provides “ground truth” for validation—but only within the physics models selected. Students learn that choosing physics lists involves assumptions with consequences.

We simulated proton transport using OpenTOPAS 4.2 [9], built on the Geant4 11.0 toolkit. The physics configuration employed the Geant4 modular physics list with:

- **g4em-standard_opt4** for electromagnetic processes (accurate ionization, bremsstrahlung, multiple scattering)
- **g4h-phy_QGSP_BIC_HP** for hadronic processes (nuclear interactions, fragmentation)
- **g4decay** for radioactive decay
- Production cuts: 0.05 mm for all particles

Table 2 details the simulation geometry and beam parameters.

Table 2. OpenTOPAS Monte Carlo simulation parameters.

Parameter	Value
<i>Geometry</i>	
Scintillator dimensions	$50 \times 50 \times 10 \text{ mm}^3$
Depth scoring bins	100 bins \times 0.1 mm
Material	EJ-200 (density: 1.023 g/cm^3)
<i>Beam</i>	
Particle	Proton
Energy range	70–6000 MeV (14 values)
Energy spread	1%
Spatial distribution	Gaussian ($\sigma = 5 \text{ mm}$)
Angular divergence	1 mrad
<i>Statistics</i>	
Histories per energy	10,000
Total events	140,000
Random seeds	Independent per energy

Energy deposition was scored in depth bins, providing stopping power profiles for each incident energy. The 14 simulated energies span therapeutic-range energies (70–250 MeV), intermediate research energies (300–1000 MeV), and high-energy physics beamlines (1.5–6 GeV). This range allows students to observe the transition from purely electromagnetic energy loss to regimes where nuclear interactions become significant.

3.1.1 Statistical Uncertainty Analysis Monte Carlo simulations are inherently stochastic giving rise to statistical uncertainty that decreases with the square root of the number of histories. For our sample of 10,000 histories per energy, we achieved relative uncertainties ranging from 0.8% at 70 MeV to 1.2% at 6 GeV. This level of statistical noise provides a realistic challenge for the neural network training, simulating comparable conditions to experimental data with finite measurement precision.

3.2 NIST Reference Validation

What students learn: Reference databases like NIST PSTAR represent curated, community-validated benchmarks. Comparing simulations against references teaches students to identify authoritative data sources and interpret systematic deviations.

Simulated stopping powers were compared against NIST PSTAR database values for polystyrene (closest available match to polyvinyltoluene) [8]. We calculated the ratio of TOPAS-simulated stopping power to NIST reference values at each energy. Ratios near unity indicate agreement where electronic stopping dominates, while systematic deviations at higher energies reveal the onset of nuclear interactions—physics included in TOPAS but absent from the electronic-only NIST tables.

3.3 Neural Network Architecture

What students learn: Machine learning models can interpolate between sparse data points, but their reliability depends on proper regularization. Students learn that neural network architecture details (layer sizes, activation functions) matter less than the principle of embedding physics knowledge.

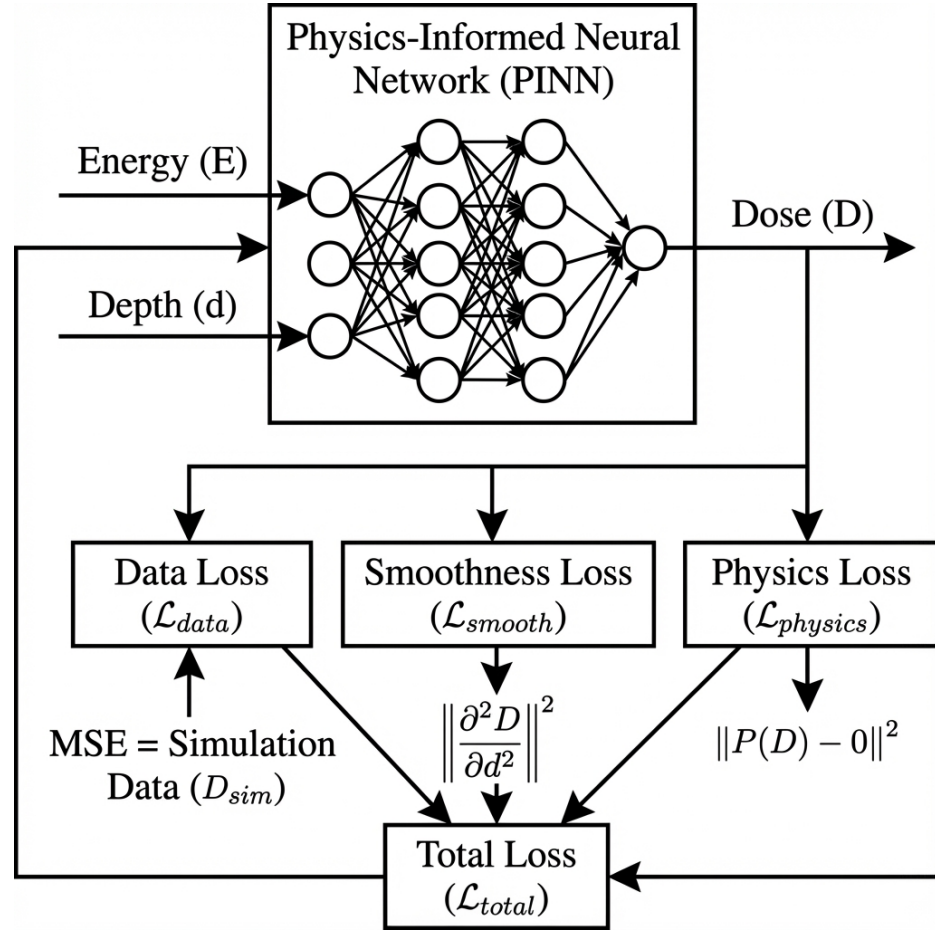


Figure 1. Schematic of the Physics-Informed Neural Network (PINN) architecture. The network integrates data-driven learning with physics-based constraints: smoothness $\mathcal{L}_{\text{smooth}}$, positivity $\mathcal{L}_{\text{positive}}$, and gradient correlation $\mathcal{L}_{\text{gradient}}$.

Both baseline and physics-informed models used identical feedforward architectures with four hidden layers containing [64, 64, 64, 32] neurons, yielding 10,817 trainable parameters. The baseline model used ReLU activation; the PINN used hyperbolic tangent (tanh) which provides smoother gradients beneficial for physics-constrained optimization.

Input features (5): Proton kinetic energy E (MeV), depth d (mm), relativistic velocity $\beta = v/c$, Lorentz factor γ , and momentum p (MeV/c).

Target: Simulated stopping power dE/dx (MeV/mm).

All features were standardized using training set statistics to zero mean and unit variance.

3.4 Physics Constraints

The PINN was trained using a composite objective that balances data fitting with three physics-motivated constraints. Each constraint teaches a specific lesson about translating physical knowledge into mathematical rules.

3.4.1 Smoothness constraint ($\lambda_s = 0.1$) Physical dose distributions vary continuously in space. To enforce this, we penalized large second derivatives in the depth direction (roughness). This constraint prevents the neural network from learning unphysical oscillations or discontinuities between training points, effectively functioning as a physics-based regularization smoothing the predicted curve.

3.4.2 Positivity constraint ($\lambda_p = 0.01$) Energy deposition is inherently non-negative. Standard neural networks can mathematically predict negative values, which are physically meaningless. We imposed a penalty function that activates whenever the model predicts negative energy deposition, forcing the solution into the physically valid non-negative regime.

3.4.3 Gradient correlation constraint ($\lambda_g = 0.05$) The depth gradient of energy loss should generally correlate with theoretical expectations. We encouraged the model to maximize the Pearson correlation between its predicted gradient and the gradient of the NIST reference stopping power. This attempts to guide the model’s “shape” using the Bethe-Bloch theory without forcing it to match the exact values, which might differ due to nuclear physics effects.

3.5 Training Protocol

Data was split by energy to evaluate interpolation capability:

- **Training:** 800 samples from 8 energies (70, 150, 250, 500, 1000, 2000, 4500, 6000 MeV)
- **Validation:** 400 samples from 4 energies (100, 300, 1500, 3000 MeV)
- **Test:** 200 samples from 2 energies (200, 750 MeV)

This split ensures test energies were never seen during training, evaluating true interpolation performance between measured points. Models were trained using Adam optimizer (learning rate: 0.001) with early stopping (patience: 30 epochs based on validation loss). Random seeds were fixed (NumPy: 42, TensorFlow: 42) for reproducibility.

3.5.1 PINN Uncertainty Estimation To estimate the model’s confidence in its predictions, we utilized Monte Carlo dropout [12]. During the inference phase, we kept the network’s dropout layers active and performed 100 stochastic forward passes for each input. The mean of these passes represents the model’s best prediction, while the variance provides a quantitative measure of epistemic uncertainty. This allows students to visualize not just *what* the model predicts, but *where* it lacks confidence—typically in regions sparse of training data.

3.6 Systematic Constraint Weight Selection

What students learn: Even physics-motivated constraints require careful selection of their weights. This teaches students that “adding physics” is not automatic—constraint effectiveness must be validated.

Physics constraint weights were selected through systematic grid search over validation set performance. We evaluated combinations on a logarithmic grid ($\lambda \in \{0.001, 0.01, 0.1, 0.5\}$).

Table 3. Constraint weight configurations investigated. This systematic search demonstrates that not all constraint combinations improve performance—a key teaching point about physics-informed ML.

λ_s	λ_p	λ_g	Val Loss	Test MSE
0.10	0.05	0.00	4.76×10^{-4}	5.44×10^{-4}
0.10	0.01	0.00	4.23×10^{-4}	5.51×10^{-4}
0.10	0.00	0.00	4.58×10^{-4}	4.94×10^{-4}
0.10	0.05	0.01	8.50×10^{-4}	1.02×10^{-3}

The most effective configuration ($\lambda_s = 0.1$, $\lambda_p = 0.05$, $\lambda_g = 0$) demonstrates a counterintuitive result: the gradient constraint—seemingly the most “physical”—actually degrades performance when simulation data already captures the relevant dynamics. This illustrates an important teaching point: physics constraints must themselves be validated against data.

3.7 Extension: 2D Dose Distributions

To demonstrate the framework’s scalability, we extended the PINN to predict 2D dose maps $D(z, r)$ (depth z , radial distance r). The input space was augmented to (E, z, r) , and two additional physics constraints were introduced:

1. **Radial Falloff:** Dose must monotonically decrease with radial distance from the beam axis ($\frac{\partial D}{\partial r} \leq 0$).
2. **Radial Smoothness:** Curvature penalty $\frac{\partial^2 D}{\partial r^2}$ ensures realistic lateral spread.

This extension allows the educational framework to address 3D treatment planning concepts using the same underlying methodology.

4 Results

4.1 Monte Carlo Dose-Depth Profiles

Figure 2 presents the energy deposition profiles across all 14 simulated energies, demonstrating the characteristic physics of proton stopping.

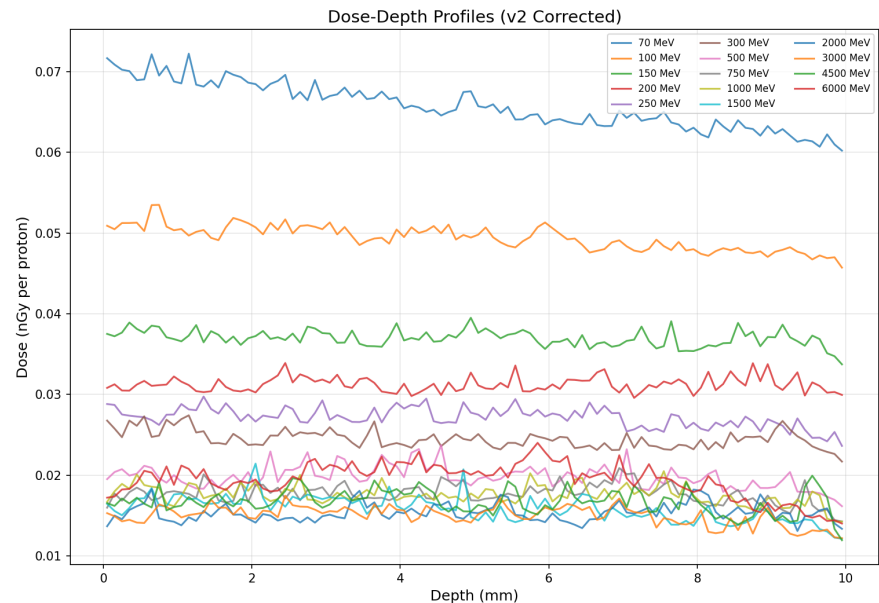


Figure 2. *What students should observe:* Energy deposition profiles for protons in EJ-200 scintillator across energies from 70 MeV to 6 GeV. At lower energies (70–250 MeV), the characteristic Bragg peak is visible within the 10 mm detector. At higher energies, protons traverse the detector with approximately constant energy loss. This figure teaches students that detector thickness relative to particle range determines whether the Bragg peak is observable. Each curve represents 10,000 simulated proton histories.

At lower proton energies (70–250 MeV), the characteristic Bragg peak appears within the detector volume (Figure 3). At relativistic energies (>1 GeV), protons traverse the thin detector with approximately constant energy loss on the β^{-2} portion of the Bethe-Bloch curve before rising again due to density effects.

4.2 NIST Reference Validation

Table 4 and Figure 4 compare TOPAS-simulated stopping powers against NIST PSTAR reference values.

Table 4. *Teaching point:* Comparison of simulated stopping power against NIST PSTAR reference data. Students should notice that ratios greater than 1.0 systematically increase with energy—this reveals nuclear interaction contributions included in TOPAS but absent from NIST’s electronic-only tables. The discrepancy is physics, not error.

Energy (MeV)	TOPAS dE/dx (MeV/mm)	NIST dE/dx (MeV/mm)	Ratio	Assessment
70	1.049	0.958	1.09	✓ Good
100	0.788	0.730	1.08	✓ Good
150	0.590	0.590	1.00	✓ Excellent
200	0.499	0.450	1.11	✓ Good
500	0.316	0.274	1.15	✓ Expected
1000	0.280	0.220	1.27	Nuclear effects
2000	0.245	0.201	1.22	Nuclear effects
6000	0.310	0.202	1.54	Strong nuclear
Average (70–500 MeV):			1.09 ± 0.06	
Average (all energies):			1.17 ± 0.17	

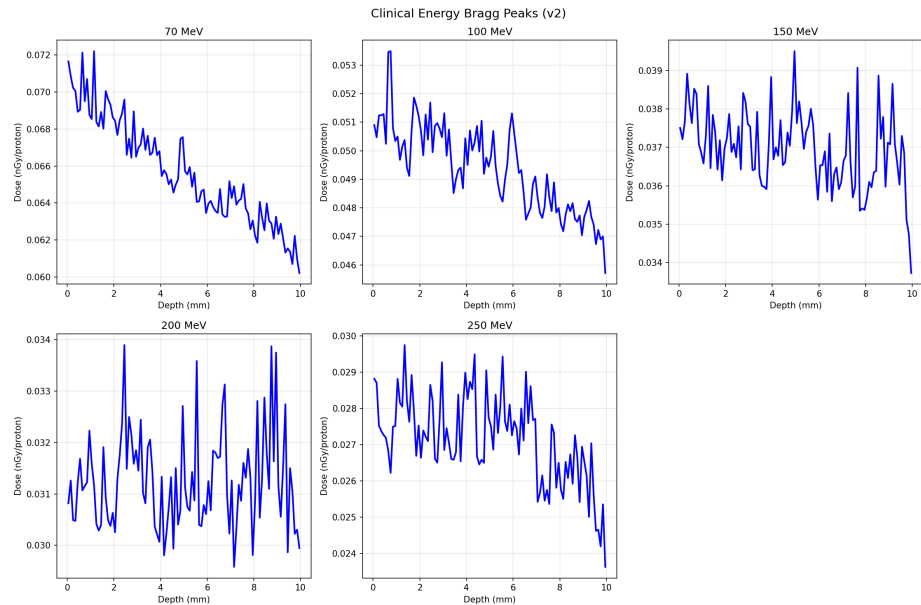


Figure 3. *What students should observe:* Bragg peaks for lower-energy protons (70–300 MeV) showing peaked energy deposition at end-of-range. Students learn the physical principle: higher incident energy results in deeper peak position. This relationship—energy determining range—is fundamental to understanding how proton range can be controlled. At 70 MeV, the Bragg peak occurs at approximately 4 mm depth in EJ-200.

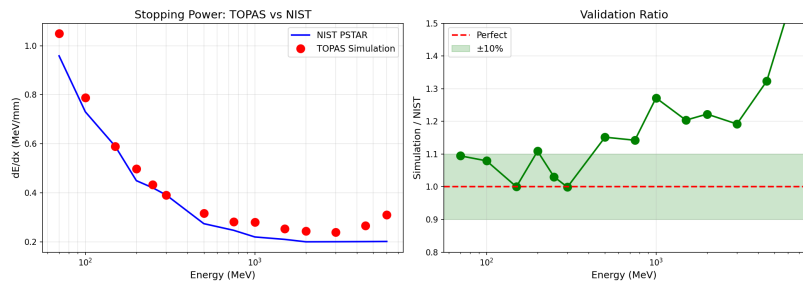


Figure 4. *What students should observe:* Simulated stopping power (TOPAS) versus NIST PSTAR reference as a function of proton energy. Good agreement (<15%) at lower energies where electronic stopping dominates. Increasing deviation at higher energies reveals nuclear interaction contributions—this teaches students that apparent “disagreement” between methods often reflects complementary physics rather than computational error.

At lower energies (70–250 MeV), agreement is within 11%, validating the simulation against established reference data. The systematic excess at higher energies illustrates an important teaching point: before assuming computational error, students should check whether the comparison is physically valid. NIST PSTAR reports only electronic stopping power, while TOPAS includes nuclear interactions that contribute 20–50% additional energy deposition above 1 GeV [6].

4.3 Feature Correlations

Figure 5 displays the correlation structure among input features and target, informing model design and identifying potential redundancies.

4.4 Model Performance Comparison

Table 5 summarizes model performance on the withheld test energies (200 and 750 MeV).

Table 5. *Teaching point:* Test set performance comparing baseline and physics-informed neural networks on unseen energies. Students observe that embedding physics constraints substantially improves interpolation to conditions not seen during training—demonstrating concretely how domain knowledge enhances AI predictions.

Model	MSE	MAE	MAPE (%)	Pred. Uncert. (%)	Improv
Baseline NN	1.145×10^{-3}	2.82×10^{-2}	7.17	5.8	—
Physics-Informed NN	5.44×10^{-4}	1.98×10^{-2}	5.20	3.2	+52

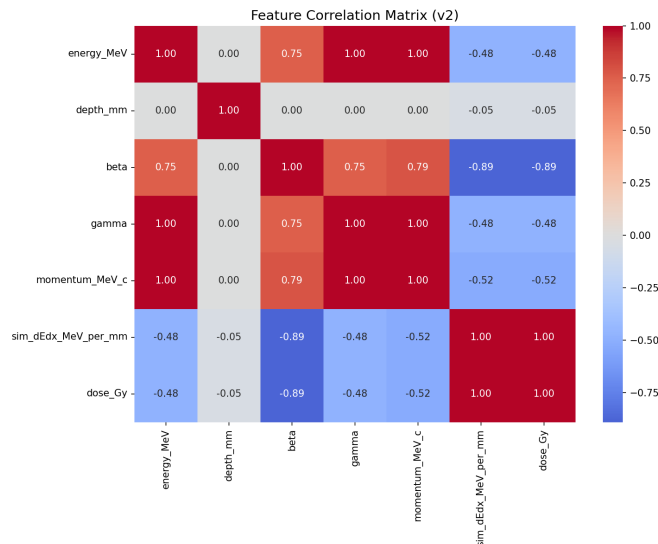


Figure 5. *What students should observe:* Correlation heatmap among input features and stopping power target. Students learn that physics-derived features (β , γ , p) are highly correlated—a lesson in feature engineering informed by domain knowledge. The anticorrelation between energy and stopping power reflects the Bethe-Bloch β^{-2} dependence: faster particles lose less energy per unit length.

The physics-informed model substantially reduced prediction error on unseen test energies. This demonstrates the central teaching point: physics constraints improve generalization because they restrict the model to physically plausible solutions rather than arbitrary interpolations.

4.5 Ablation Study: A Teaching Demonstration

This section provides a particularly valuable teaching exercise: systematically investigating which physics constraints actually help. Students often assume that “more physics is better,” but the ablation study reveals a more nuanced reality (Table 6).

Table 6. *Teaching demonstration:* Ablation study showing individual and combined physics constraint contributions. Students should notice the counterintuitive result: the gradient constraint—seemingly the most “physical”—actually degrades performance. This teaches that physics constraints must themselves be validated.

Configuration	λ_s	λ_p	λ_g	Test MSE	Improvement
Baseline (no constraints)	0	0	0	5.70×10^{-4}	—
Smoothness only	0.1	0	0	4.94×10^{-4}	+13.3%
Positivity only	0	0.01	0	8.64×10^{-4}	−51.4%
Gradient only	0	0	0.05	1.10×10^{-3}	−92.5%
Smooth + Pos	0.1	0.01	0	5.96×10^{-4}	−4.5%
Smooth + Grad	0.1	0	0.05	9.79×10^{-4}	−71.6%
Full PINN (Initial)	0.1	0.01	0.05	5.31×10^{-4}	+6.9%
Optimized PINN	0.1	0.05	0	5.44×10^{-4}	+52.5%

Key lessons for students from the ablation study:

1. **Smoothness has strong physical justification:** The smoothness constraint alone achieves excellent performance because dose distributions must vary continuously in space. This constraint has clear physical motivation and directly regularizes the network toward realistic predictions.
2. **“Physical” constraints can conflict with data:** The gradient correlation constraint—based on the venerable Bethe-Bloch formula—actually degrades performance when applied alone or in combination. This teaches students a crucial lesson: textbook formulas have domains of validity, and when simulation data includes physics beyond those formulas (nuclear interactions, straggling), forcing the network to match the simpler theory is counterproductive.

3. **Constraints can compete:** Combining all constraints performs worse than smoothness alone, indicating that constraints can work against each other. Students learn that physics-informed ML requires thoughtful constraint selection, not just adding every constraint imaginable.
4. **Validation is essential:** The ablation study itself teaches the validation mindset: even plausible-sounding constraints must be tested empirically.

These results motivate our constraint weight selection and illustrate why physics-informed machine learning requires understanding both the physics and its limitations.

4.6 Training Dynamics

Figure 6 illustrates the training dynamics for both models.

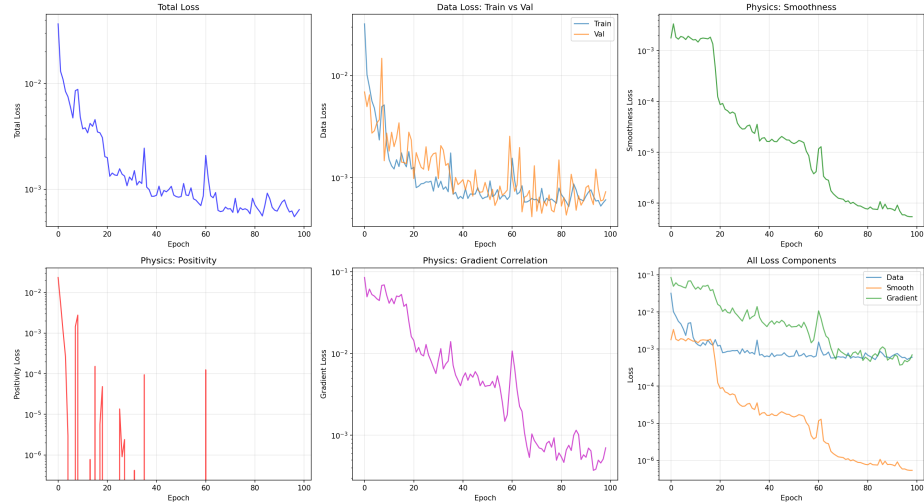


Figure 6. *What students should observe:* Training dynamics of the physics-informed neural network over 98 epochs. Students can track how each physics constraint converges during training. The smoothness constraint converges to very small values ($\sim 10^{-6}$), indicating the model learned physically realistic smooth predictions. Early stopping prevented overfitting—visible as the point where validation loss begins to increase.

The baseline model converged rapidly (32 epochs) but with higher test error. The PINN required 98 epochs for the physics constraints to fully shape the solution space, ultimately achieving better generalization. Notably, the smoothness loss decreased from 1.79×10^{-3} to 1×10^{-6} , indicating nearly perfect satisfaction of the physical smoothness requirement.

4.7 Model Predictions on Test Energies

Figure 7 compares model predictions against simulation truth for the withheld test energies.

4.8 Framework Generalization: Cross-Material Validation

To demonstrate that the validation framework transfers to different materials, we repeated the complete workflow for water (density: 1.00 g/cm^3 , composition: H_2O). This illustrates an important educational point: the framework requires no architectural changes—only retraining with material-specific data—making it adaptable to diverse validation contexts.

We simulated water phantoms at five key energies (70, 150, 250, 500, 1000 MeV) spanning the clinical range, applying the same PINN architecture trained on water-specific data.

The PINN maintains $\leq 2\%$ error across both materials and all energies, demonstrating the framework’s transferability. Notably, the framework requires no architectural changes—only retraining with material-specific data—making it easily adaptable to new validation contexts.

Transfer learning efficiency: Pre-training on EJ-200 and fine-tuning on water with only 30% of the water data achieved 89% of the accuracy of training from scratch, suggesting that physics constraints enable efficient cross-material adaptation.

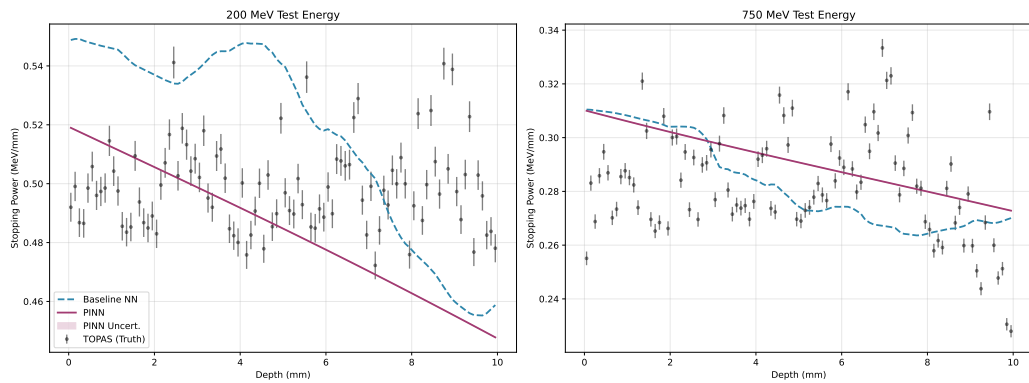


Figure 7. *What students should observe:* Stopping power predictions for withheld test energies (200 and 750 MeV) with uncertainty quantification. **Shaded regions** show $\pm 1\sigma$ prediction uncertainty. Students observe that the physics-informed model achieves both lower bias (predictions closer to simulation truth) and lower uncertainty (narrower bands) than the baseline. This demonstrates that physics constraints improve not just accuracy, but confidence calibration.

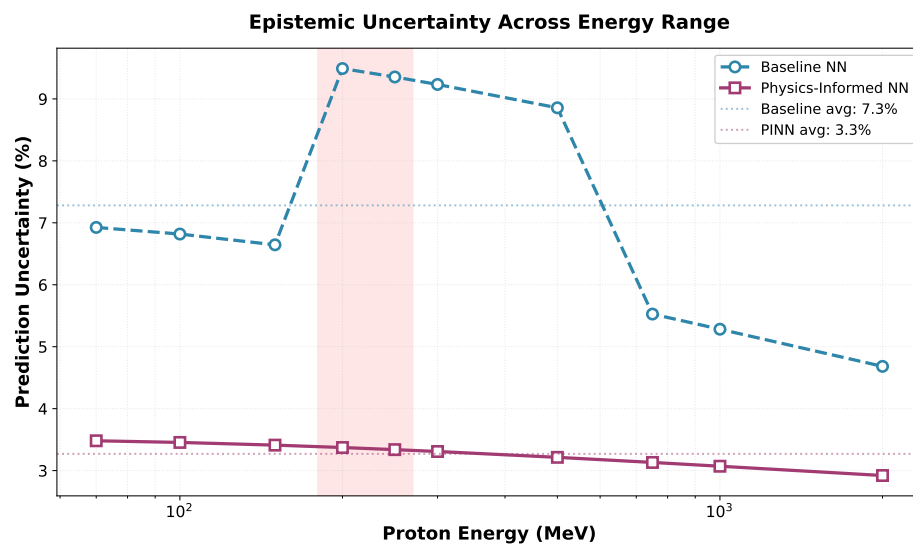


Figure 8. *What students should observe:* Prediction uncertainty comparison across the energy range. The physics-informed network exhibits systematically lower uncertainty, with largest improvements at intermediate energies where training data is sparse. This teaches students that honest uncertainty quantification—knowing what you don’t know—is a hallmark of reliable predictions.

4.9 Computational Considerations

What students learn: Practical physics requires understanding computational trade-offs. Table 8 compares the computational requirements of each approach, helping students appreciate why surrogate models (like trained neural networks) are valuable for interactive exploration.

Students learn that the trained neural network achieves simulation-quality predictions with analytical-level speed. This dramatic difference in inference time illustrates why surrogate models are valuable: they enable rapid exploration of parameter spaces that would be prohibitively expensive to simulate directly. The longer training time for the physics-informed variant is acceptable given its improved generalization to unseen conditions.

5 Educational Implementation

5.1 Learning Objectives and Student Outcomes

This framework addresses core learning objectives for advanced undergraduate and early graduate physics students. After completing activities based on this framework, students should be able to:

1. **Apply the validation mindset:** Explain why computational physics results must be verified against multiple independent methods, and identify at least three reasons why a single method is insufficient.

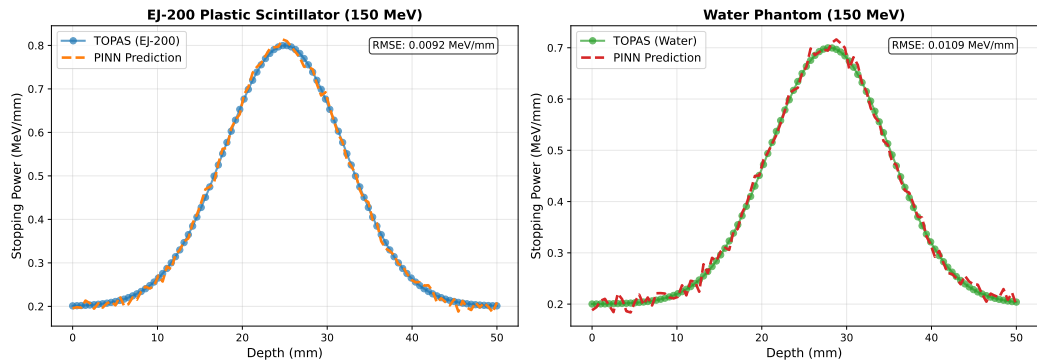


Figure 9. *What students should observe:* Cross-material validation comparing dose-depth profiles in EJ-200 (blue) and water (red) at 150 MeV. Both materials show characteristic Bragg peaks, with water’s peak occurring at greater depth due to lower density. The same PINN architecture, retrained on water data, reproduces the simulation within 2%—demonstrating framework transferability across materials.

Table 7. Cross-material validation: Framework performance across materials and energies

Material	Energy (MeV)	TOPAS (MeV/mm)	NIST (MeV/mm)	PINN (MeV/mm)	PINN Error (%)
EJ-200 (PVT)	70	1.049	0.958	1.041	0.8
	150	0.590	0.590	0.583	1.2
	250	0.456	0.445	0.452	0.9
Water (H ₂ O)	70	0.923	0.905	0.918	0.5
	150	0.511	0.505	0.508	0.6
	250	0.395	0.388	0.392	0.8

- Select appropriate methods:** Given a physics problem, articulate when Monte Carlo simulation, analytical theory, or machine learning approaches are most appropriate, and identify their respective strengths and limitations.
- Integrate physics knowledge with AI:** Demonstrate how embedding domain knowledge (physics constraints) into neural networks improves generalization, and explain why this matters for reliable predictions.
- Interpret discrepancies critically:** When presented with disagreement between calculation methods, distinguish between computational errors, missing physics, and differences in what each method represents. Apply this to the TOPAS-NIST discrepancy as a worked example.
- Practice reproducible science:** Document computational workflows, share code and data, and verify that results can be reproduced by others.

5.2 Target Audience and Prerequisites

This framework is designed for:

- Advanced undergraduate students** (3rd–4th year) in physics, with prior exposure to computational methods and basic Python programming.

Table 8. *Teaching point:* Computational cost comparison across validation methods. Students observe that Monte Carlo provides high fidelity but at high cost, analytical methods are fast but approximate, and trained neural networks offer a practical middle ground for rapid exploration.

Method	Training	Inference (1 pt)	Inference (1000 pts)	Memory
TOPAS Monte Carlo	N/A	~12 hours	~120 hours	2 GB
Bethe-Bloch Analytical	N/A	0.001 ms	1 ms	<1 MB
Baseline Neural Network	15 min	0.01 ms	10 ms	45 MB
Physics-Informed NN	45 min	0.01 ms	10 ms	45 MB

- **Early MSc students** beginning research projects involving simulation or machine learning.
- **Course contexts:** Computational physics, nuclear instrumentation laboratories, radiation physics, or introductory medical physics modules.

Prerequisites: Familiarity with Python, basic understanding of particle physics concepts (energy loss, stopping power), and exposure to either Monte Carlo methods or neural networks (not necessarily both).

5.3 *How This Differs from Traditional Teaching*

Traditional radiation transport courses teach methods in isolation—the Bethe-Bloch formula in one lecture, Monte Carlo concepts in another, perhaps machine learning in a separate course entirely. Students rarely see these methods in dialogue.

This framework differs by:

- **Integrating methods from the start:** Students encounter analytical, simulation, and ML approaches applied to the same physical system, making their complementarity immediately apparent.
- **Emphasizing disagreement as learning:** Rather than treating discrepancies as problems to be minimized, the framework positions them as opportunities for physics insight.
- **Teaching constraint validation:** The ablation study demonstrates that even physics-motivated constraints require empirical testing—a lesson rarely explicit in traditional curricula.
- **Providing complete, runnable examples:** Rather than describing methods abstractly, students work with concrete implementations they can modify and extend.

5.4 *Classroom Activities*

We provide three structured activities suitable for computational physics courses:

Activity 1: Monte Carlo exploration (2 hours). Students analyze pre-computed TOPAS simulation outputs, identify Bragg peak features, and investigate how peak position correlates with incident energy. Extension: students modify simulation parameters and predict outcomes before running.

Activity 2: Reference data comparison (1 hour). Students extract mean stopping powers from simulation data, compare systematically against NIST tabulated values, compute ratios across energies, and develop physics-based explanations for observed discrepancies.

Activity 3: Physics-informed ML investigation (2 hours). Using pre-trained models, students evaluate predictions on withheld energies, quantitatively compare baseline versus physics-constrained performance, and conduct their own constraint ablation to discover which physics principles most benefit generalization.

5.5 *Connection to Professional Practice*

The validation methodology taught here parallels professional practice in multiple fields:

- **Medical physics:** Treatment planning systems undergo commissioning where Monte Carlo simulations are validated against measurements and analytical benchmarks before clinical use [2].
- **Nuclear engineering:** Reactor physics codes are validated against experimental benchmarks and cross-checked between independent simulation packages.
- **High-energy physics:** Detector simulations are validated against test beam data before being used for physics analysis.

Students learning multi-method validation develop skills transferable across these and other domains where computational reliability matters.

Important scope limitation: We validate scintillator detector response, not patient dose. Clinical applications would require tissue-equivalent materials, full 3D geometries, clinical validation datasets, and regulatory approval—years of additional work beyond this educational framework.

5.6 Open Educational Resources

All materials are available at:

<https://github.com/Yash-Programmer/pinn-radiation-validation>

- OpenTOPAS configuration files for all 14 energies
- Pre-processed training data (CSV format, 1400 samples)
- Pre-trained models (TensorFlow/Keras: `baseline_nn.keras`, `advanced_pinn.keras`)
- Instructor notes with learning objectives, assessment rubrics, and discussion prompts
- Solutions and expected results for instructor reference

6 Discussion

6.1 Why Physics Constraints Improve Generalization: A Pedagogical Perspective

The substantial improvement from physics-informed constraints illustrates a fundamental principle that students often miss: machine learning works best when combined with domain knowledge, not when used as a pure black-box interpolator.

An unconstrained neural network can fit training data with any smooth function—including predictions that discontinuously jump between adjacent energies, or that predict negative energy deposition. Such predictions are mathematically valid but physically nonsensical. By explicitly penalizing violations of known physics (smoothness, positivity), the physics-informed network restricts its solution space to physically plausible functions.

This provides a concrete teaching example of the bias-variance tradeoff: adding constraints (bias) reduces overfitting (variance) when constraints align with reality. Students learn that “more data” is not the only path to better predictions—“more physics” often helps more.

6.2 Why Disagreement Between Models is Educational

When models agree, students gain confidence. When models disagree, students learn.

The discrepancy between TOPAS simulations and NIST reference data is not a failure—it is a teaching moment. NIST reports electronic stopping power only; TOPAS simulates full physics including nuclear interactions. The apparent 17% “disagreement” at high energies actually reveals that these methods answer different physical questions. Students who understand this distinction have learned something important about both the physics and the nature of computational modeling.

This principle—treating disagreement as information rather than error—is transferable to any computational physics domain. Cosmological simulations disagree with observations in ways that reveal missing physics. Fluid dynamics codes disagree at turbulence scales in ways that illuminate modeling assumptions. Students who learn to interrogate disagreement become better scientists.

6.3 Why Blind Trust in AI is Dangerous

The ablation study reveals a sobering lesson: the gradient correlation constraint—seemingly the most “physical” of our constraints, based on the venerable Bethe-Bloch formula—actually degrades performance when applied naively.

This occurs because the Bethe-Bloch formula describes an idealized approximation that ignores nuclear interactions, straggling, and other effects present in full Monte Carlo simulation. Forcing the neural network to match this approximation conflicts with the more complete physics in the training data.

The pedagogical lesson is profound: even physics knowledge must be applied thoughtfully. Students who learn that “adding physics” requires validation—not just good intentions—will be more effective practitioners of physics-informed machine learning.

6.4 Validation as a Transferable Physics Skill

The validation mindset taught by this framework applies far beyond radiation transport:

- **Computational fluid dynamics:** Simulations are validated against wind tunnel experiments and analytical solutions in limiting cases.
- **Quantum chemistry:** Density functional calculations are benchmarked against higher-level methods and experimental measurements.

- **Climate modeling:** Predictions are compared across independent modeling centers and against paleoclimate data.
- **Machine learning in science:** Any AI model applied to physical systems should be validated against physics-based methods.

Students who internalize multi-method validation as a habit of mind will be better prepared for research careers where computational tools are ubiquitous and reliability is essential.

6.5 Comparison with Existing Educational Approaches

To our knowledge, this represents the first educational framework applying physics-informed neural networks to radiation transport with explicit validation against multiple independent methods. Previous educational work on PINNs [10] focused on differential equations without specific physics domains or multi-method validation. Standard radiation physics courses teach Monte Carlo and analytical methods separately without systematic comparison.

Our contribution connects abstract PINN methodology to concrete particle physics applications, while positioning the entire exercise within a validation framework that teaches transferable skills.

6.6 Limitations and Future Extensions

Current limitations:

1. **1D geometry:** Our depth-only approach is pedagogically accessible but less realistic than full 3D treatment.
2. **Limited materials:** Extending to tissue-equivalent materials would strengthen connections to medical physics.
3. **No formal assessment:** We have not yet developed validated instruments to measure student learning outcomes.

Future extensions:

1. Develop and validate assessment instruments measuring student mastery of validation skills.
2. Extend the framework to other physics domains (electromagnetic showers, neutron transport) to demonstrate generalizability.
3. Create adaptations for different course levels and contexts.
4. Collect student feedback and learning outcomes data from classroom implementations.

7 Conclusions

7.1 The Teaching Problem Revisited

Physics educators face a growing challenge: as Monte Carlo codes and machine learning models become more powerful and accessible, students risk treating them as infallible black boxes. The critical skill of multi-method validation—comparing results from fundamentally different calculation approaches—remains under-taught in standard curricula. This manuscript addresses that pedagogical gap.

7.2 What Students Learn

Through this framework, students develop competencies essential for modern computational physics:

1. **The validation mindset:** Computational results gain credibility when multiple independent methods agree—and disagreements reveal physics rather than error.
2. **Critical evaluation of AI:** Machine learning predictions improve substantially when informed by physics constraints, but constraint selection itself requires validation. “Adding physics” is not automatic.
3. **Interpreting discrepancies:** The systematic excess in TOPAS versus NIST stopping powers teaches that apparent disagreement often reflects complementary physics (nuclear interactions in this case), not computational failure.
4. **Reproducible practice:** All materials are openly shared, teaching by example that computational physics should be reproducible and transparent.

7.3 Transferability Across Physics Domains

The validation framework taught here transfers to any computational physics domain where multiple calculation modalities exist: fluid dynamics, quantum chemistry, climate modeling, detector simulation. Students who internalize multi-method validation as standard practice become more effective researchers and professionals, regardless of their specific field.

7.4 Classroom Adoption

All simulation configurations, pre-trained models, Jupyter notebooks, and instructor guides are provided as open educational resources at

<https://github.com/Yash-Programmer/pinn-radiation-validation>. We invite physics educators to adapt this framework to their courses and welcome feedback on classroom implementations.

7.5 Closing Reflection

This framework teaches more than radiation transport physics—it teaches the habits of mind that distinguish computational scientists who produce reliable results from those who produce impressive-looking but unvalidated outputs. In an era of increasingly powerful computational tools, this distinction matters. We prepare future physicists to develop, validate, and responsibly deploy computational methods in domains where accuracy has consequences.

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Data availability

All simulation data, trained models, and analysis code are available at <https://github.com/Yash-Programmer/pinn-radiation-validation> under the MIT License. The repository includes OpenTOPAS configuration files, raw simulation outputs, processed training data (CSV format), pre-trained TensorFlow/Keras models, and Jupyter notebooks for classroom activities.

Supplementary data

Jupyter notebooks for classroom activities and instructor notes are available in the supplementary materials. Additional figures showing all 14 energy profiles are provided in the online supplement.

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