

Physics-informed deep learning-based Monte Carlo dose prediction for BNCT

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***Keywords :** BNCT, TPS, physics-informed, dose prediction, residual learning

1. Introduction

Boron neutron capture therapy (BNCT) is a targeted radiotherapeutic modality that utilizes boron-10-containing compounds that selectively accumulate in target cells. Upon irradiation with a thermal neutron beam, the nuclear capture reaction $^{10}\text{B}(n, \alpha)^7\text{Li}$ generates high linear energy transfer (LET) charged particles that destroy malignant cells [1]. BNCT requires Monte Carlo (MC) particle transport to accurately model the dose produced by complex neutron interactions. Although MC calculation provides high physical fidelity, its computational cost limits rapid evaluation of candidate beam arrangements during treatment planning. This study proposes a physics-informed deep learning model that combines a 3D MedNeXt [2] with Swin3D attention [3] to predict multi-component BNCT dose distributions from patient anatomy and two-port beam parameters.

2. Methods and Results

2.1. Dataset and pre-processing

The GLIS-RT open dataset [4] was used to construct the dataset. After preprocessing, 190 patients were divided into training, validation, and test sets of 151, 28, and 11 patients, respectively. For each patient, 50 randomly sampled two-port beam configurations were calculated with the GPU-accelerated MC code RT² [5], yielding 7,550 training, 1,400 validation, and 550 test samples. CT images, five anatomical masks, and four physical dose components were resampled to $64 \times 128 \times 128$ voxels.

2.2. Network architecture and training details

The proposed network uses MedNeXt blocks in a four-level encoder-decoder structure and shifted-window Swin3D attention at the deepest feature level and bottleneck. Beam directions were represented as unit vectors and injected into the network by feature-wise linear modulation (FiLM). Spatial beam geometry was additionally encoded as differentiable 3D ray features. The network predicted boron, nitrogen,

gamma, and hydrogen dose components as residual corrections to analytical depth-dose priors. A shared single-beam network and weighted superposition enforced linearity with respect to the two beam weights. The training objective combined region and high-dose weighted L1, multiscale, dose-gradient, RBE-consistency, and dose-volume histogram losses. For augmentation, one of eight exact axial-plane dihedral transformations (90° rotations and flip) was applied consistently to the anatomy, dose, beam directions, and beam centers. The model was optimized with AdamW and exponential moving-average weights; the checkpoint with the lowest validation loss was evaluated.

2.3. Results of BNCT dose prediction

Total RBE dose was normalized by the peak MC dose of each test configuration. Across all 550 test configurations, the proposed model achieved body and target mean absolute errors (MAEs) of 0.00387 ± 0.00169 and 0.01517 ± 0.00768 , respectively. The absolute target $D_{95\%}$ error was 0.00541 ± 0.00568 , while the global gamma pass rate of 2%/2 mm and 3%/3 mm were $95.74 \pm 4.19\%$ and $98.43 \pm 1.84\%$, respectively, using a 10% dose cutoff. Relative to the 3D U-Net backbone model, body MAE, target MAE, and target $D_{95\%}$ error decreased by 49.5%, 51.8%, and 72.1%, respectively, and the 2%/2 mm gamma pass rate increased from 77.79% to 95.74%. Compared with the 3D U-Net backbone using the same physics inputs, the corresponding errors decreased by 10.9%, 13.9%, and 24.4%, and the gamma pass rate increased from 93.57% to 95.74%.

Table I: Quantitative evaluation results

	3D U-Net w/o phys. inputs	3D U-Net w phys. inputs	Proposed
Body MAE	0.0077 ± 0.0046	0.0043 ± 0.0020	0.0039 ± 0.0017
Target MAE	0.0315 ± 0.0190	0.0176 ± 0.0088	0.0152 ± 0.0077
Target $\Delta D_{95\%}$	0.0174 ± 0.0197	0.0074 ± 0.0084	0.0055 ± 0.0060
Target $\Delta D_{95\%}$	0.0194 ± 0.0214	0.0072 ± 0.0078	0.0054 ± 0.0057
Target $\Delta D_{50\%}$	0.0258 ± 0.0222	0.0104 ± 0.0108	0.0090 ± 0.0093
Target $\Delta D_{5\%}$	0.0255 ± 0.0245	0.0183 ± 0.0165	0.0148 ± 0.0136
Target $\Delta D_{2\%}$	0.0283 ± 0.0265	0.0209 ± 0.0188	0.0173 ± 0.0151
Target ΔD_{mean}	0.0224 ± 0.0204	0.0105 ± 0.0102	0.0086 ± 0.0087
γ (2%/2mm)	77.7871 ± 13.8868	93.5705 ± 5.0210	95.7402 ± 4.1934
γ (3%/3mm)	89.0426 ± 10.2410	97.7157 ± 2.1937	98.4273 ± 1.8371

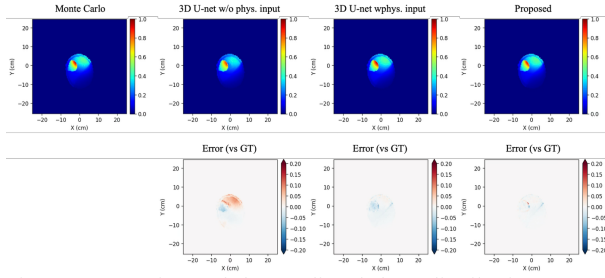


Fig. 1. Comparison of the predicted dose distribution across comparative methods

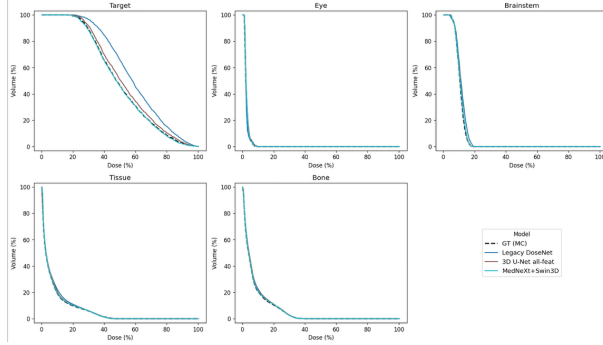


Fig. 2. Comparison of the dose-volume histogram across comparative methods

3. Conclusions

The proposed physics-informed deep learning model accurately predicted MC-based 3D BNCT dose distributions over diverse patient anatomies and beam configurations. Combining local convolutional modeling, windowed 3D attention, component-wise dose priors, exact beam superposition, and geometry-consistent augmentation improved both voxel-level accuracy and clinically relevant target-dose agreement. These results support the model as a rapid surrogate for MC dose calculation in BNCT treatment planning research, while further validation on independent clinical datasets remains necessary.

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