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Systematic benchmarking of Monte Carlo Codes for accelerator-based BNCT neutron production targets

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Beam-shaping assembly (BSA) design using Monte Carlo techniques for accelerator-based boron neutron capture therapy (BNCT) requires accurate modelling of light-ion reactions on thin or thick targets, which define the neutron source term for subsequent beam shaping. Geant4 11.1.3, PHITS 3.33, FLUKA 4-4.0 and MCNP 6.3 have been benchmarked for thick-target neutron yield and spectra from 7Li(p,n)7Be, 9Be(p,n)9B, 9Be(d,n)10B, C(d,n)N, and the inverse-kinematics reaction p(7Li,n)7Be in the low-energy regime relevant to accelerator-based BNCT.
Using each code's recommended physics settings, predictions of total neutron yield, forward (0 degrees) yield, neutron energy spectra and angular distributions were compared with compiled experimental data. To quantify agreement, metrics of mean relative error and sMAPE for yields and Pearson Correlation Coefficient for spectral shapes were reported. Single-core throughput for each code on a fixed workstation is provided as a simple computational performance indicator.
Results show varying levels of agreement between the codes depending on the reaction type, energy range, and beam characteristics. Across most reactions, Geant4, MCNP and PHITS reproduce total and forward yields within typical experimental scatter, while PHITS shows the most consistent agreement with experimental energy spectra for 9Be(p,n)9B. The largest discrepancies occur near threshold energies and for p(7Li,n)7Be, where none of the default models capture angular behaviour observed during experiment. Under our settings, PHITS delivered the highest single-threaded throughput per history.
These results clarify the strengths and limitations of widely used codes for accelerator-based BNCT target modelling and provide a practical basis for selecting and tuning models when generating neutron source input for BSA design and optimisation.

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