Geant4 Collaboration Meeting 2024

Benchmarking Monte Carlo codes for the modelling of low-energy neutron production target reactions

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Accelerator-Based Neutron Sources (ABNS)

Due to high cost and limited availability of nuclear research reactors, **development of ABNS has gained momentum.**

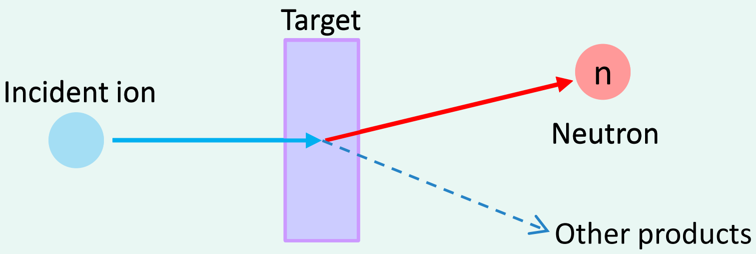
Compact ABNS:

(p,n)

(d,n)

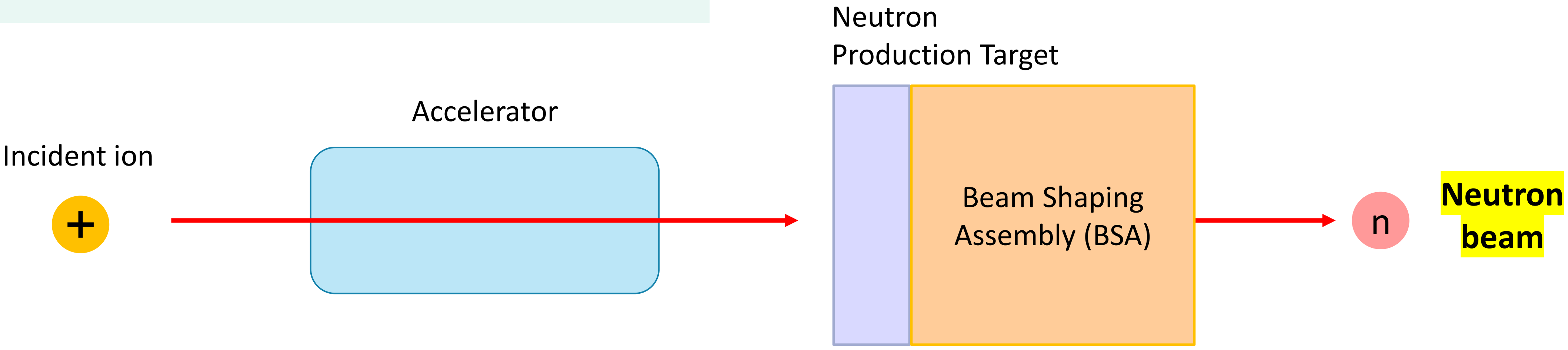
(α,n)

(x,n)



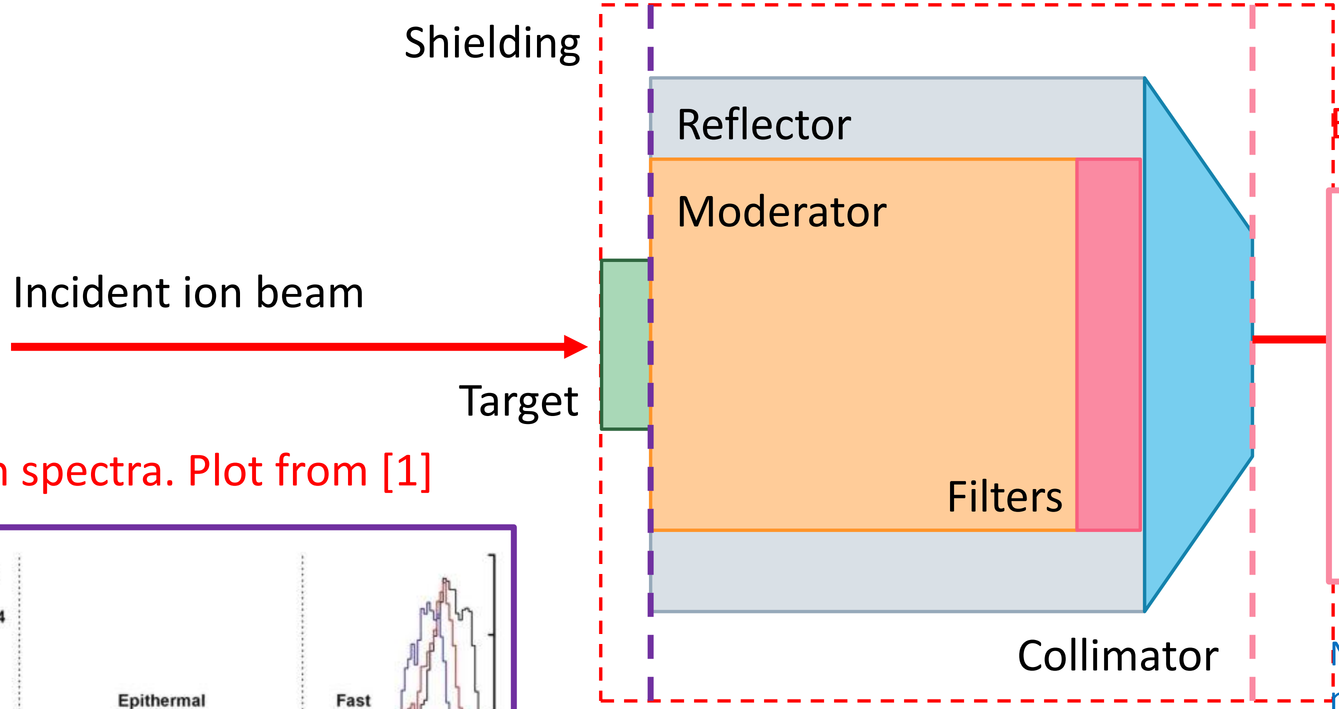
Advantages:

- Can be switched on/off (safety considerations)
- Lower cost
- Easier to maintain
- Smaller system
- Allows for better locations

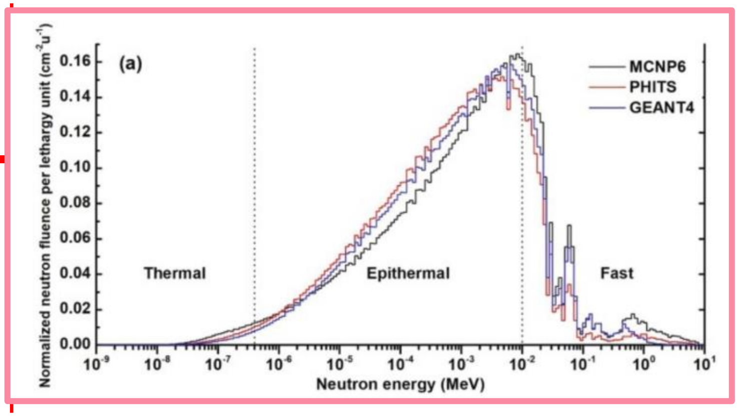


ABNS: The Beam Shaping Assembly (BSA)

A beam shaping assembly (BSA) is used to **modify the characteristics of the raw neutron beam** that is output from the target of the ABNS

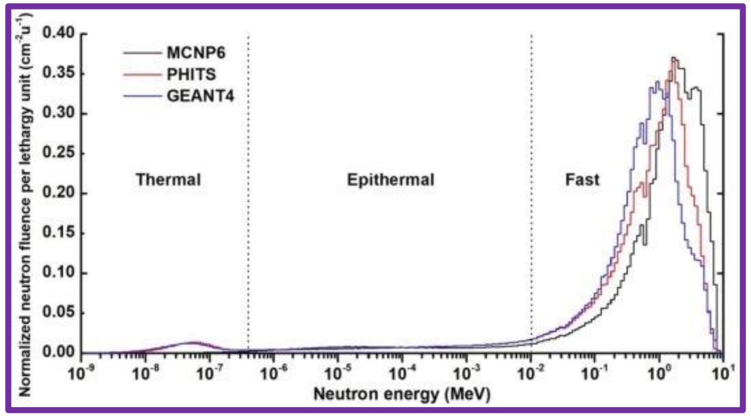


Epithermal neutron spectra. Plot from [1]



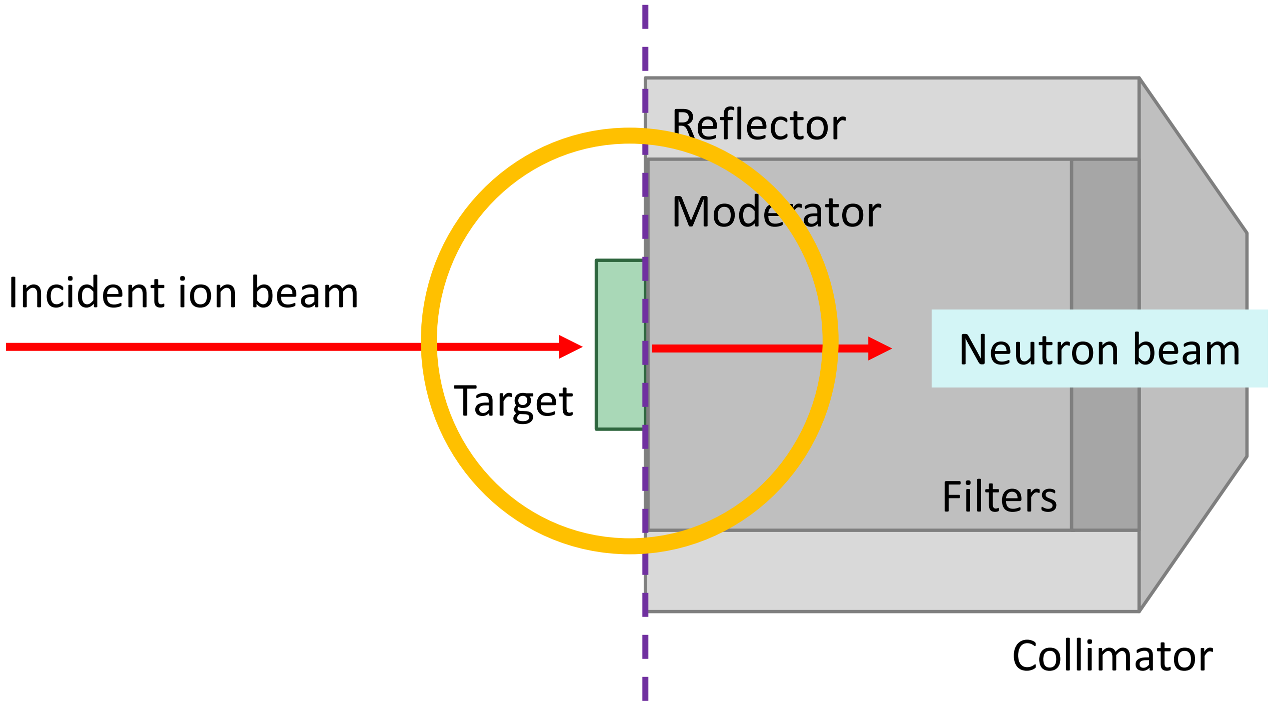
Note: For thermal/epithermal beams, either more moderator or low-energy incident ions are needed

Fast neutron spectra. Plot from [1]



[1] - Lee et al, 2020. *NIM B*, **478**

ABNS: The Beam Shaping Assembly (BSA)



This study focuses on the target output!

[1] - Lee et al, 2020. *NIM B*, **478**

Benchmarking Monte Carlo codes for AB-BNCT relevant neutron production reactions

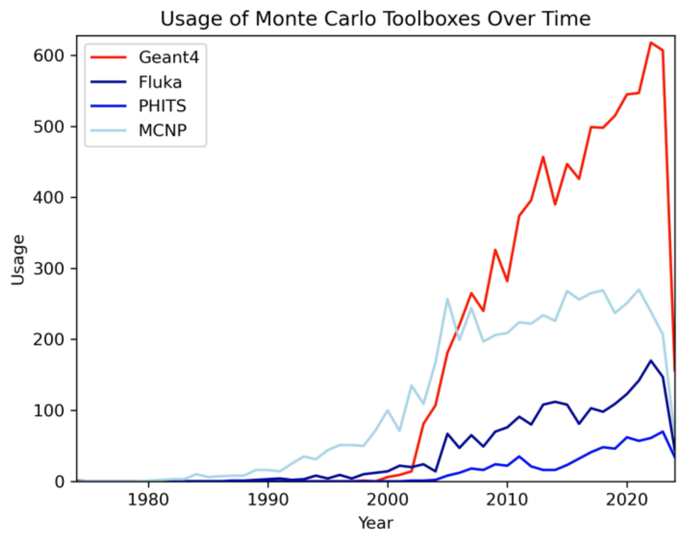
Aim:

To evaluate the performance of Geant4 for the simulation of accelerator-based boron neutron capture therapy (AB-BNCT) relevant neutron production reactions:

- Benchmark **Geant4 against available experimental results** (thick target yields)
- At the same time, benchmark **Geant4 against other available Monte Carlo codes**

Monte Carlo codes:

- **Geant4 v11.1.3**
- MCNP v6.3
- PHITS v3.33
- FLUKA (CERN) v4-40



AB-BNCT relevant reactions

Reaction	Incident Ion	Target Material	Threshold energy (MeV)
$^{9}Be(p,n)^{9}B$	Proton	Beryllium	2.06
$^{7}Li(p,n)^{7}Be$		Lithium	1.88
$^{9}Be(d,n)^{10}B$	Deuteron	Beryllium	0, 1
$^{13}C(d,n)^{14}N$		Carbon	0
$p(^{7}Li,n)^{7}Be$*	Lithium	Proton (polypropylene)	13.098

* Reaction being investigated for use by Okamura et al. At Brookhaven National Laboratory (BNL) [3]

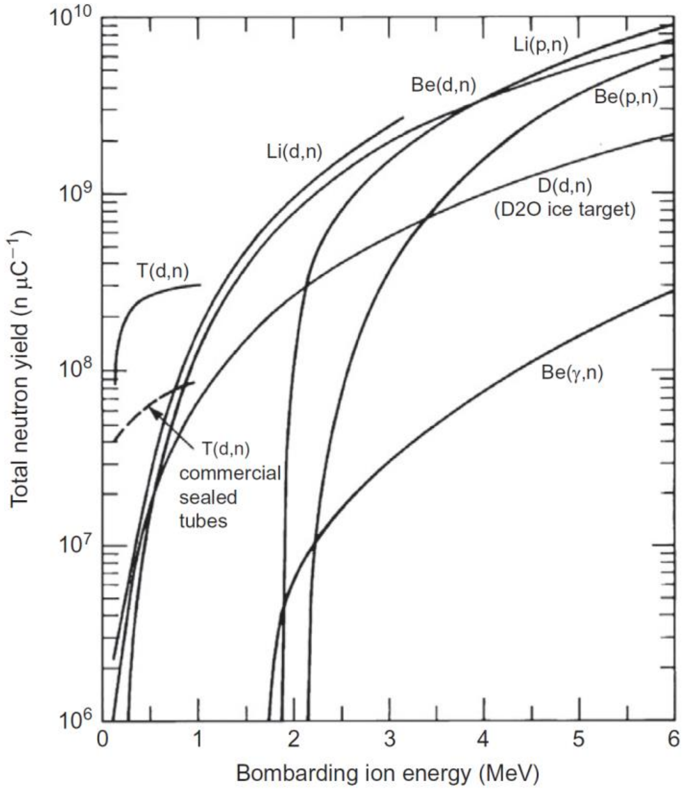


Figure. Neutron yield for low-energy particle beam reactions with a thick target [2].

Simulation Geometry and Scoring

Total production yield

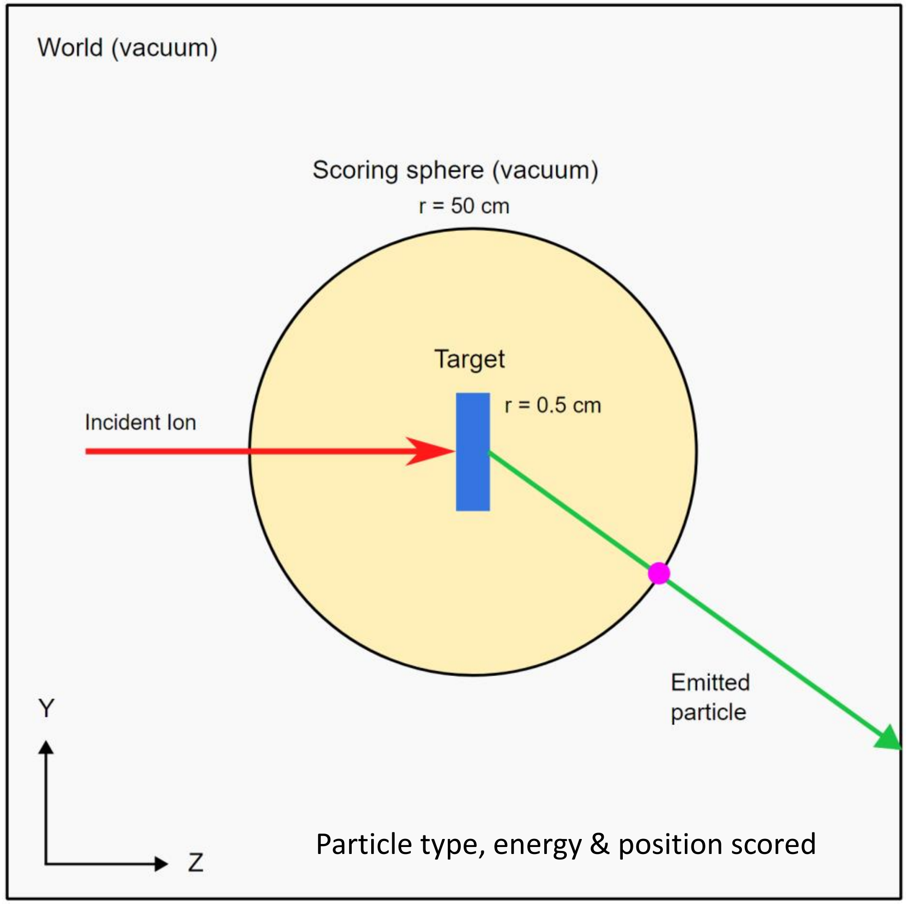
- Dictates source efficiency / irradiation times
- Useful for informing which reaction suits the needs of the accelerator system

Angular distribution

- Determines degree of beam collimation
- Informs BSA reflector and collimator design

Neutron energy

- Informs the degree of moderation and shielding needed



Cross section data and transport models

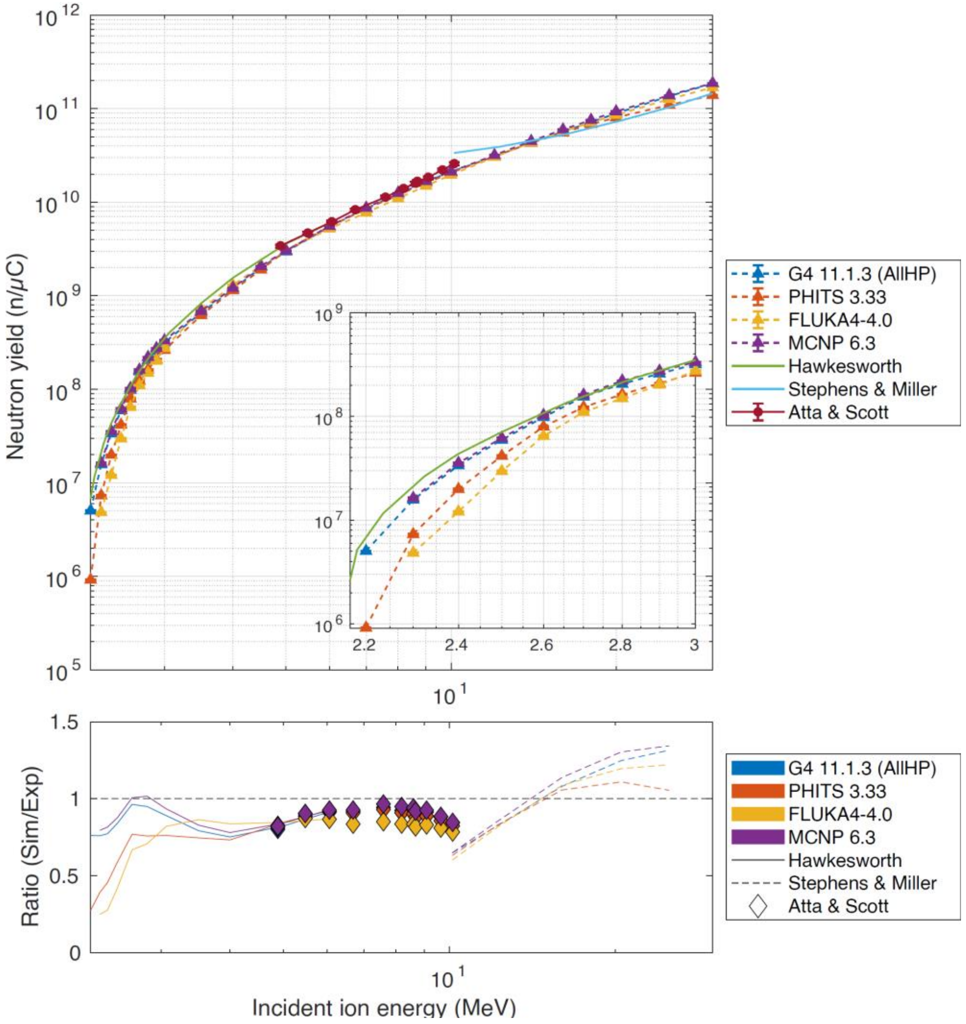
Physics list QGSP_BIC_AllHP has been used

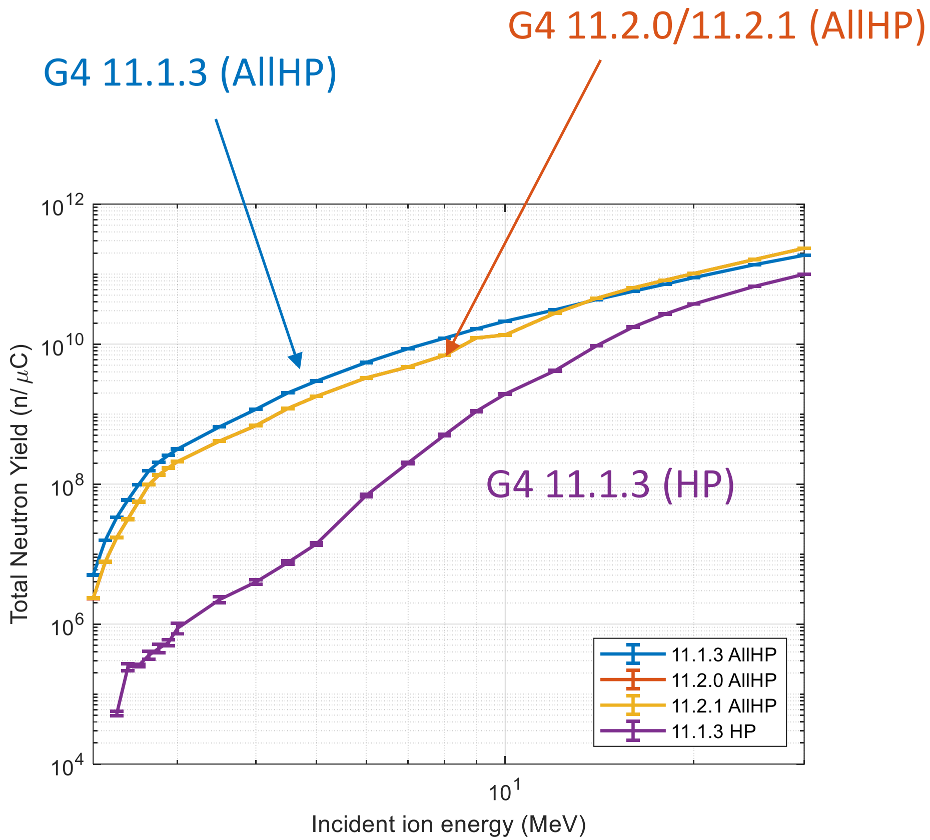
Geant4 v11.1.3 has been used for this study.
Further explanation in the next slides

Table 3. Cross section data libraries and models for particle transport used in each Monte Carlo code.

	Geant4	PHITS	FLUKA	MCNP
Proton	TENDL-2019, ENDF/B-VIII.0	JENDL-5	PEANUT model	ENDF/B-VII.0
Deuteron	TENDL-2019, JENDL/DEU-2020	JENDL-5	PEANUT model	ISABEL model (default) JENDL/DEU-2020 (added ACE files)
Heavy ions	Binary Cascade model	INCL model	RQMD, Boltzmann Master Equation models	LAQSM03.03 model
Neutron	JEFF-3.3	JENDL-4, JENDL-5	JEFF-3.3	ENDF/B-VII.1
Thermal Scattering	JEFF-3.3, ENDF/B-VIII.0	JENDL-4	JEFF-3.3	ENDF/B-VII.1

$^{9}Be(p,n)^{9}B$ reaction – Total neutron yield



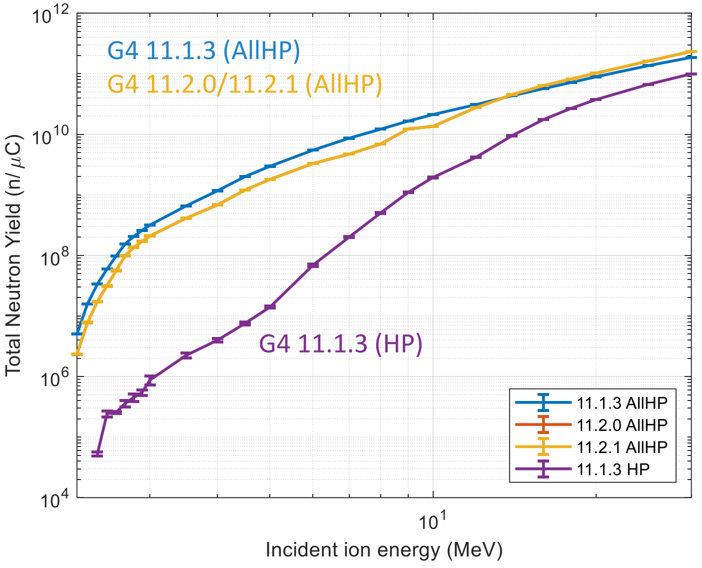


	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.166	0.05
G4 11.2.1 AllHP	0.449	0.05
G4 11.1.3 HP	0.872	0.20
PHITS	0.202	0.10
FLUKA	0.242	0.08
MCNP	0.156	0.07

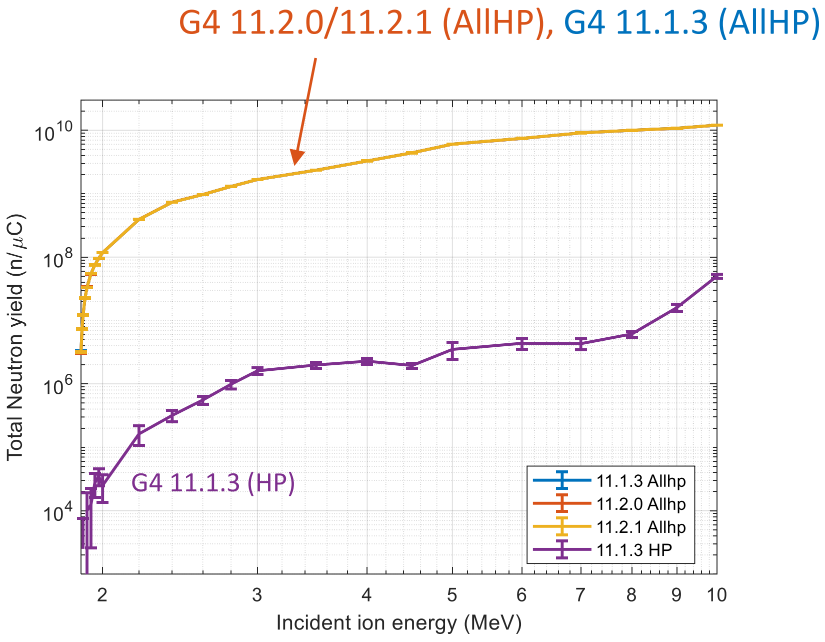
Note: MCNP and Geant4 are in agreement on this plot

Total neutron yield

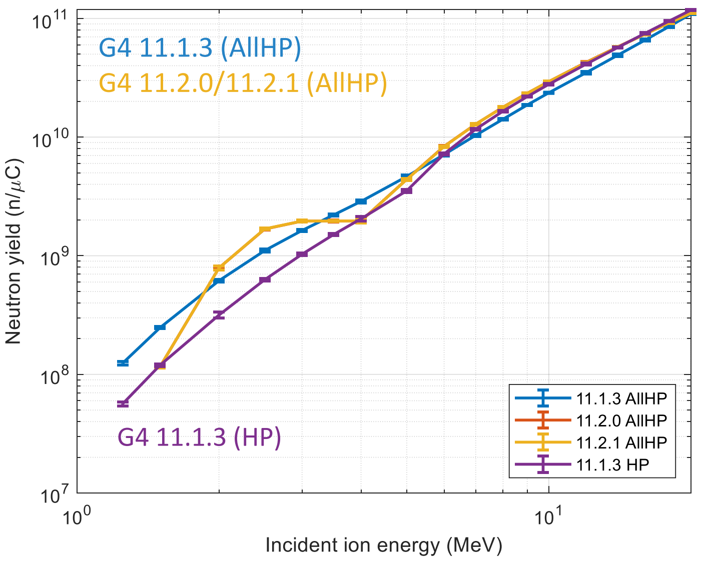
$^{9}Be(p,n)^{9}B$



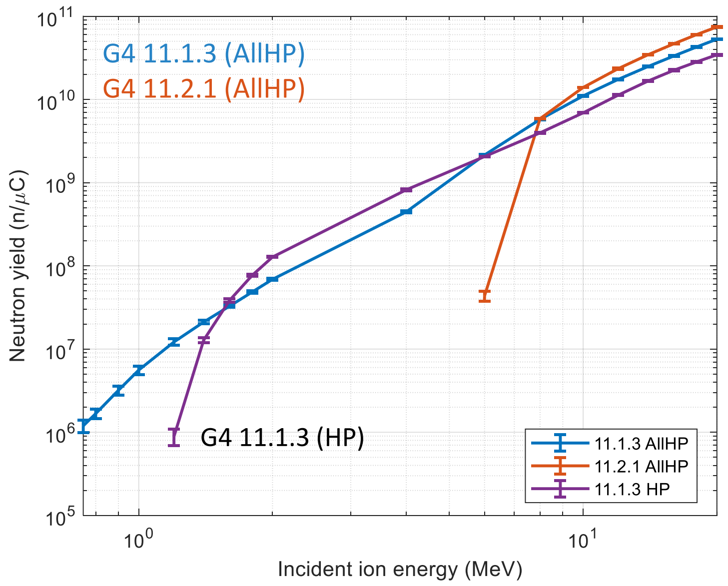
$^{7}Li(p,n)^{7}Be$



$^{9}Be(d,n)^{10}B$



C(d,n)N



Total neutron yield

Geant4 v11.1.3 AllHP has been chosen for benchmarking against other codes

Geant4 v11.1.3 AllHP performs the best against experimental datasets for total neutron yield compared to v11.2 series

$^{9}Be(p,n)^{9}B$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.166	0.05
G4 11.2.1 AllHP	0.449	0.05
G4 11.1.3 HP	0.872	0.15
PHITS	0.202	0.10
FLUKA	0.242	0.08
MCNP	0.156	0.07

$^{7}Li(p,n)^{7}Be$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.147	0.04
G4 11.2.1 AllHP	0.147	0.04
G4 11.1.3 HP	1.000	0.00
PHITS	0.117	0.07
FLUKA	0.094	0.06
MCNP	0.174	0.09

$^{9}Be(d,n)^{10}B$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.151	0.04
G4 11.2.1 AllHP	0.218	0.08
G4 11.1.3 HP	0.418	0.16
PHITS	0.183	0.06
FLUKA	0.188	0.07
MCNP	0.150	0.05

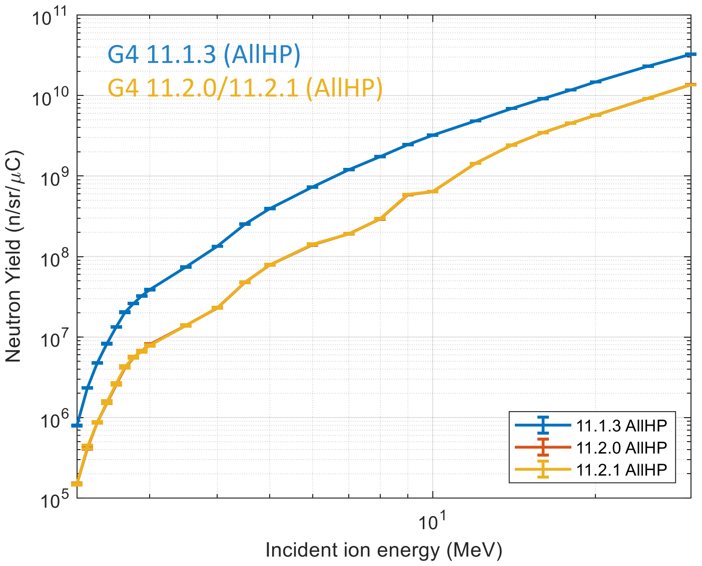
C(d,n)N

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.474	0.131
G4 11.2.1 AllHP	0.896	0.147
G4 11.1.3 HP	0.513	0.090
PHITS	0.491	0.138
FLUKA	0.641	0.107
MCNP	0.493	0.086

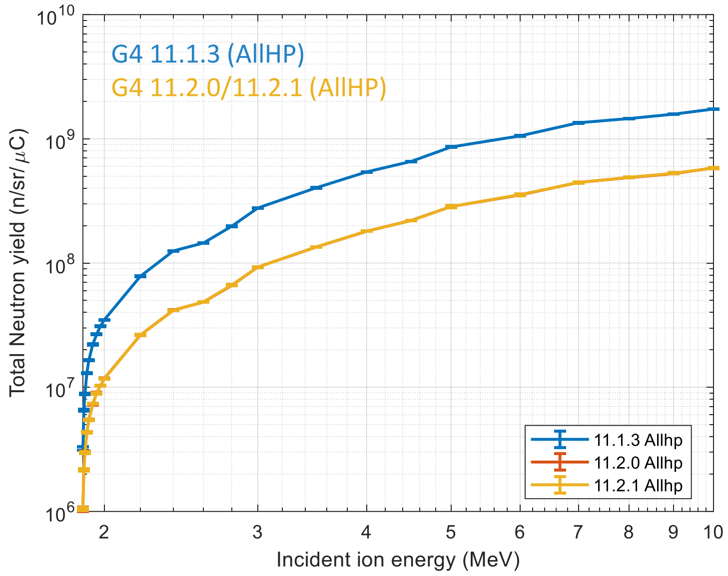
Neutron yield at 0º (forward direction)

Reactions simulated using v11.2.x present lower yields in the forward direction compared to v11.1.3

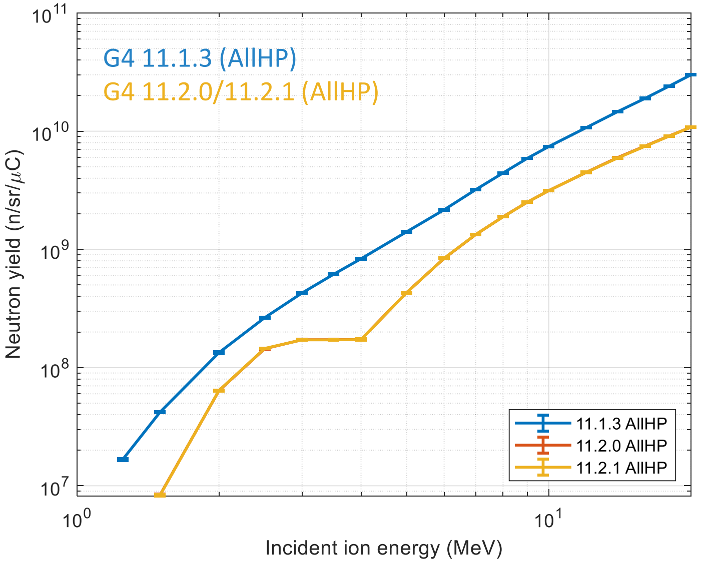
$^{9}Be(p,n)^{9}B$



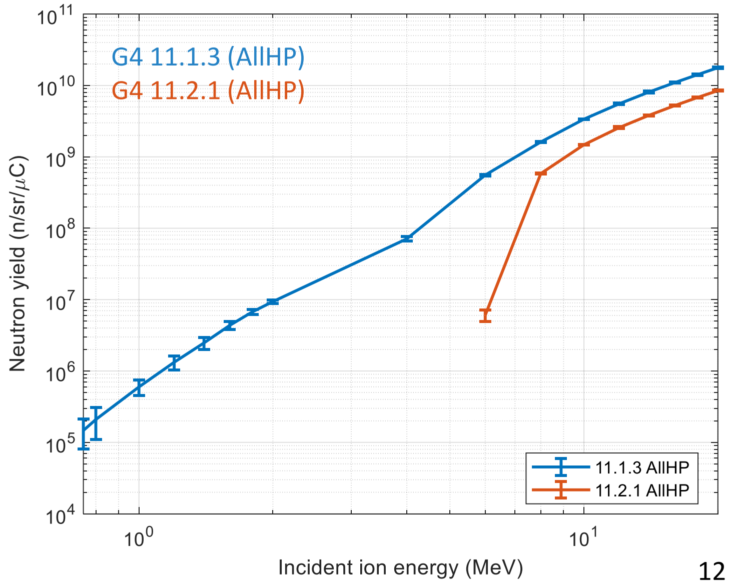
$^{7}Li(p,n)^{7}Be$



$^{9}Be(d,n)^{10}B$



C(d,n)N



Neutron yield at 0^o (forward direction)

Geant4 v11.1.3 AllHP has been chosen for benchmarking against other codes

Geant4 v11.1.3 outperforms v11.2.x in all cases

$^9Be(p,n)^9B$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.335	0.19
G4 11.2.1 AllHP	0.685	0.15
PHITS	0.218	0.16
FLUKA	0.367	0.15
MCNP	0.368	0.21

$^7Li(p,n)^7Be$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.439	0.18
G4 11.2.1 AllHP	0.605	0.15
PHITS	0.482	0.25
FLUKA	0.564	0.41
MCNP	0.454	0.29

$^9Be(d,n)^{10}B$

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.290	0.15
G4 11.2.1 AllHP	0.655	0.13
PHITS	0.287	0.17
FLUKA	0.420	0.10
MCNP	0.274	0.15

C(d,n)N

	$\overline{MRE}$	σ
G4 11.1.3 AllHP	0.328	0.21
G4 11.2.1 AllHP	-	-
PHITS	0.333	0.19
FLUKA	0.488	0.22
MCNP	0.306	0.19

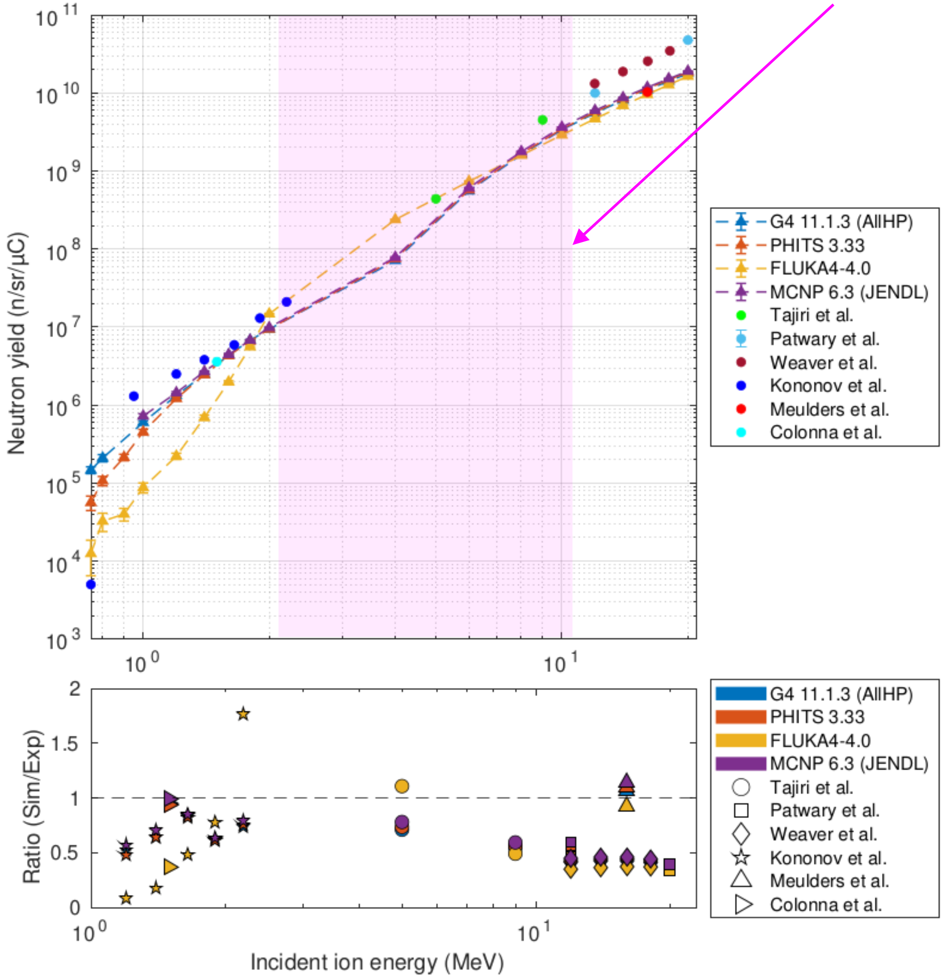
Note about Available Experimental Datasets

There are many gaps in the available experimental data for all reactions of interest.

- **More data points need to be collected** across the relevant incident ion energy ranges for future MC benchmarking.
- **Available thick target yields (TTY)** relating to neutron yield, energy spectra and angular distribution data **have been collated.**
- There is currently no relevant experimental datasets for the p(7Li,n)7Be reaction

Example: Neutron yield
C(d,n)N, 0°

Gap in experimental data between ~2 – 10 MeV



Neutron Spectra – $^{9}Be(p,n)^{9}B$

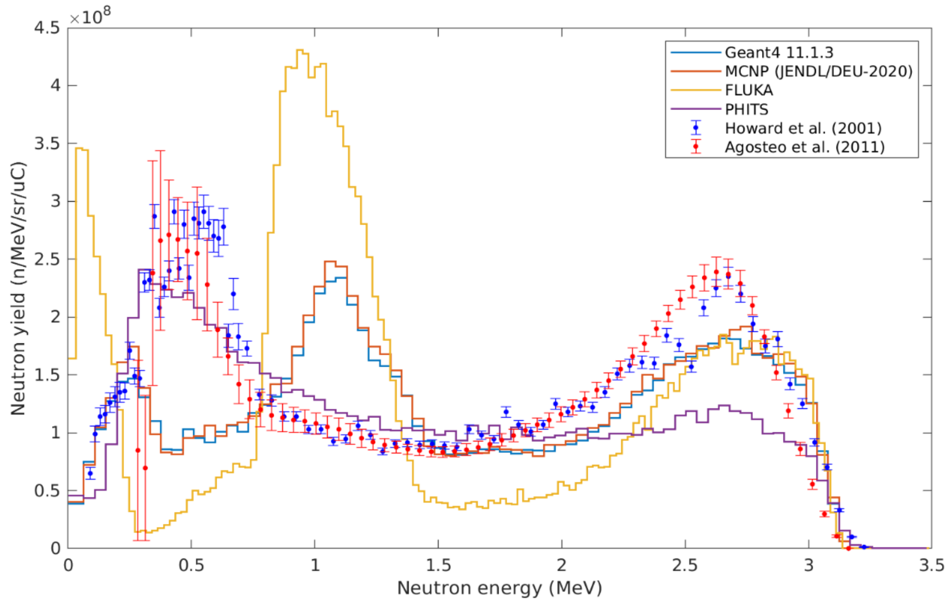
Using **Geant4 v11.1.3** for benchmarking

Pearson Correlation Coefficient (PCC) used to quantify overall agreement of shape

$$PCC = \frac{\sum_{i=1}^{n}(S_i - \overline{S})(R_i - \overline{R})}{\sqrt{\sum_{i=1}^{n}(S_i - \overline{S})^2 \sum_{i=1}^{n}(R_i - \overline{R})^2}}$$

Geant4 v11.1.3 does not produce good agreement with experimental data at 0º for $^{9}Be(p,n)^{9}B$

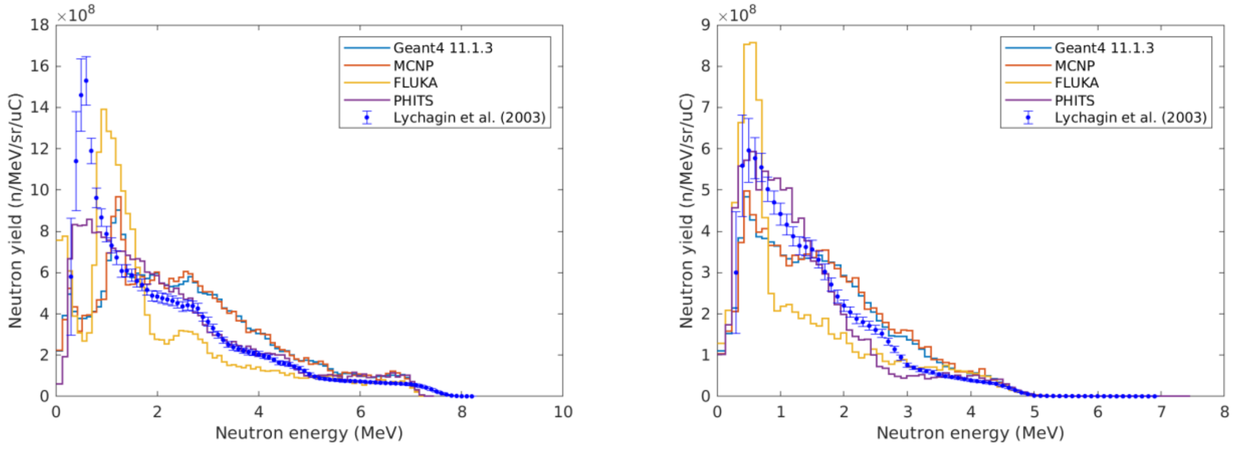
5 MeV (0º)



	Howard et al.	Agosteo et al.
Geant4	0.107	0.260
PHITS	0.789	0.599
FLUKA	-0.251	-0.048
MCNP	0.081	0.233

PCC =

9 MeV (0º)



(a) $\theta = 0^\circ$ (b) $\theta = 140^\circ$

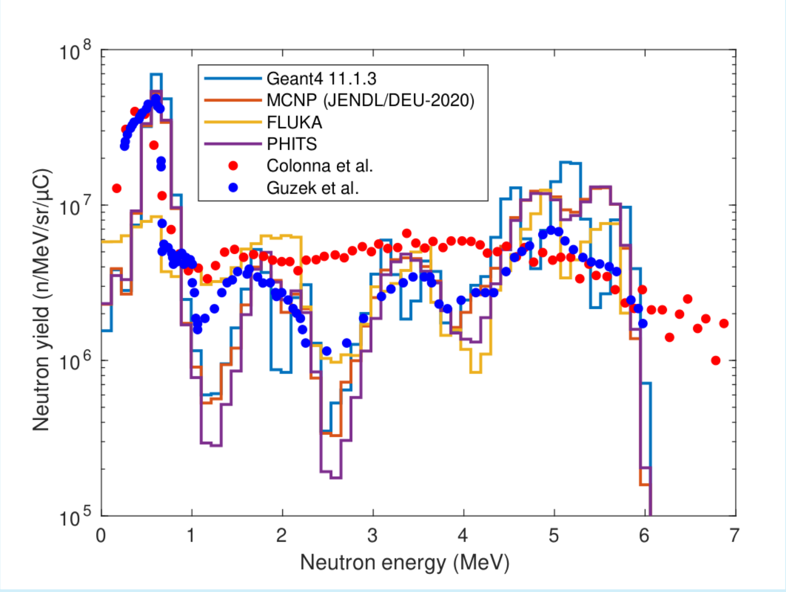
	0º	140º
Geant4	0.693	0.957
PHITS	0.930	0.970
FLUKA	0.693	0.821
MCNP	0.687	0.954

PCC =

Neutron Spectra – $^{9}Be(d,n)^{10}B$

Using **Geant4 v11.1.3** for benchmarking

1.5 MeV

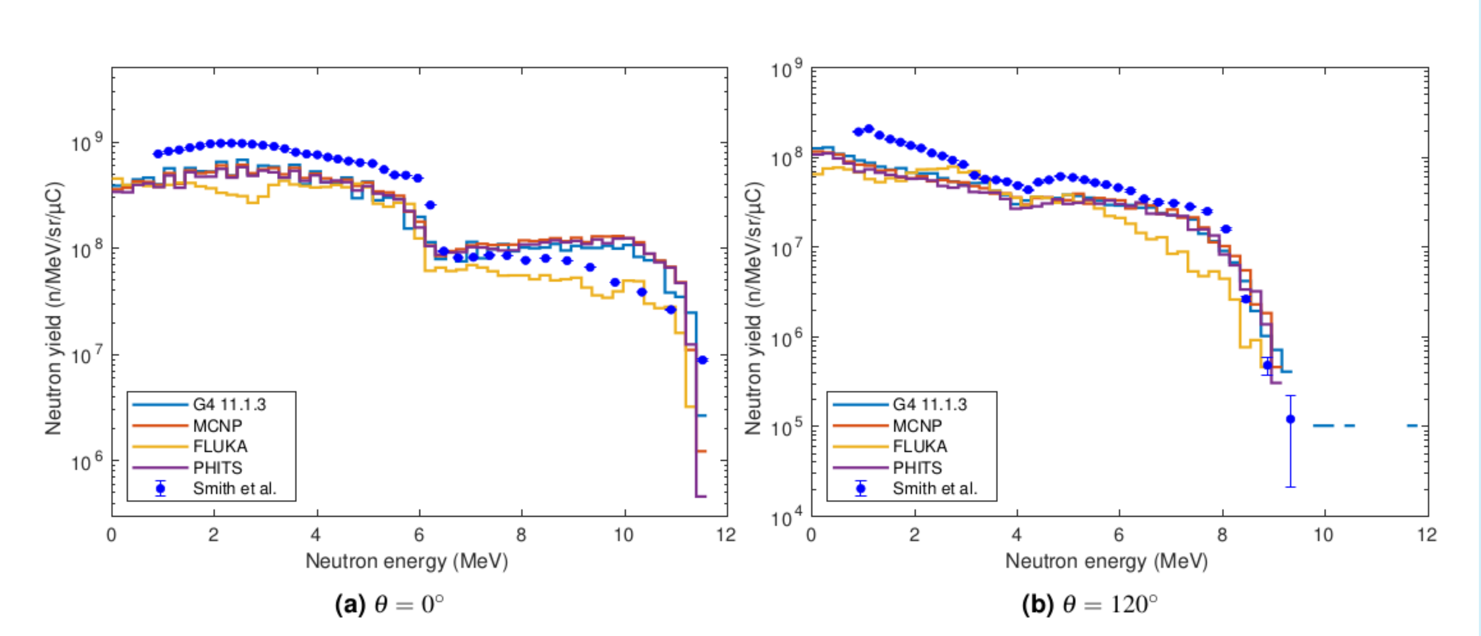


Geant4 11.1.3 produces spectral minima at energies consistent with Guzek et al.

PCC =

	Guzek et al.
Geant4	0.746
PHITS	0.799
FLUKA	0.483
MCNP	0.795

7 MeV



(a) $\theta = 0^{\circ}$ **(b)** $\theta = 120^{\circ}$

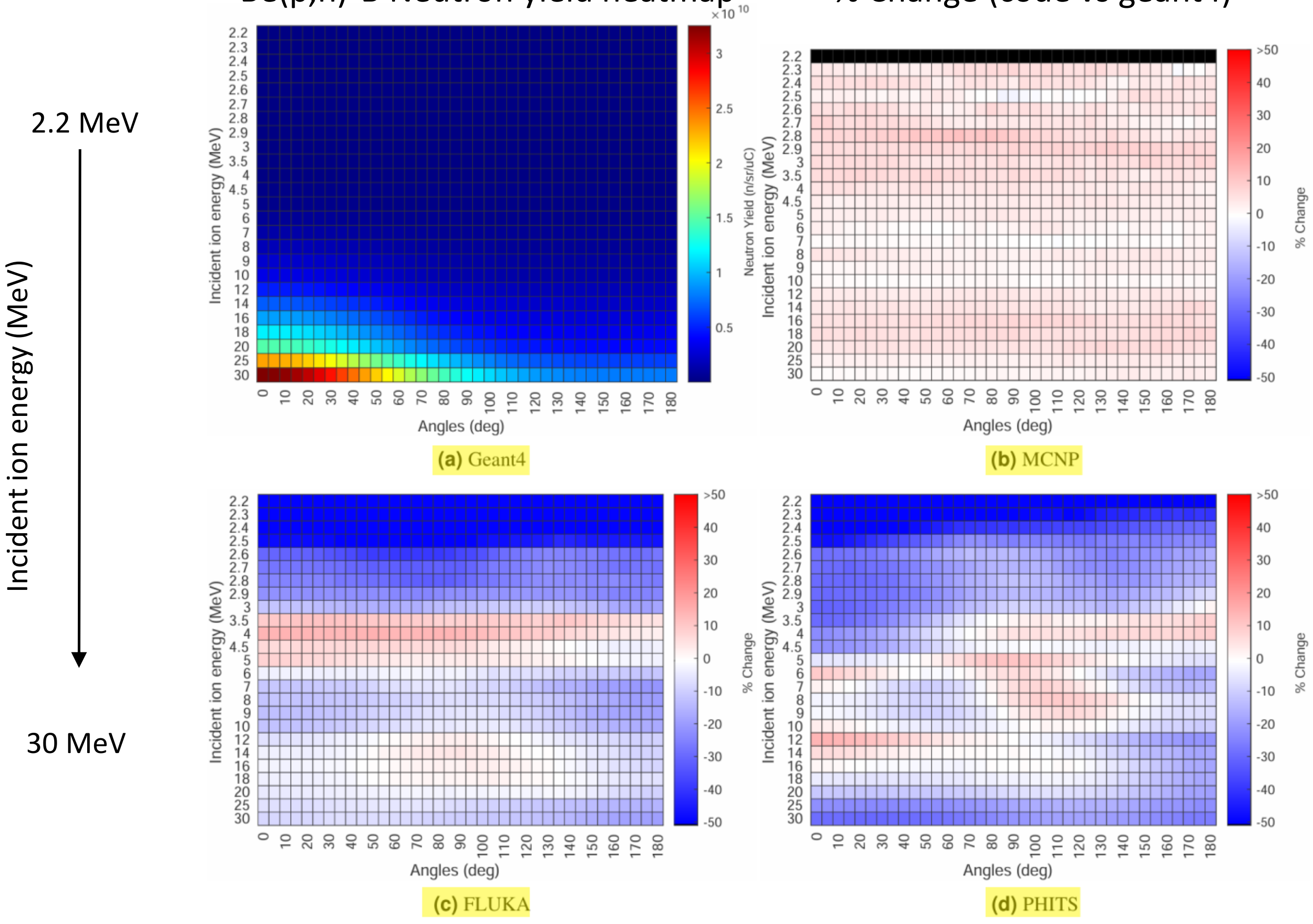
PCC =

	0°	120°
Geant4	0.979	0.965
PHITS	0.980	0.958
FLUKA	0.930	0.784
MCNP	0.980	0.953

Global Inter-code Comparison - Neutron yield

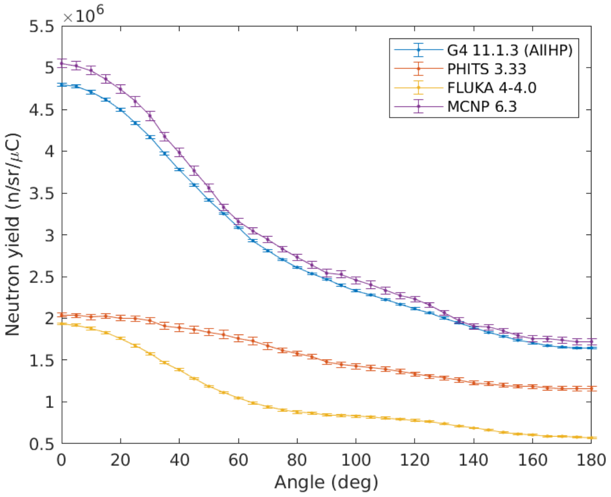
Using **Geant4 v11.1.3** for benchmarking

$^{9}Be(p,n)^{9}B$ Neutron yield heatmap | % Change (code vs geant4)

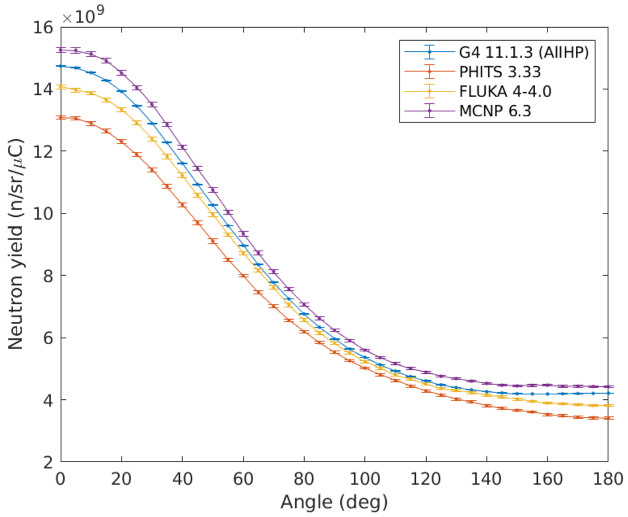


- High variability at lower incident ion energies (Ei)
- Geant4 and MCNP present similar yields across all incident ion energies and angles

2.4 MeV



20 MeV



Global Inter-code Comparison - Neutron yield

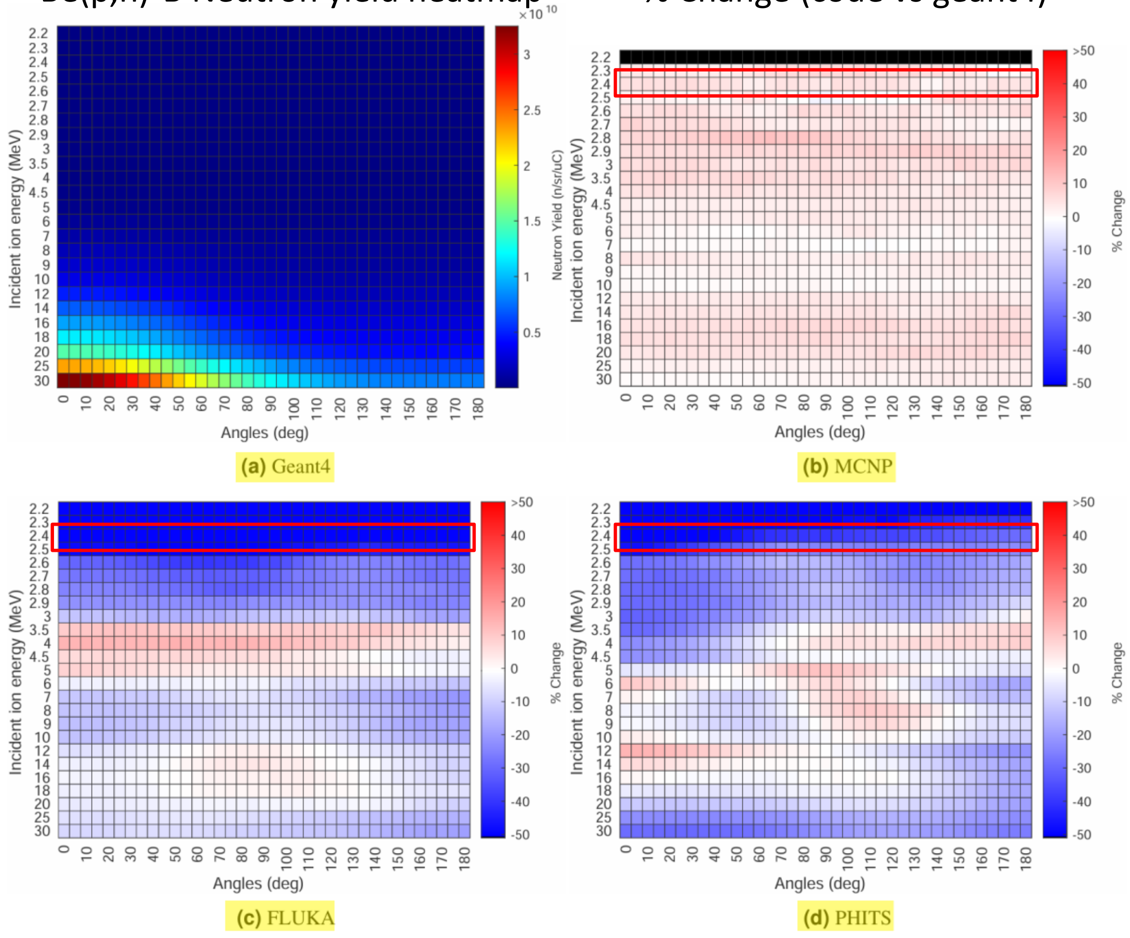
Using **Geant4 v11.1.3** for benchmarking

$^{9}Be(p,n)^{9}B$ Neutron yield heatmap | % Change (code vs geant4)

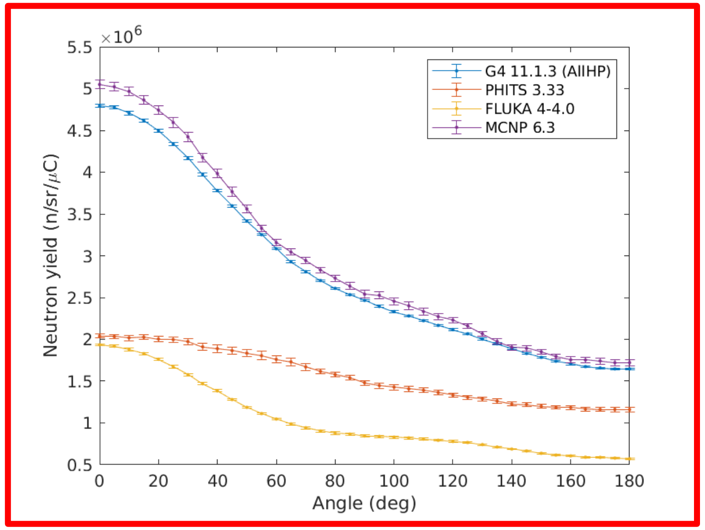
2.2 MeV

Incident ion energy (MeV)

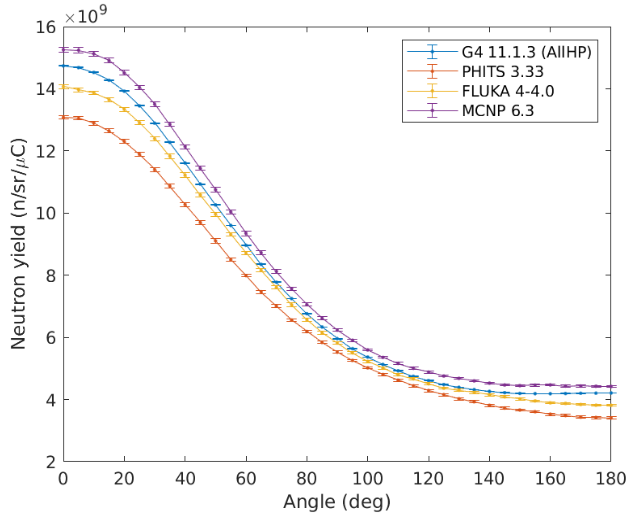
30 MeV



2.4 MeV



20 MeV



- High variability at lower incident ion energies (Ei)
- Geant4 and MCNP present similar yields across all incident ion energies and angles

Global Inter-code Comparison - Neutron yield

Using **Geant4 v11.1.3** for benchmarking

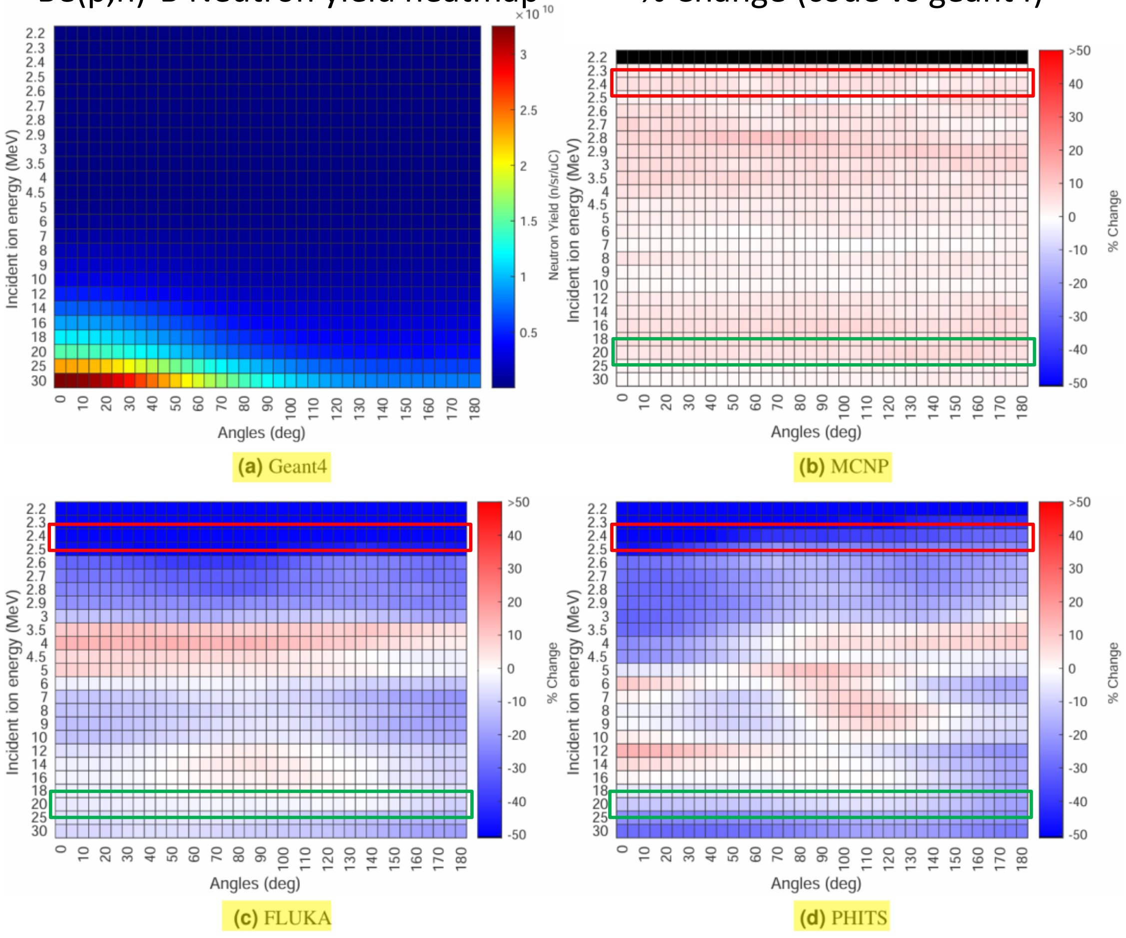
^{9}Be(p,n)^{9}B Neutron yield heatmap

% Change (code vs geant4)

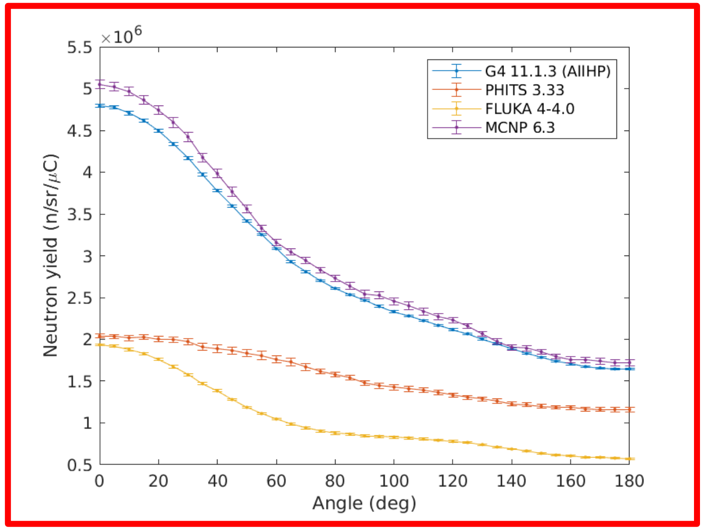
2.2 MeV

Incident ion energy (MeV)

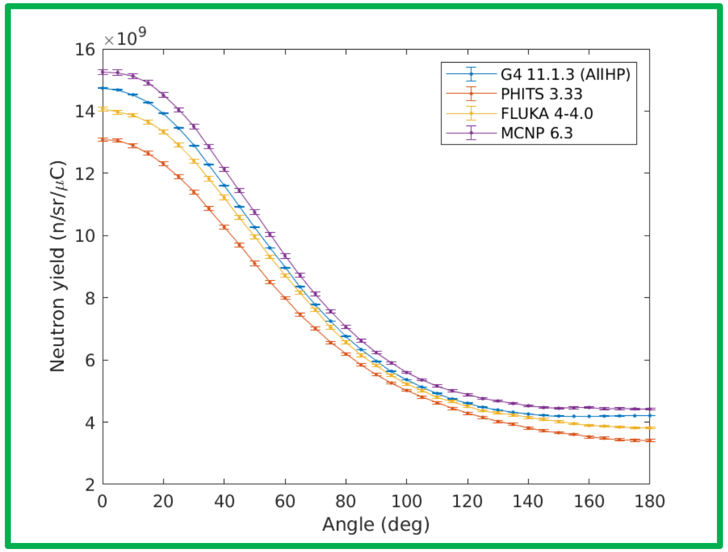
30 MeV



2.4 MeV



20 MeV



- High variability at lower incident ion energies (Ei)
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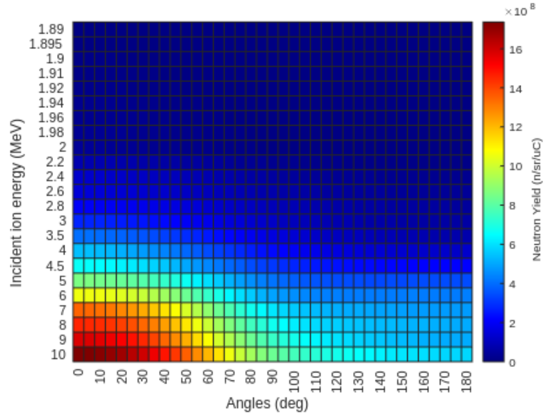
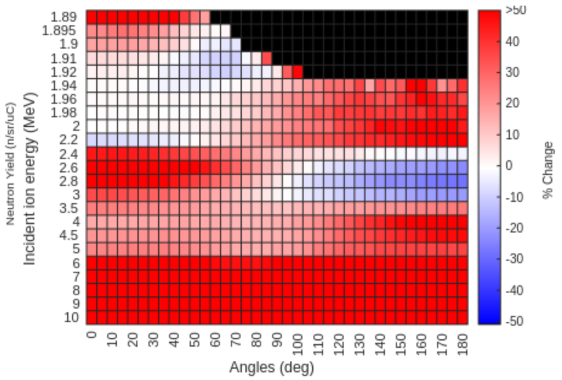
Inter-code Comparison - Neutron yield

Using **Geant4 v11.1.3** for benchmarking

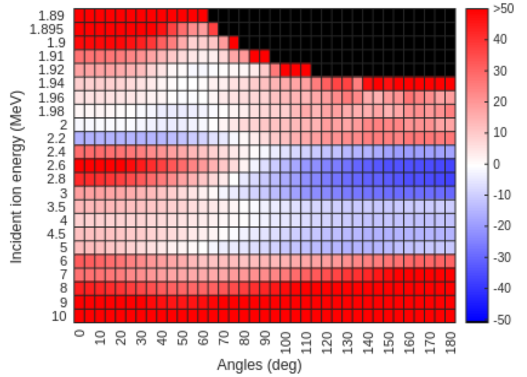
$^{7}Li(p,n)^{7}Be$



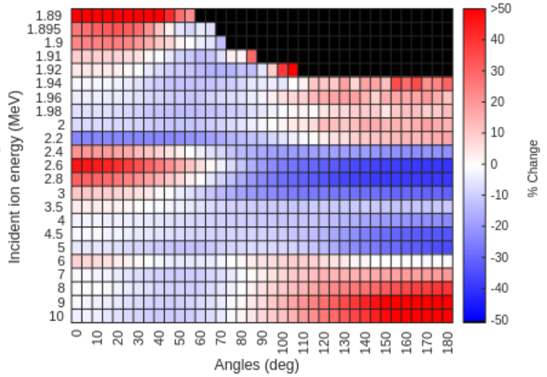
(a) Geant4



(b) MCNP

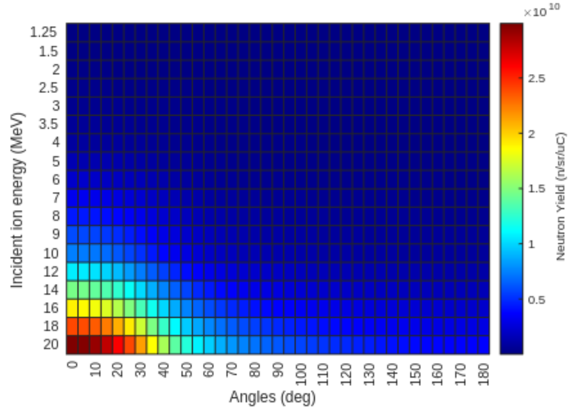


(c) FLUKA

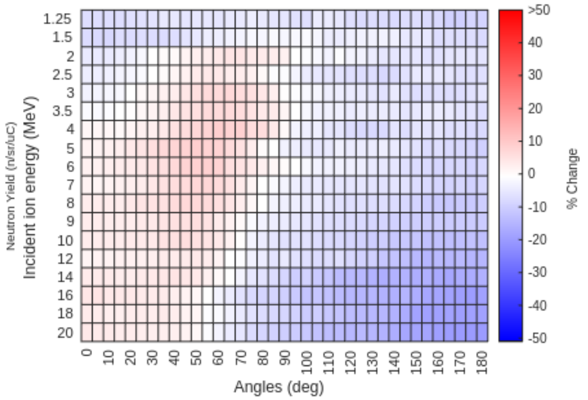


(d) PHITS

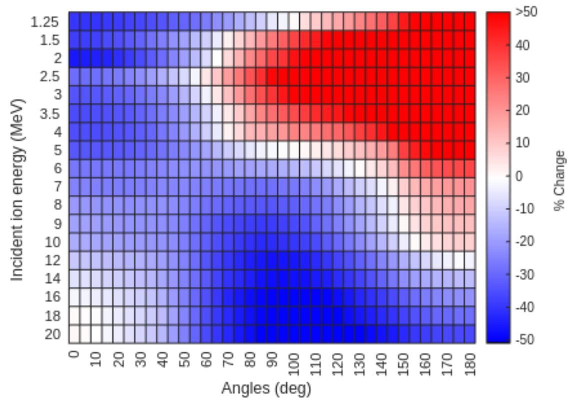
$^{9}Be(d,n)^{10}B$



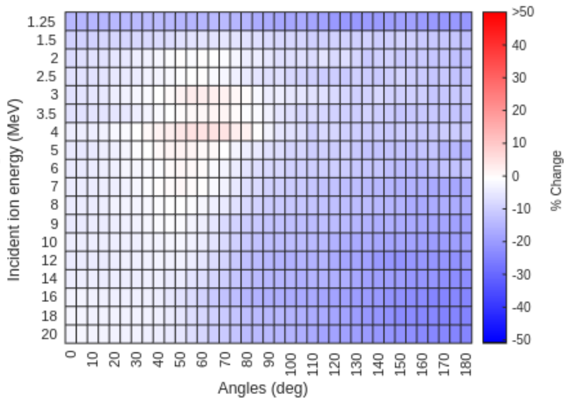
(a) Geant4



(b) MCNP



(c) FLUKA



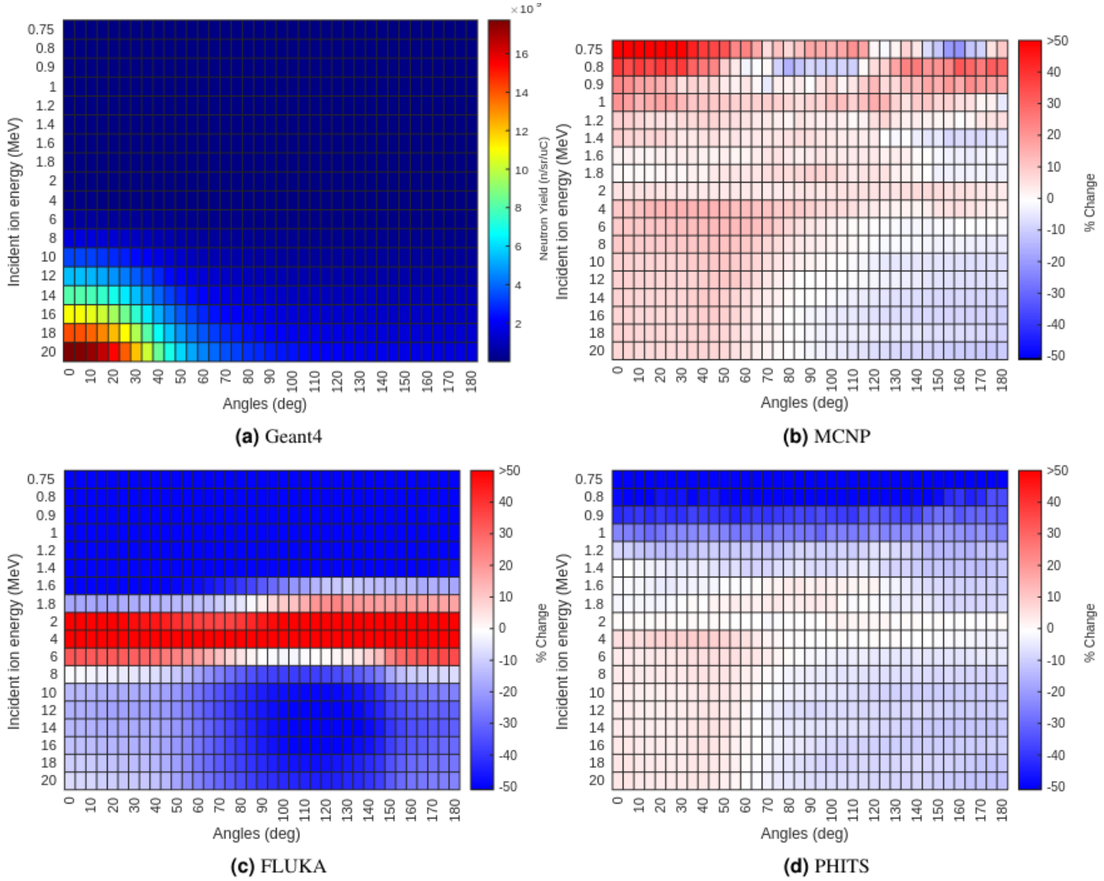
(d) PHITS

Geant4, PHITS, and MCNP are using JENDL/DEU-2020 cross sections for deuterons

Inter-code Comparison - Neutron yield

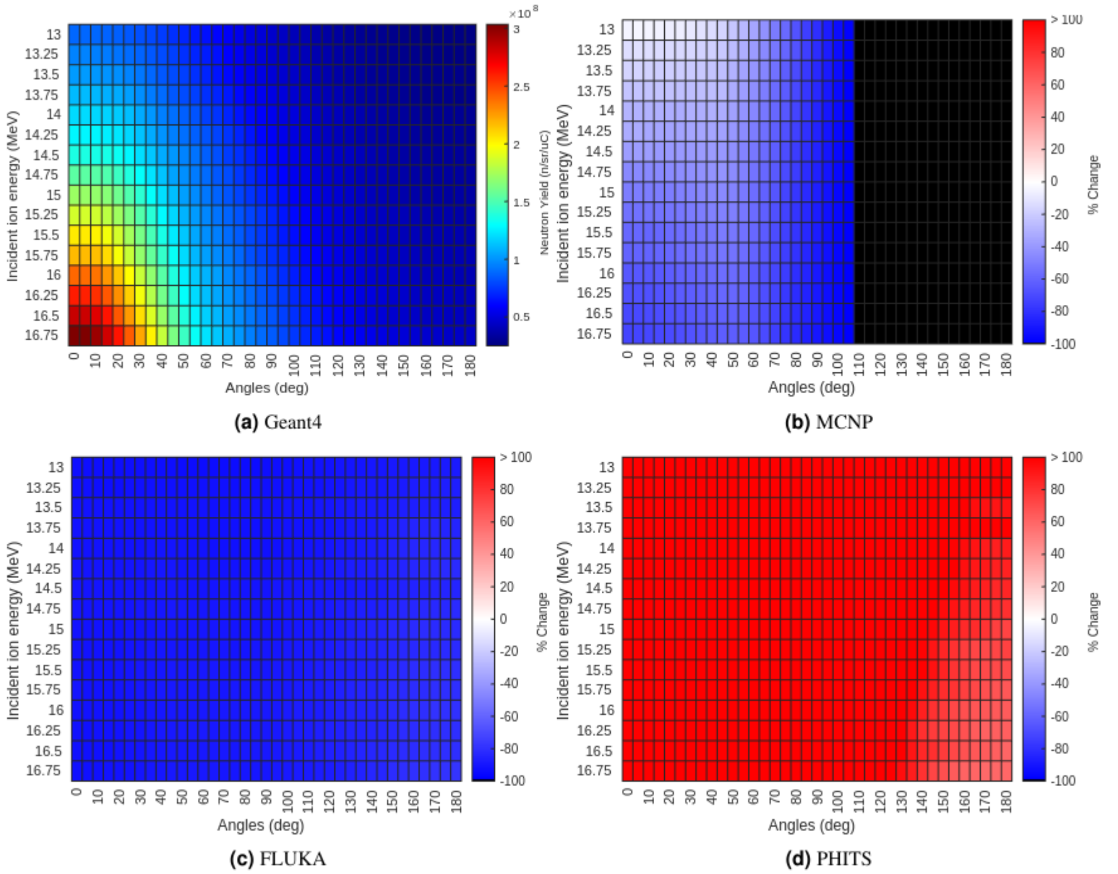
Using **Geant4 v11.1.3** for benchmarking

C(d,n)N



Geant4, PHITS, and MCNP are using JENDL/DEU-2020 cross sections for deuterons

p(^{7}Li,n)^{7}Be



Transport models for the p(Li,n) reaction do not include experimental data

Conclusion & Next Steps

The performance of Geant4 for the simulation of accelerator-based boron neutron capture therapy (AB-BNCT) relevant neutron production reactions has been evaluated

- Geant4 AllHP has been used for reactions involving proton and deuteron transport on Be, Li and C targets.
- **Geant4 v11.1.3 displays better agreement with available experimental data compared to v11.2.x** for total neutron yield and neutron yield at 0^{o} (forward direction).
- Results from Geant4 have been **compared to those from other Monte Carlo Codes (PHITS, FLUKA, MCNP)**. Code recommendation depends on the reaction and properties of interest.

Next Steps:

- Paper submission: Computer Physics Communications (or Journal of Computational Physics)
- Use this study to inform **future simulations and development of beam shaping assembly designs** for ABNSs housed at ANSTO and BNL

Thank you! Questions?

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And everyone else involved in this work!

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