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Code Inter-Comparison for Radiation Damage Related Quantities

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Outline

- Introduction
- 2013 Inter-Comparison of FLUKA, MARS and PHITS Predictions for the Neutron-Dominated Case (Mu2e & COMET Superconducting Coils)
- New Inter-Comparison with FLUKA, MARS, PHITS, SRIM and MCNP, Primarily for Neutrino Facilities
- 2 MeV to 7 TeV Intense Proton Beams on a Thin Ti Window
- 180 MeV to 7 TeV Proton Beams on a Thick Graphite Target
- Summary and To-Do List

Introduction

The first inter-comparison of FLUKA, MARS and PHITS performed in 2013 at “Radiation Effects in Superconducting Magnet Materials” (RESMM13) at KEK revealed that the codes agreed very well on DPA for the neutron-dominated case of the Mu2e and COMET SC coils.

New code inter-comparison exercise has been undertaken for this meeting for the proton-induced radiation related quantities in beam windows and targets of the existing and planned neutrino experiments. Energy deposition, fast neutron fluence, DPA, and Hydrogen/Helium gas production are all used to estimate the radiation damage levels and evaluate lifetime.

Beam energies, spot sizes, total POT and materials chosen to be representative for those in the neutrino programs. Low energies were also included to match those at the existing irradiation facilities. The highest proton beam energy of 7 TeV was added for completeness.

Motivation

Usually, benchmarking against experimental data is the way to justify the calculation results. It is not the case for such a not directly observable value as DPA. Therefore, the code prediction inter-comparison is the way to go for DPA.

Two-fold purpose of any code inter-comparison:

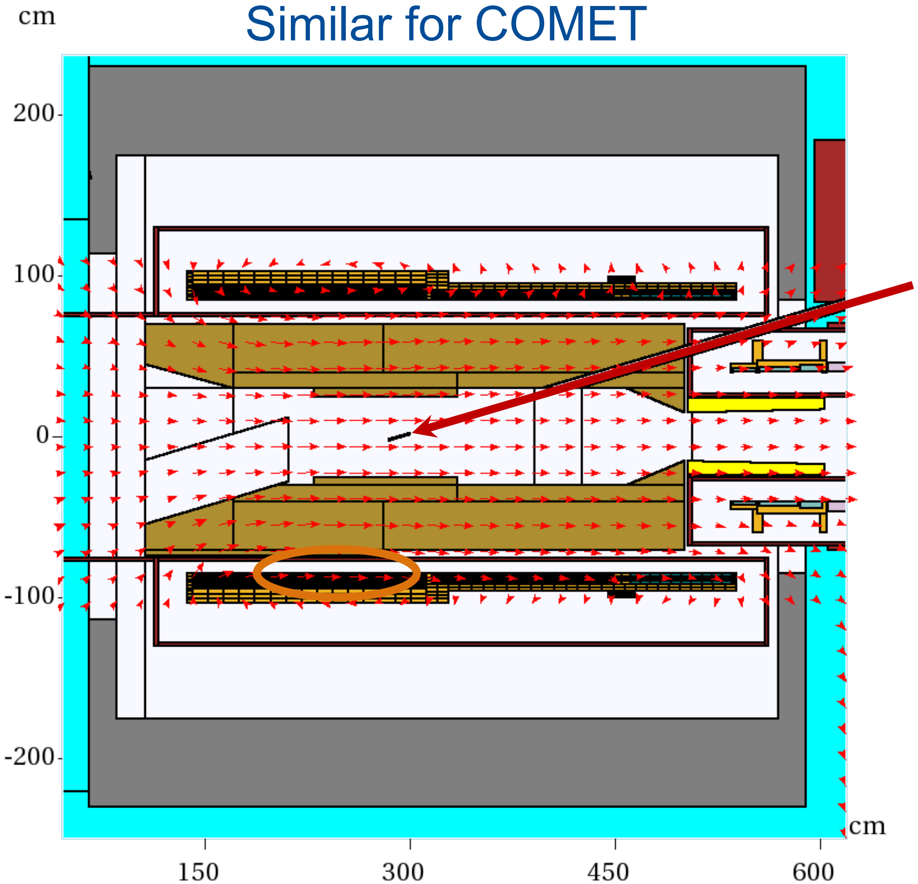
1. Find and understand uncertainties in code predictions and in our knowledge in the field

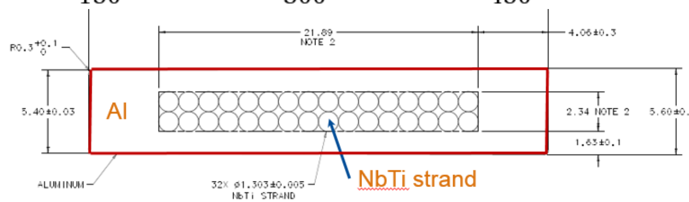
2. Identify possible issues in the codes participating and fix these

Example: Just ten years ago, the differences in DPA predicted by the high-energy codes could be as high as a factor of 10, substantially reduced since as a result of the developments induced by the code inter-comparisons.

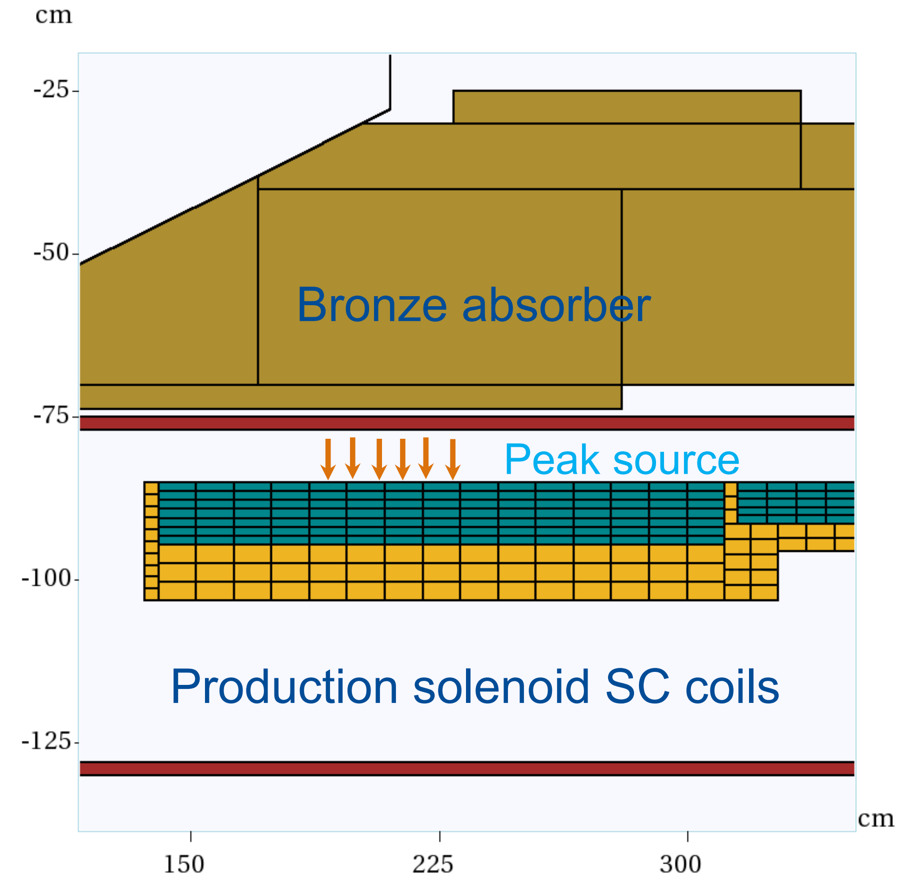
Code Intercomparison for Mu2e PS Coils

Similar for COMET

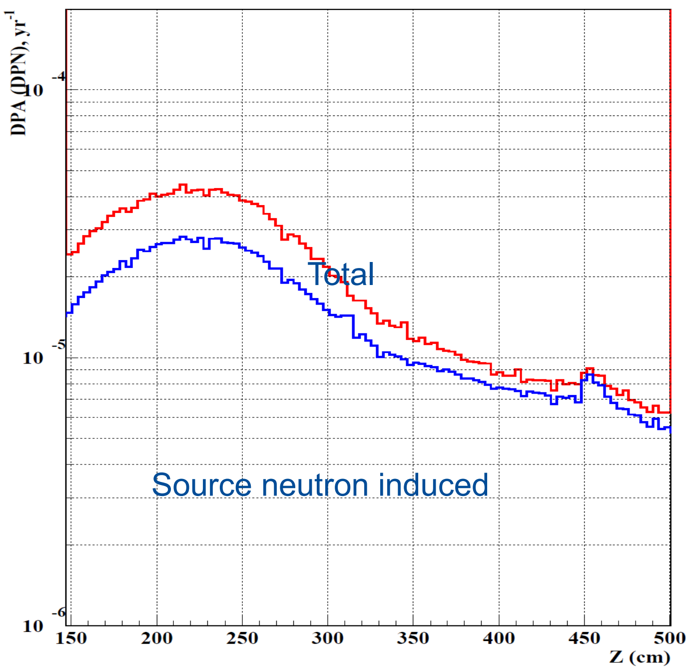


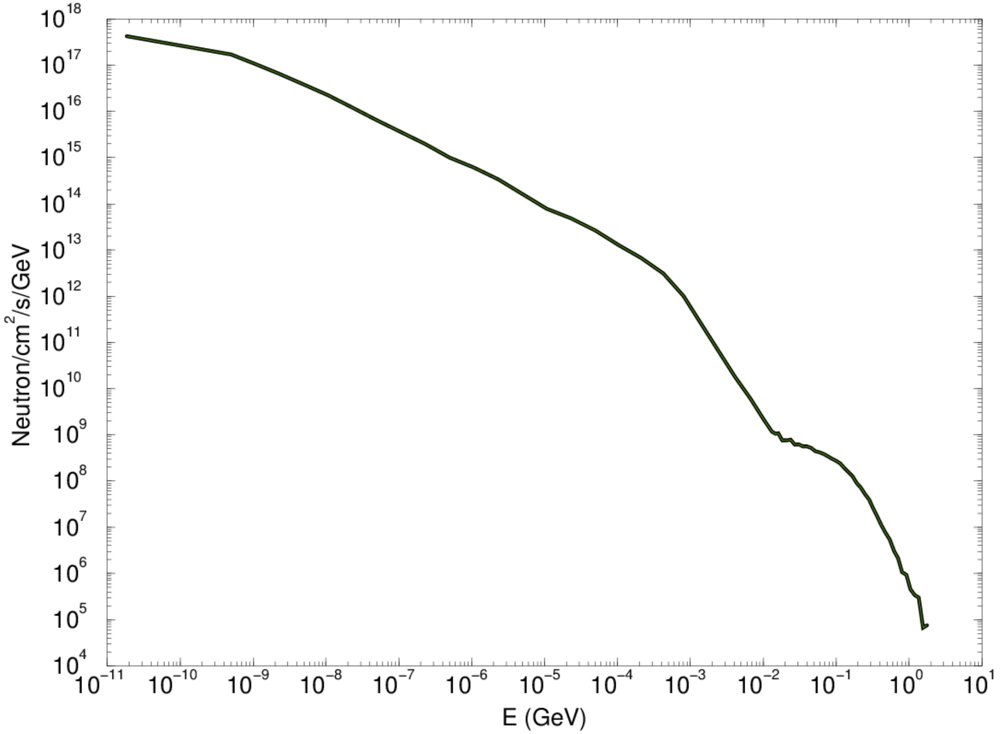


8-GeV p, 8 kW, 6.e12 p/s, $\sigma_x = \sigma_y$ = 1mm Tungsten water-cooled target (r=3mm, L=160mm). Upgrade to 100 kW @ 0. 8 GeV is considered.



Neutrons in Mu2e Production Solenoid SC Coils





Source neutron-induced DPA is ~70% of the total
Neutrons with E < 14.5 MeV are >99% of all neutrons in the PS coils
Source neutron spectrum 0.001 eV < E < 1.8 GeV impinged on Al, Cu & Al-NbTi coil blocks 10x10x10 cm^3 sub-dived along z in ten 1-cm slabs

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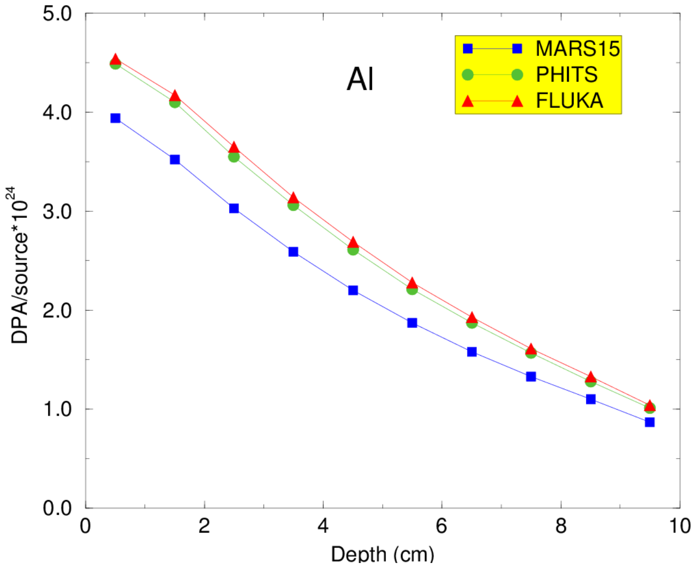
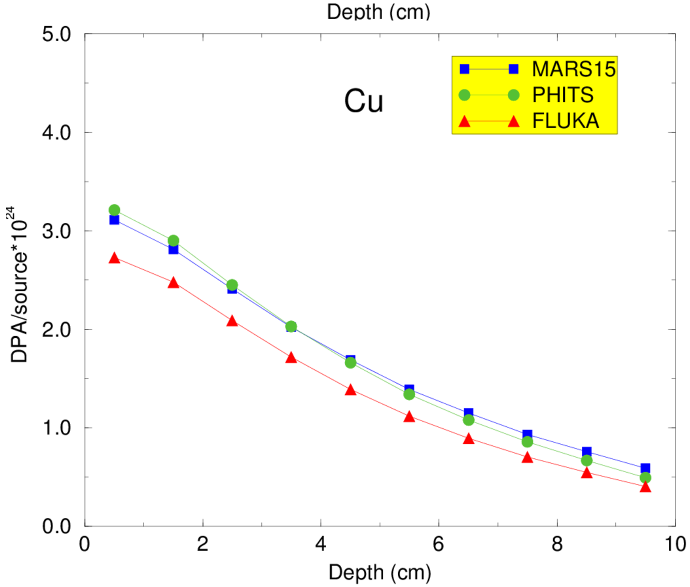
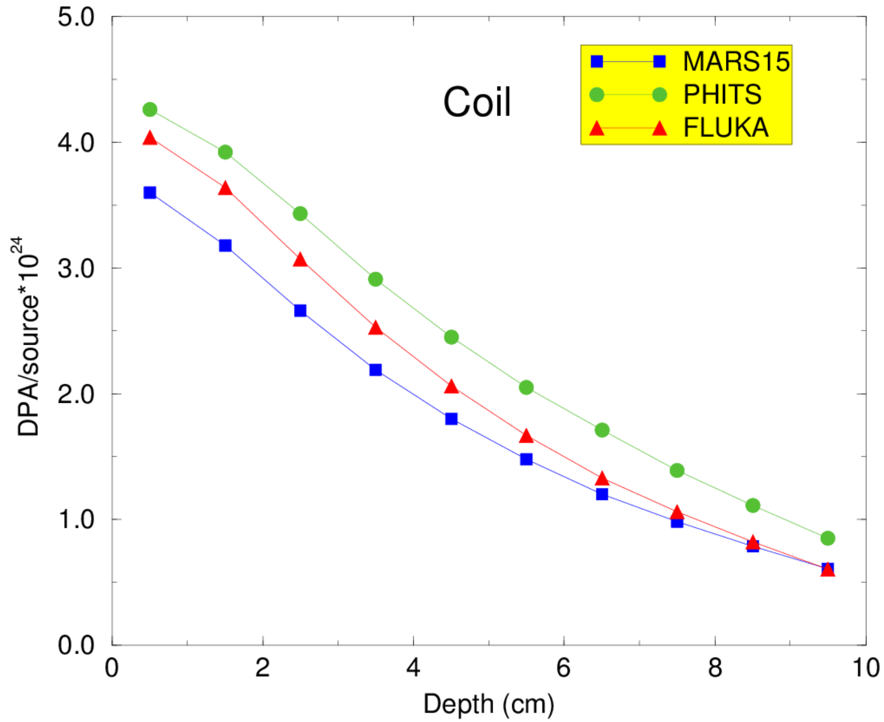
MARS15-PHITS-FLUKA DPA: Al, Coil and Cu







For low-energy neutron-dominated case in the NRT mode, three codes agreed within 10%

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Codes and Participants

- FLUKA 2017.0 (dev version), E=<20 PeV, Vasilis Vlachoudis (CERN)
- MARS15(2016) v. Aug2017, E=<100 TeV, Nikolai Mokhov (Fermilab)
- PHITS version2.96, E =< 1 TeV, Yosuke Iwamoto (JAEA)
- SRIM/TRIM 2013, Kinchin-Pease “quick calculation” mode, E =< 10 GeV, K. Ammigan (Fermilab)
- MCNP (see next page), E =< 3 GeV, David Wootan (PNNL)

DPA Models

FLUKA: Non-restricted nuclear losses converted to dpa

FLUKA-R: Restricted losses above the damage threshold converted to dpa

MARS, PHITS, SRIM, MCNP: NRT

MARS-EF: NRT with Nordlund efficiency function

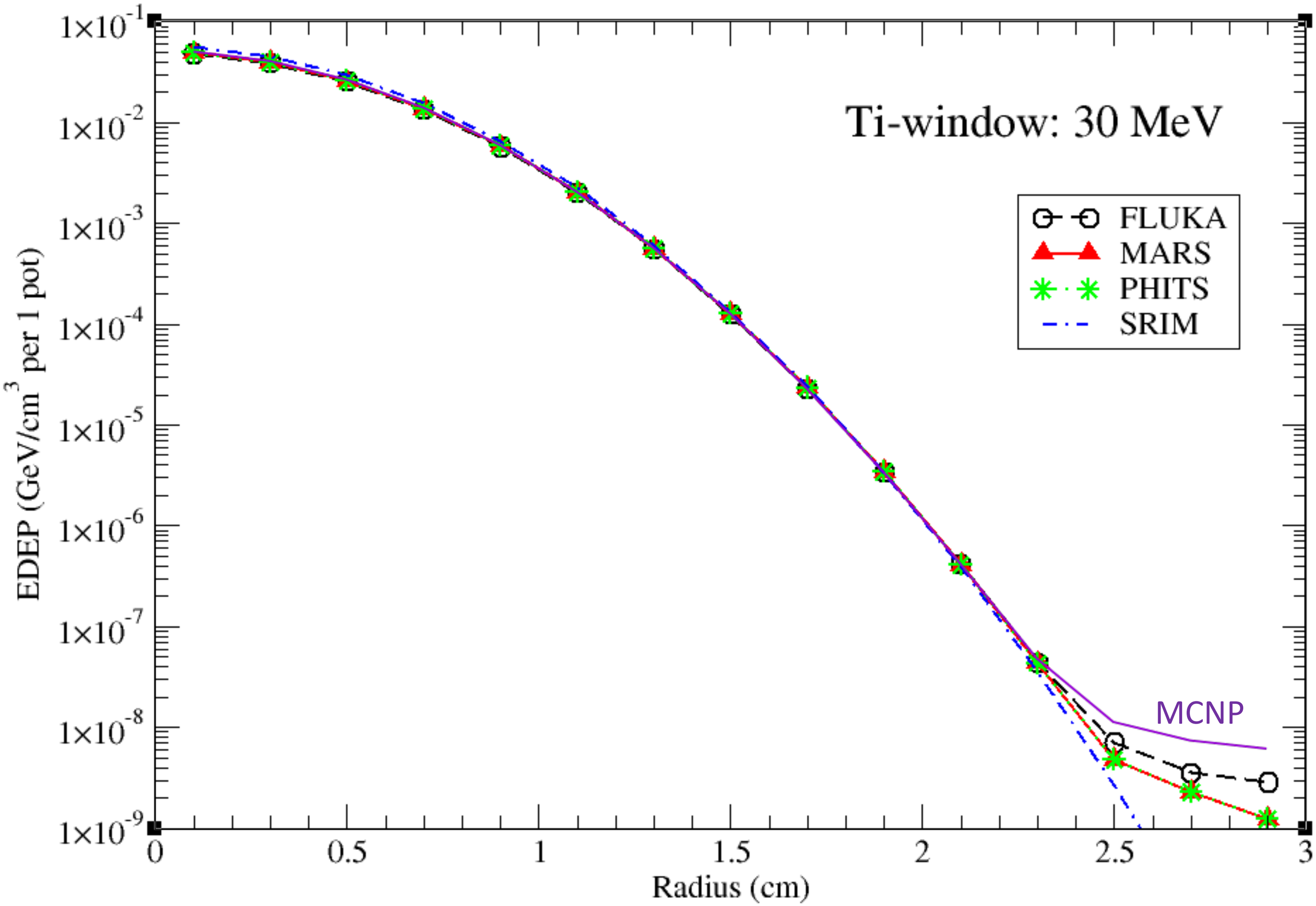
MCNP

1. MCNPX 2.7.0 and HTAPE3X (included with MCNPX 2.7.0)
2. MCNPX input included lca 8j 1 1 (use CEM03.02 model and use LAQGSM03.03 to handle all heavy-ion interactions as well as all light-ion interactions. LAQGSM also replaces FLUKA for high energy proton and neutron reactions.
3. Graphite target cross sections used 6012.24h
4. Titanium target cross sections used 22046.70c, 22047.70c, 22048.70c, 22049.70c, 22050.70c
5. Since the information passed to HTAPE3X comes only from interactions processed by the medium and high energy modules of MCNPX, low energy neutron and protons which utilize MCNPX library data do not contribute to edits by HTAPE3X of collision data
6. Energy deposition used option 16 in HTAPE3X, with the mean damage energy per zone used to calculate NRT dpa
7. Gas production used option 14 in HTAPE3X, with the total H and total He atoms stopped in each cell, including source particles
8. Alternative for Titanium to use DXS dpa and gas production cross sections up to 3GeV was not tested but should be to get more accurate gas production values

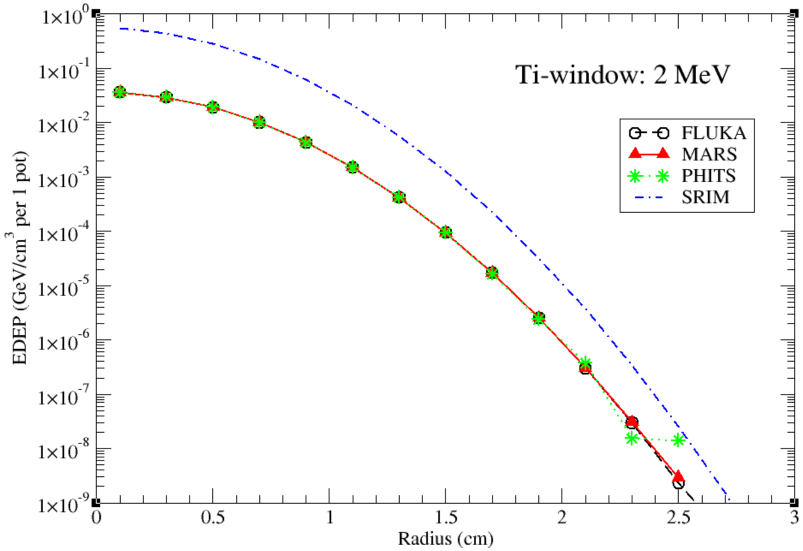
Setup 1: Beam Window

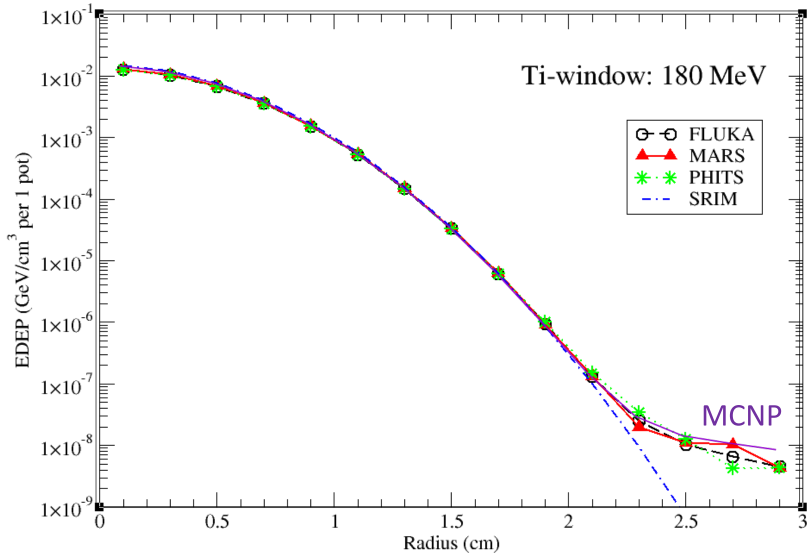
- **Material:** Ti-6Al-4V, density 4.43 g/cc: ~~weight % composition: Al 6, Fe 0.25, O 0.2, Ti 89.55, V 4.~~ It was suggested for this intercomparison to approximate it by a pure natural Ti with density 4.43 g/cc, with composite materials considered at a later time.
- **Geometry:** Disk 0.045-cm thick and 3 cm in radius, subdivided radially in 15 bins with Δr=0.2 cm
- **Proton beam:** Gaussian with $\sigma_x = \sigma_y = 0.43$ cm, 2.4e21 pot/yr
- **Proton kinetic energy (GeV):** 0.002, 0.03, 0.18, 0.8, 3, 30, 120, 400 and 7000
- **Energy threshold:** 0.001 eV for neutrons and 10 keV for everything else
- **Calculated quantities**: EDEP (GeV/cm^3 per 1 pot), DPA (1/yr), ${}_1H^1$ and ${}_2He^4$ (appm/DPA) (H-1 and He-4 stopped in the window), neutron fluence (cm^{-2} yr^{-1}) total and > 0.1 MeV. DPA and appm/DPA for the intercomparison are to be calculated with the standard NRT model; additional results with various efficiency functions are welcome.
- **Scoring:** in 15 radial bins and total in the window.

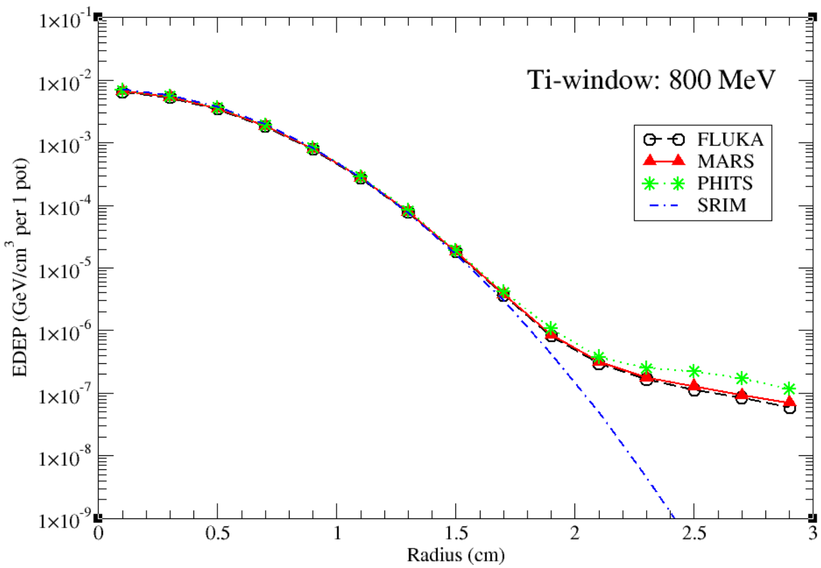
Ti-Window: EDEP @ 30 MeV

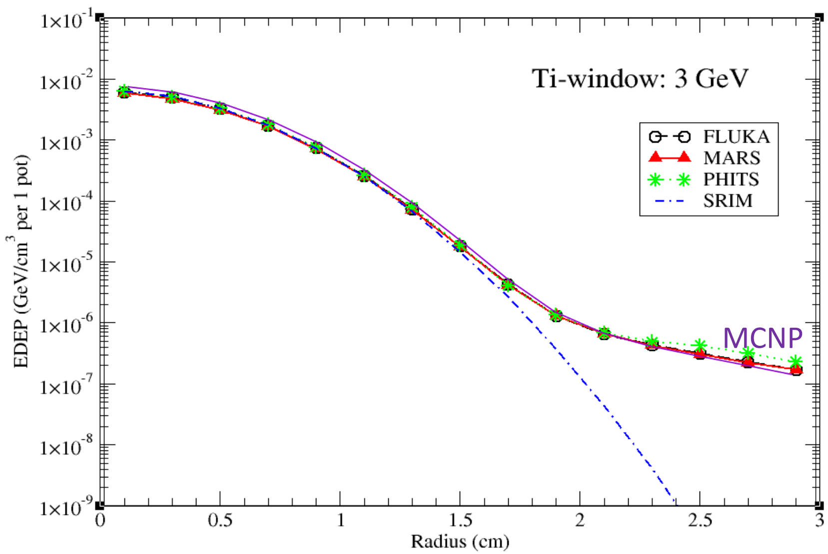


Ti-Window: EDEP @ 2, 180, 800 MeV and 3 GeV









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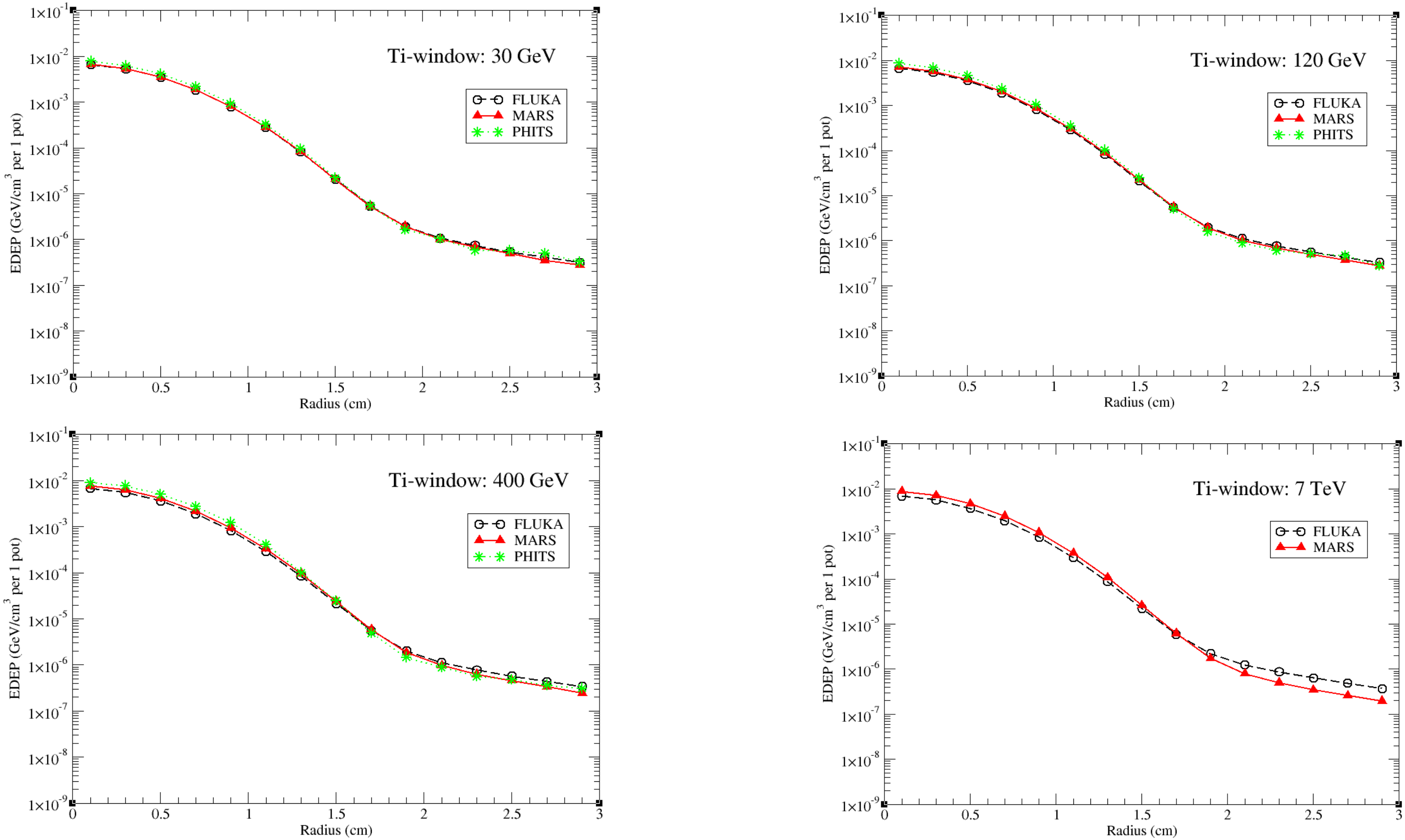
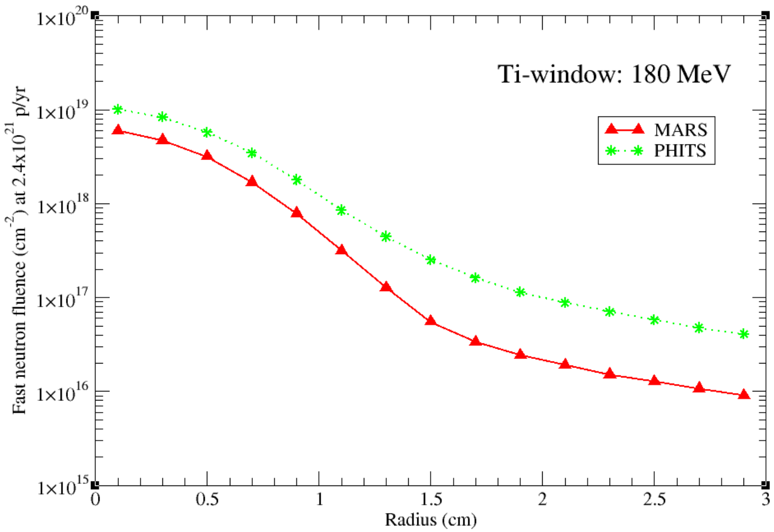
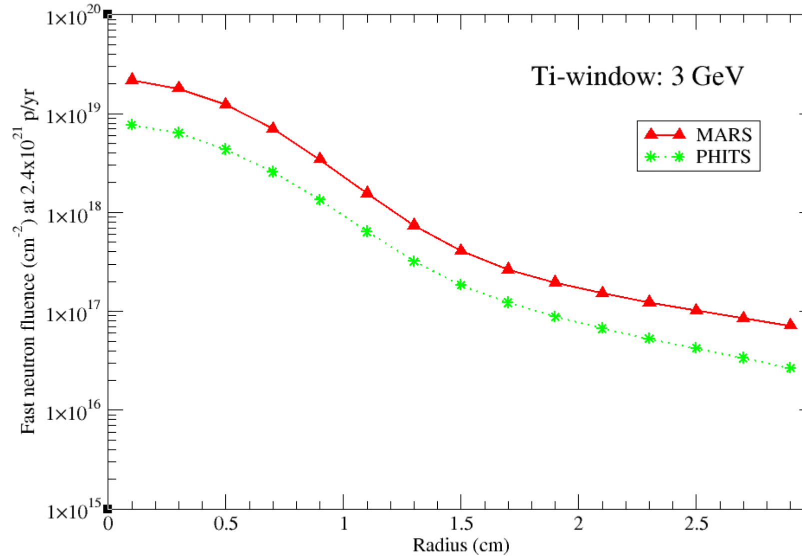
Ti-Window: EDEP @ 30, 120, 400 and 7000 GeV

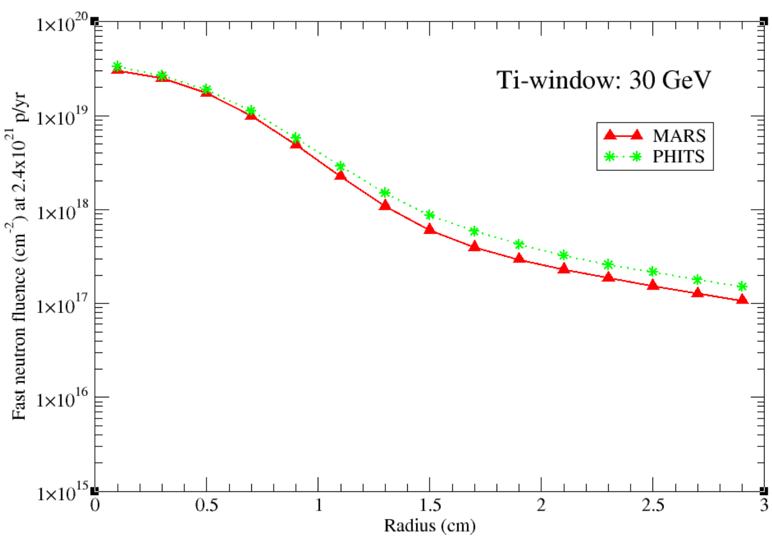


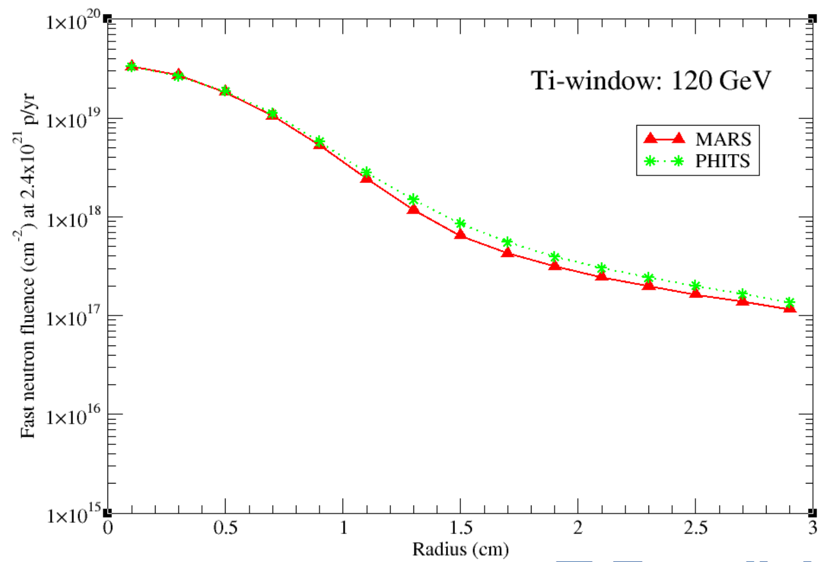
Ti-Window: Fast Neutrons @ 0.18, 3, 30 and 120 GeV



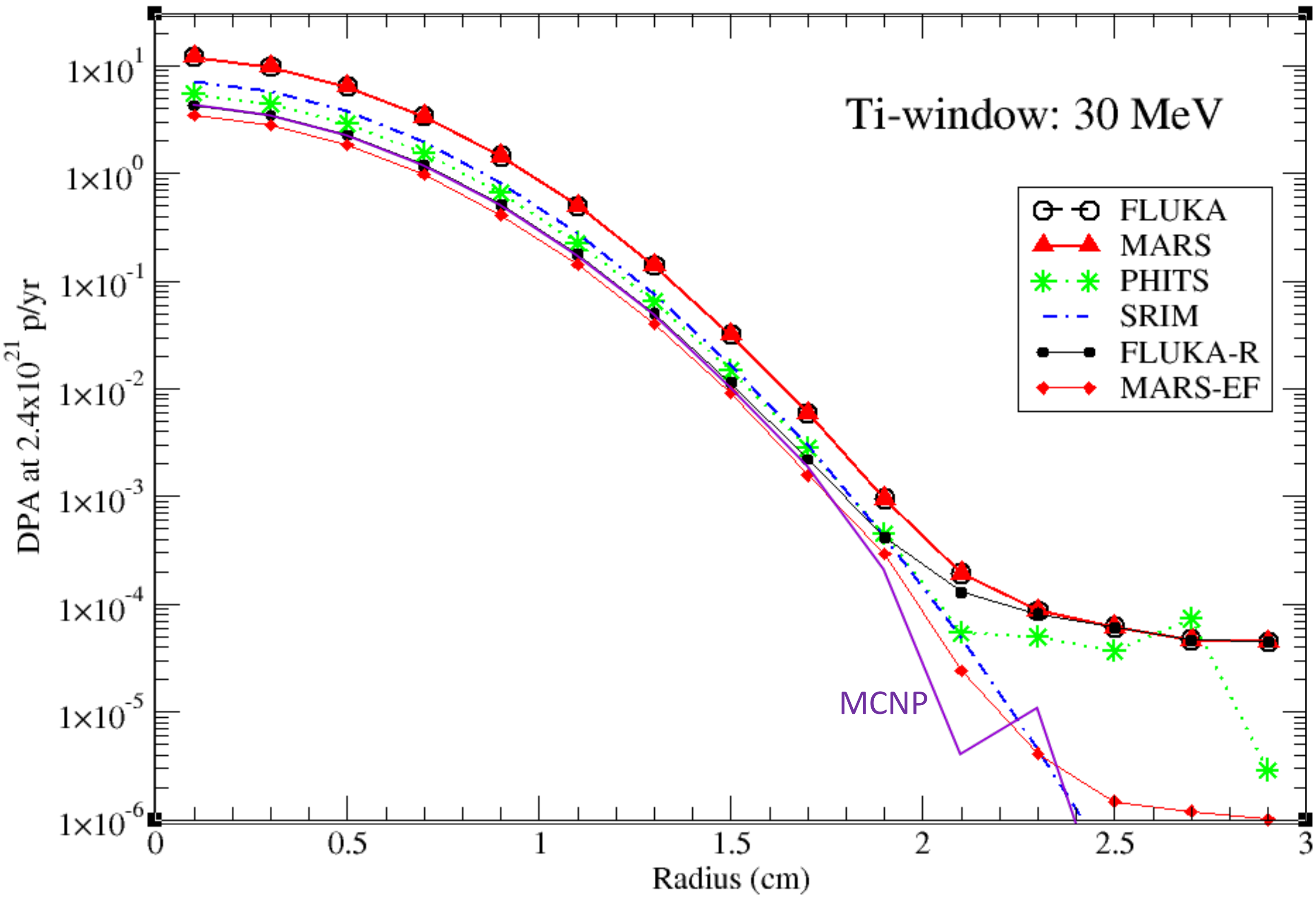


FLUKA values were not provided since there was no a request for that in the original specs.

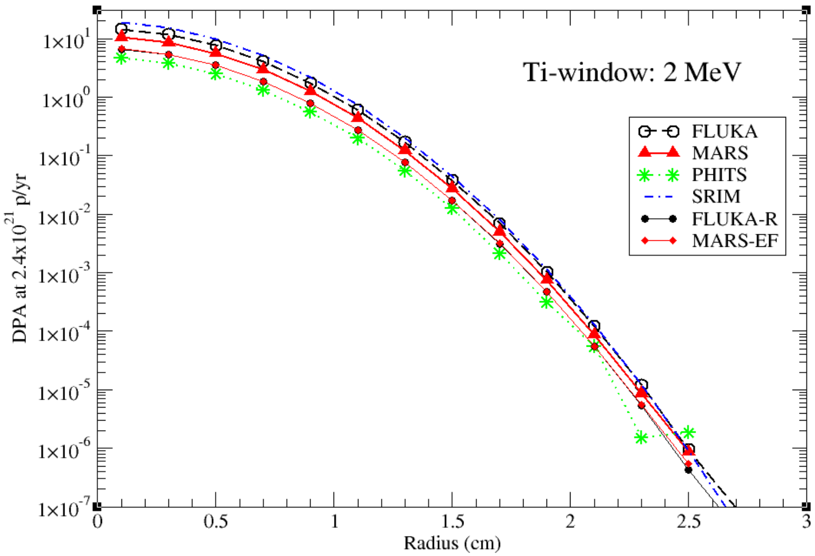


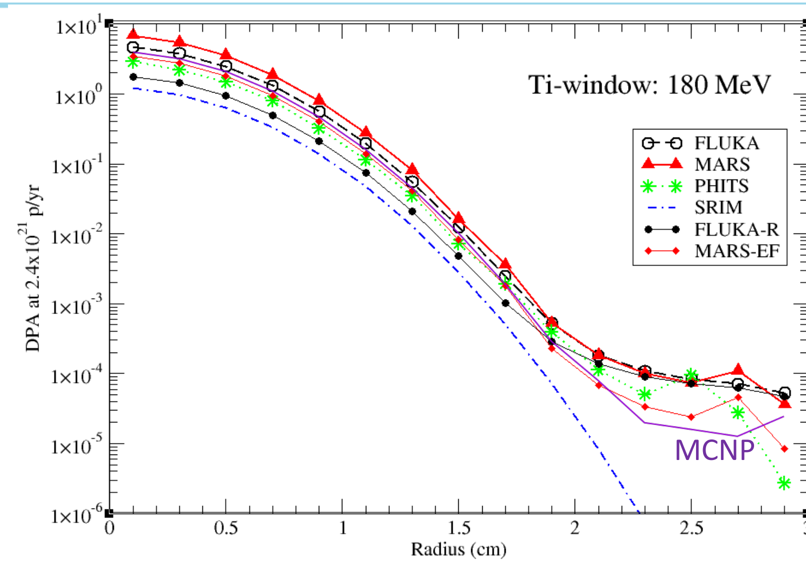


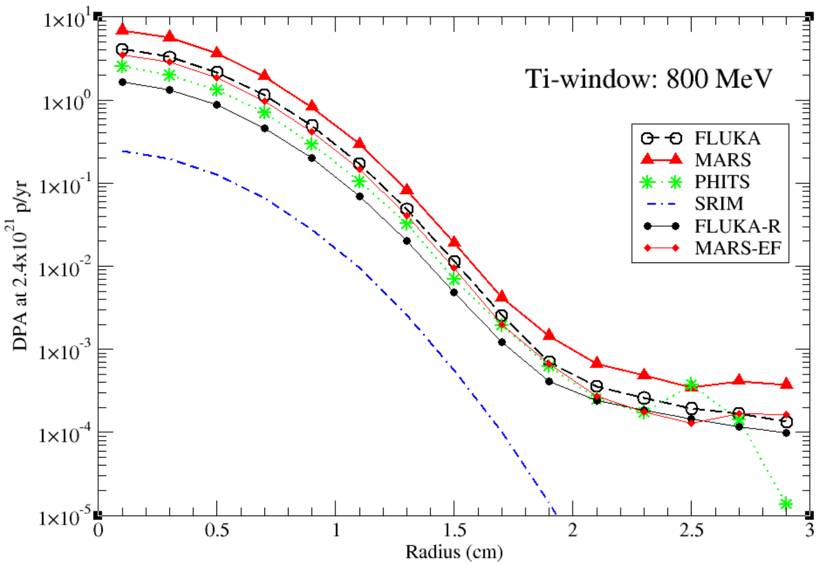
Ti-Window: DPA @ 30 MeV

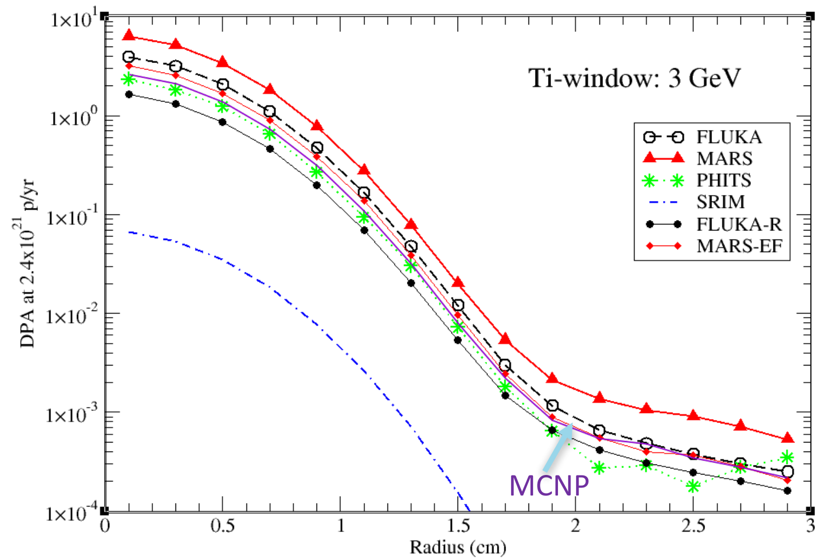


Ti-Window: DPA @ 2, 180, 800 MeV and 3 GeV









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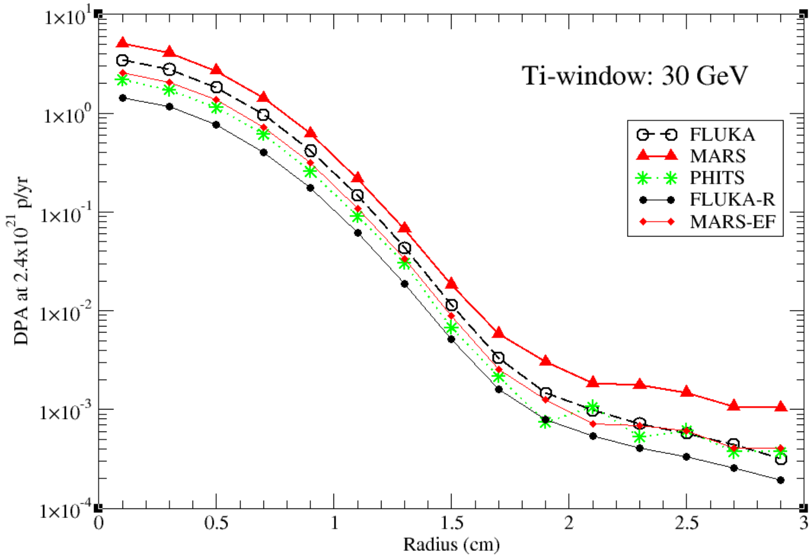
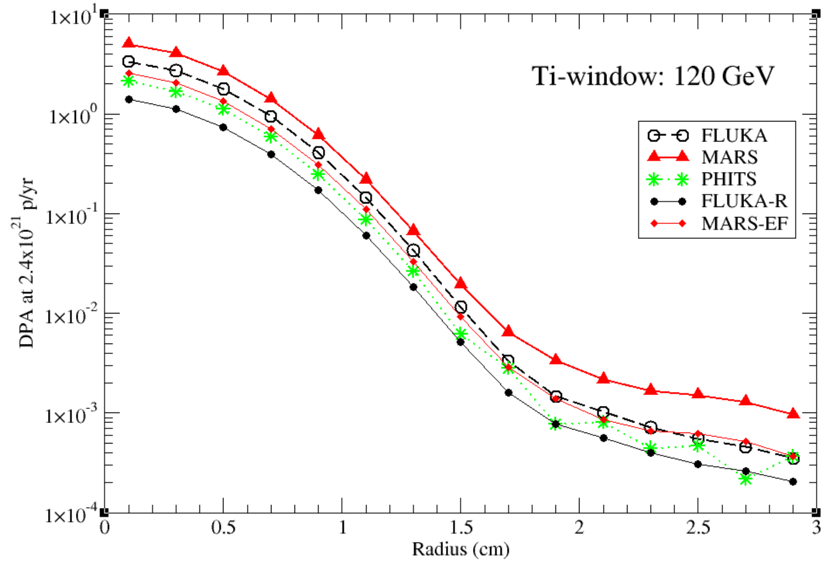
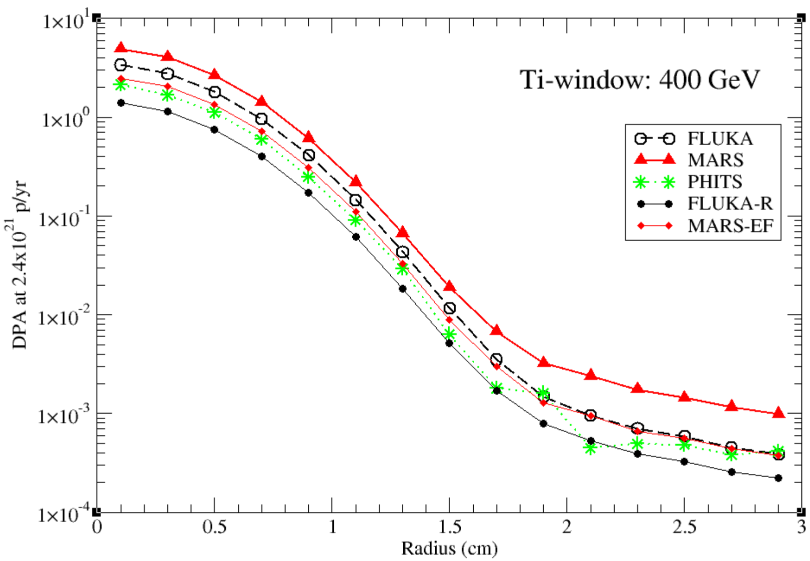
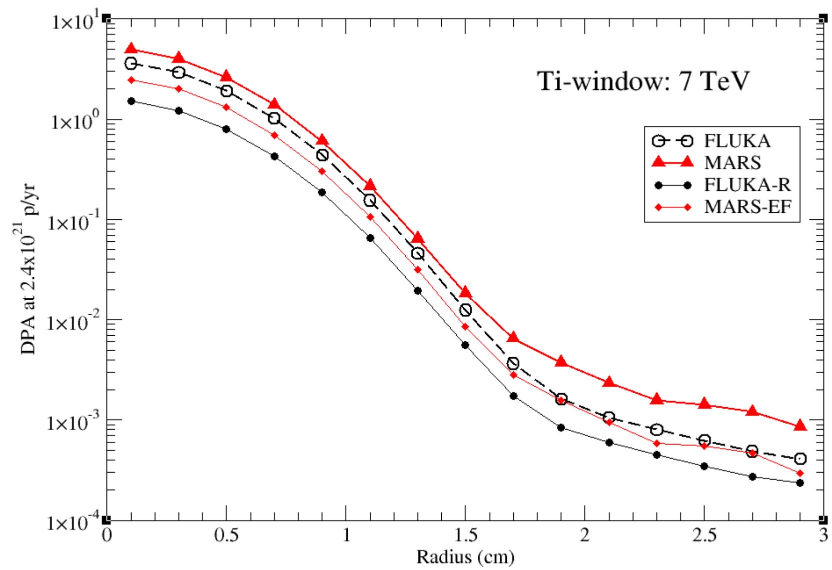
Ti-Window: DPA @ 30, 120, 400 and 7000 GeV





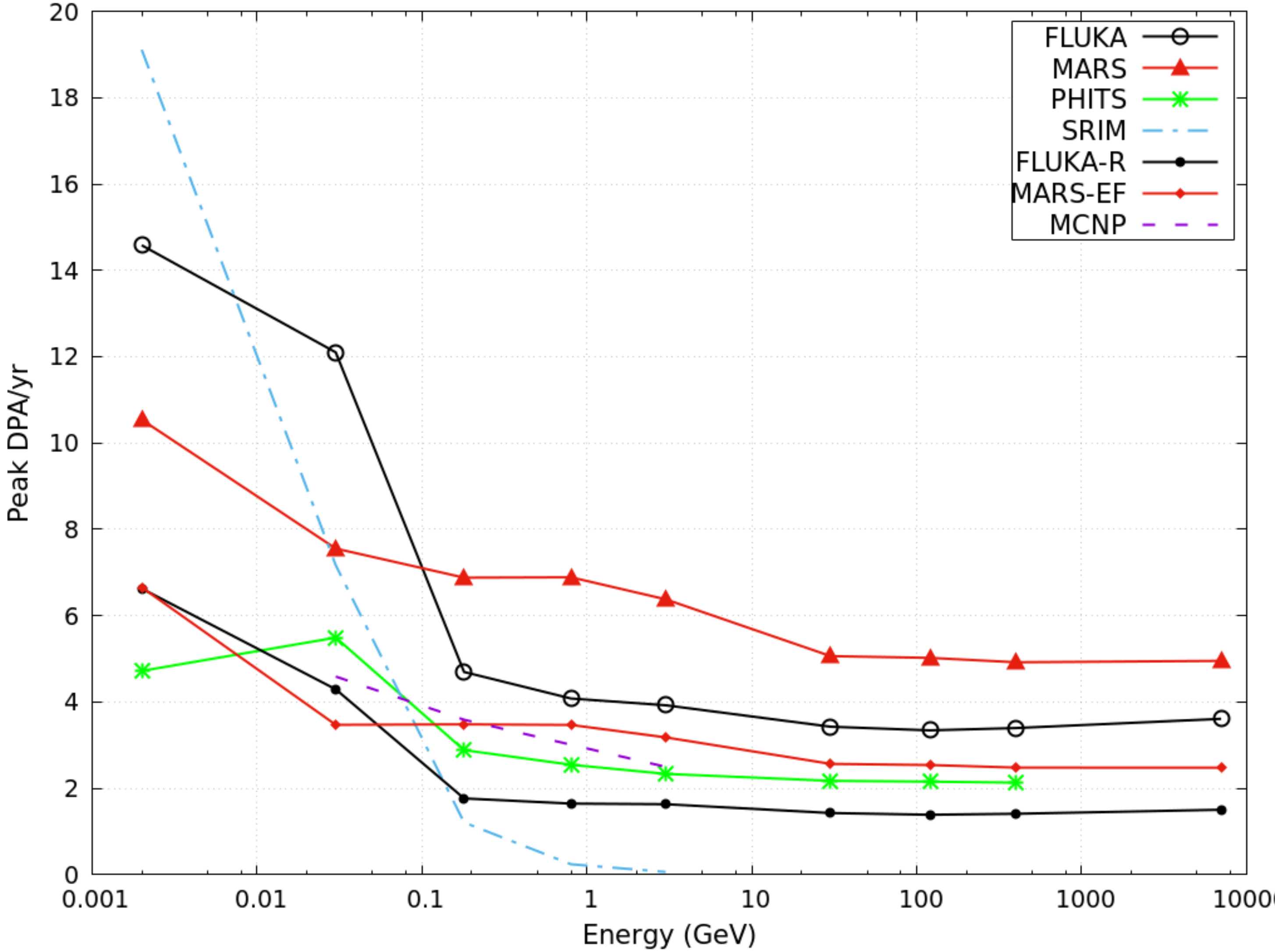




Ti Window: DPA/yr Peak

E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	SRIM	MCNP
2 MeV	14.58	6.628	10.54	6.658	4.723	19.11	-
30 MeV	12.10	4.295	7.555	3.473	5.493	7.168	4.59
180 MeV	4.697	1.768	6.881	3.484	2.886	1.211	3.59
800 MeV	4.082	1.649	6.890	3.470	2.548	0.243	-
3 GeV	3.925	1.634	6.379	3.182	2.336	0.066	2.50
30 GeV	3.429	1.430	5.064	2.568	2.175	-	-
120 GeV	3.345	1.390	5.023	2.542	2.156	-	-
400 GeV	3.398	1.412	4.922	2.482	2.134	-	-
7 TeV	3.612	1.506	4.954	2.479	-	-	-

Ti-Window: Peak DPA *vs* Proton Beam Energy



Ti Window (at axis): H appm/DPA

E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	MCNP
2 MeV	5.35×10^4	1.18×10^5	7.40×10^4	1.17×10^5	0	-
30 MeV	87.5	246.6	141.6	308.0	2.0	
180 MeV	140.1	372.1	117.8	232.6	3.05	
800 MeV	186.9	462.7	127.1	252.4	5.72	-
3 GeV	250.6	602.0	197.2	395.2	6.69	
30 GeV	279.0	669.0	294.4	580.5	9.33	-
120 GeV	274.2	659.9	318.2	628.9	9.54	-
400 GeV	270.4	650.5	341.0	676.4	9.90	-
7 TeV	273.6	656.1	355.9	711.1		-

The H appm/DPA ratio radial distributions in window are pretty flat, therefore only the values at r=0 are shown in the table

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Ti Window (at axis): He appm/DPA

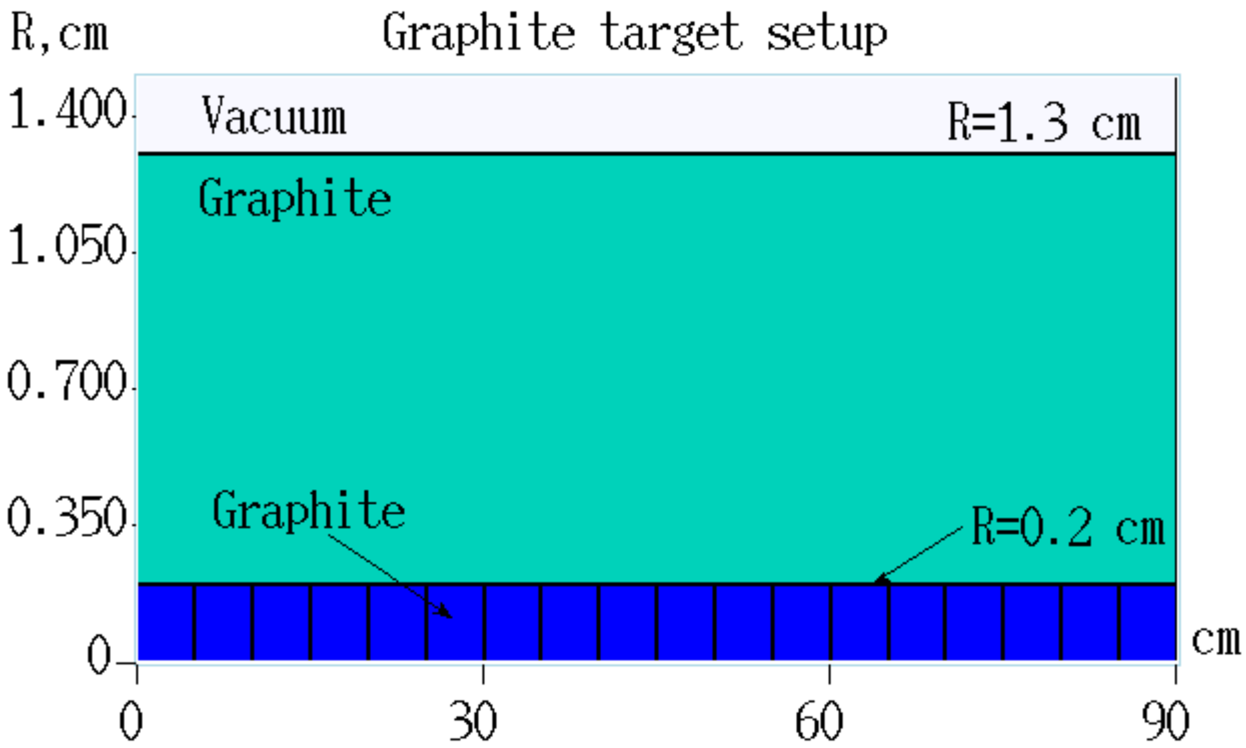
E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	MCNP
2 MeV	0	0	0	0	0	
30 MeV	13.2	37.2	19.6	42.6	0.25	
180 MeV	82.1	218.2	40.2	79.3	1.46	
800 MeV	196.8	487.2	55.0	109.1	3.89	
3 GeV	386.0	927.2	112.0	224.5	5.08	
30 GeV	488.7	1171.9	178.8	352.6	7.47	-
120 GeV	480.3	1156.0	198.5	392.2	6.73	-
400 GeV	477.4	1148.6	211.8	420.1	7.52	-
7 TeV	480.8	1152.8	215.2	429.9	-	-

The He appm/DPA ratio radial distributions in window are pretty flat, therefore only the values at r=0 are shown in the table

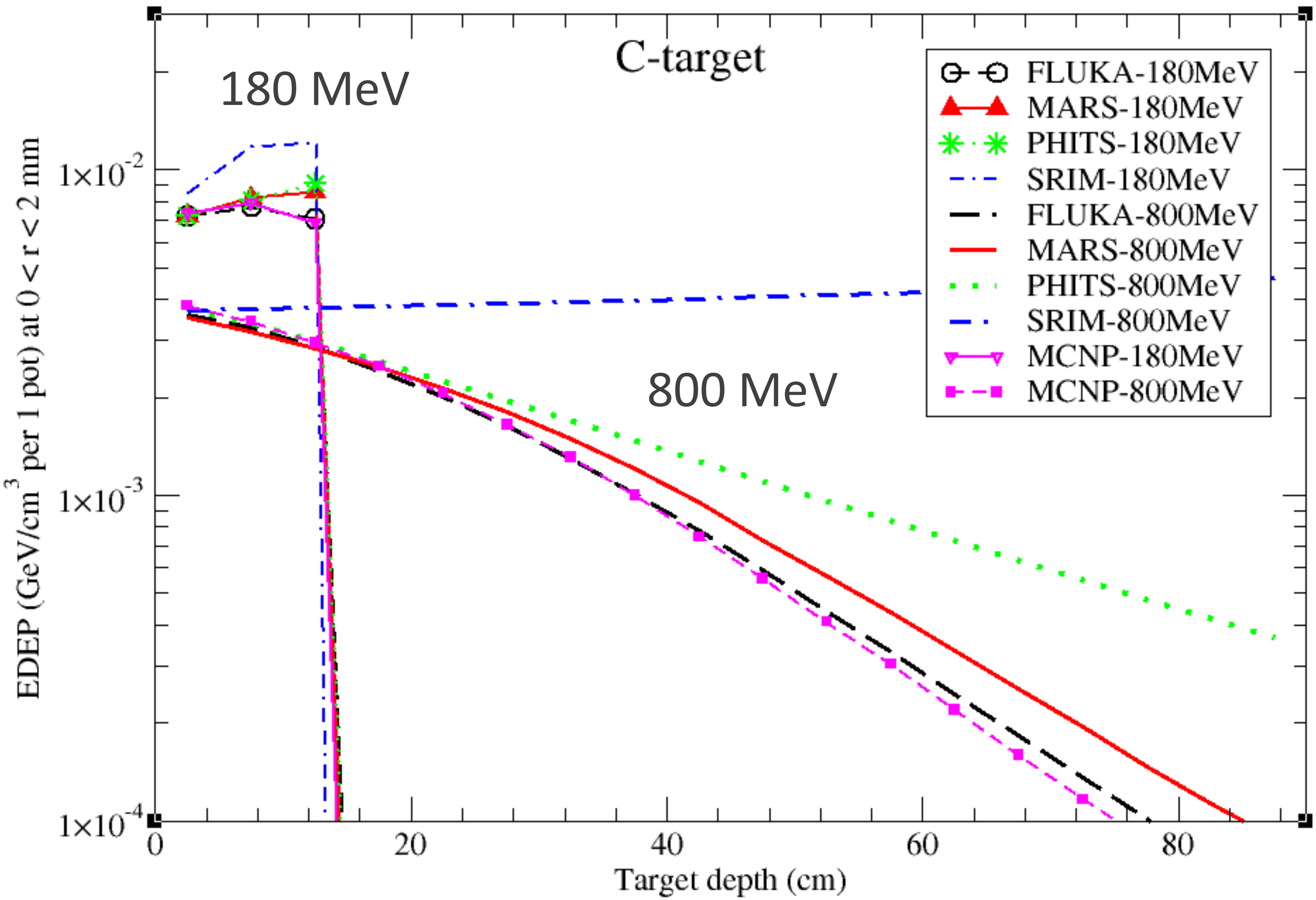
Setup 2: Graphite Target

- **Material:** IG-430U, density 1.84 g/cc, composition: pure natural C (impurities are all < 0.01 ppm wt)
- **Geometry:** cylinder 90-cm long and 1.3 cm in radius; for this intercomparison subdivided radially in two regions: 0-0.2 cm and 0.2-1.3 cm, with central region subdivided longitudinally in 18 bins with Δz=5 cm
- **Proton beam:** Gaussian with $\sigma_x = \sigma_y = 0.43$ cm, 2.4e21 pot/yr
- **Proton kinetic energy (GeV):** 0.18, 0.8, 3, 30, 120, 400 and 7000
- **Energy threshold:** 0.001 eV for neutrons and 10 keV for everything else
- **Calculated quantities:** EDEP (GeV/cm^3 per 1 pot), DPA (1/yr), ${}_1H^1$ and ${}_2He^4$ (appm/DPA) (H-1 and He-4 stopped/captured in the target), neutron fluence ($cm^{-2}\ yr^{-1}$) total and > 0.1 MeV. See above comments on H-1, He-4 and DPA models.
- **Scoring in the central radial region (r < 0.2cm, i.e. peak axial distribution):** in 18 z-bins, and total in the target. It means for both setups that at this meeting we will inter-compare just 1-D distributions as calculated with five codes. 2D distributions can be considered at a later stage.

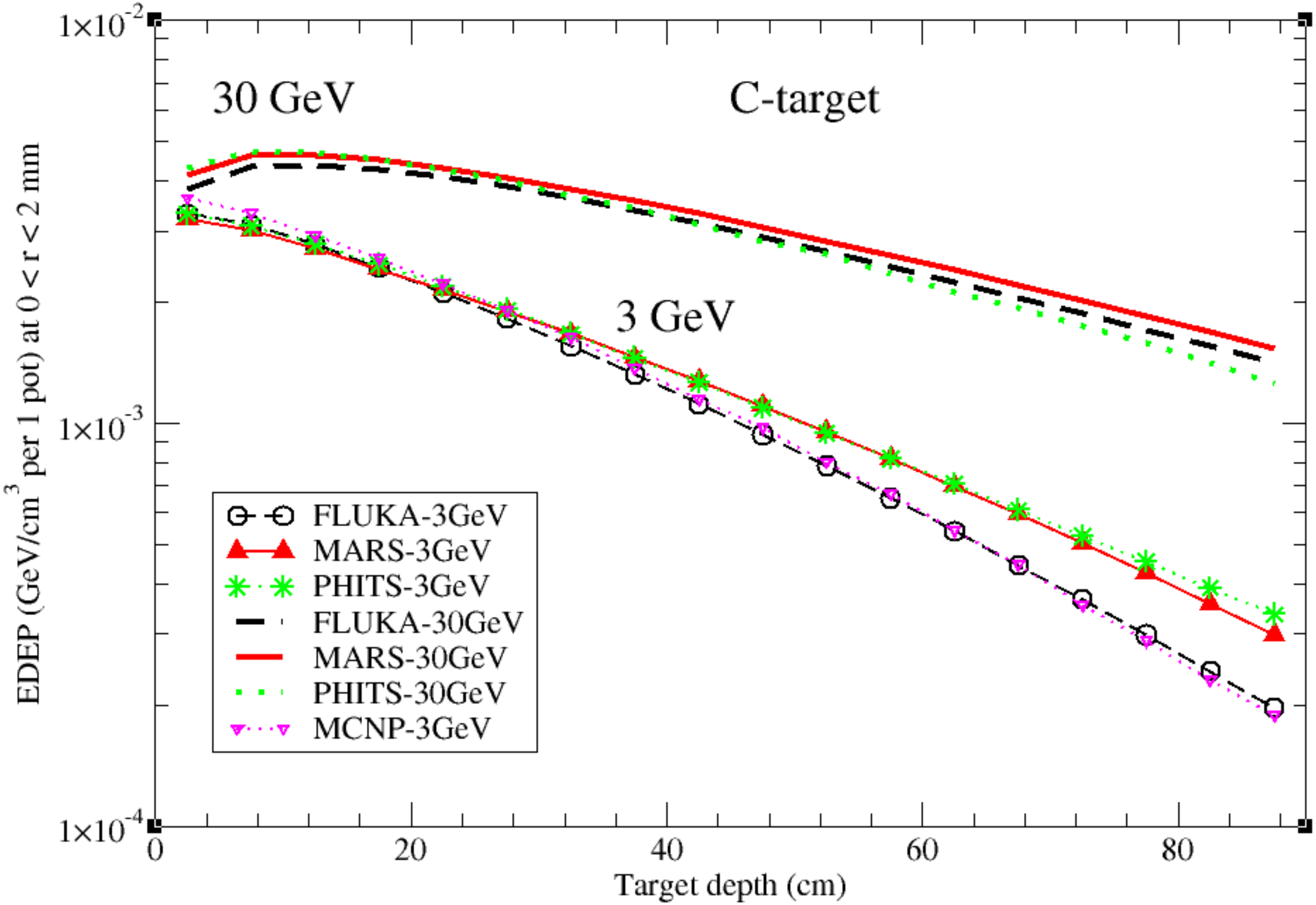
C-Target


R,cm
Graphite target setup
1.400
1.050
0.700
0.350
0
Vacuum
R=1.3 cm
Graphite
Graphite
R=0.2 cm
cm
0
30
60
90

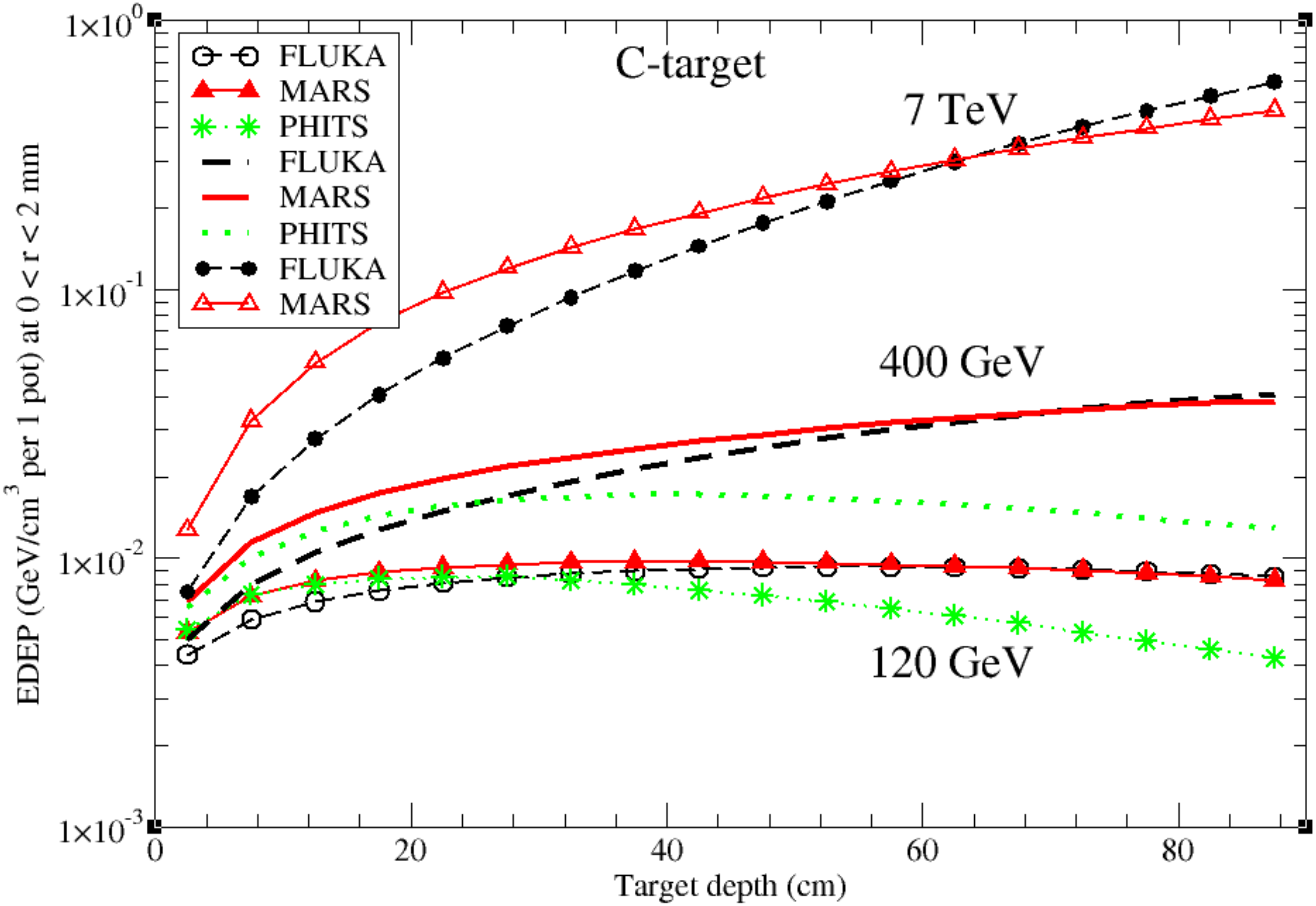
C-Target: EDEP @ 180 and 800 MeV



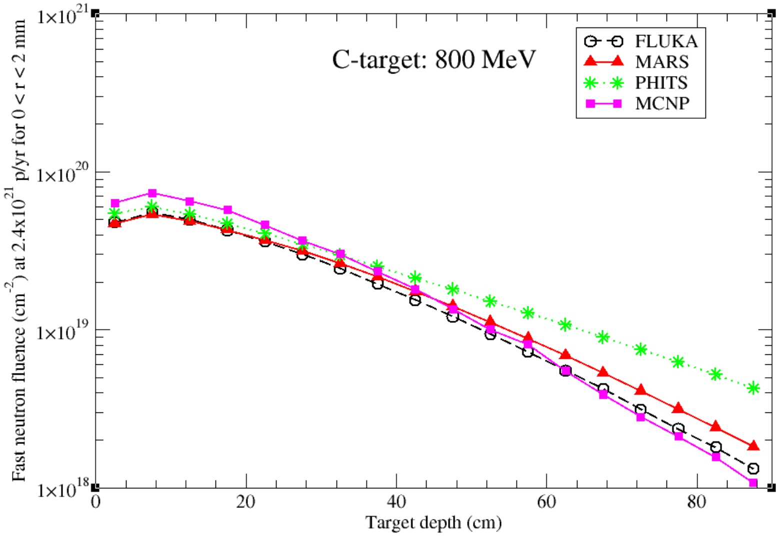
C-Target: EDEP @ 3 and 30GeV

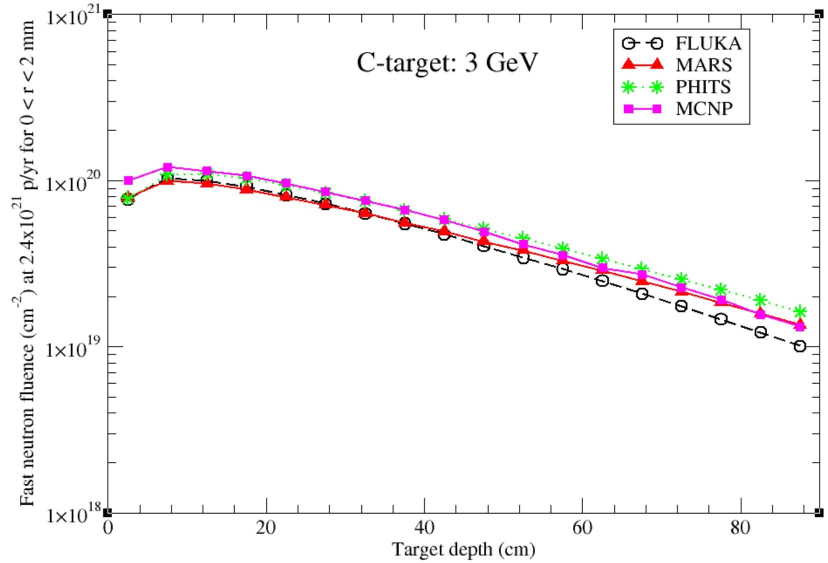


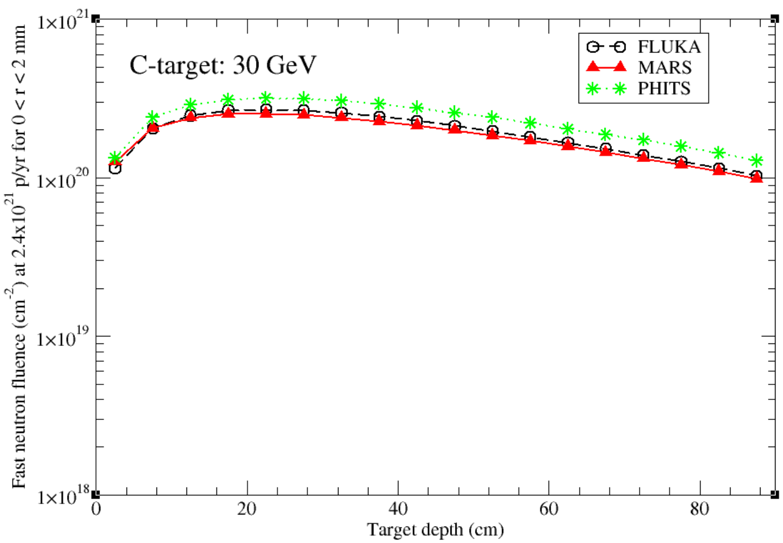
C-Target: EDEP @ 120, 400 and 7000 GeV

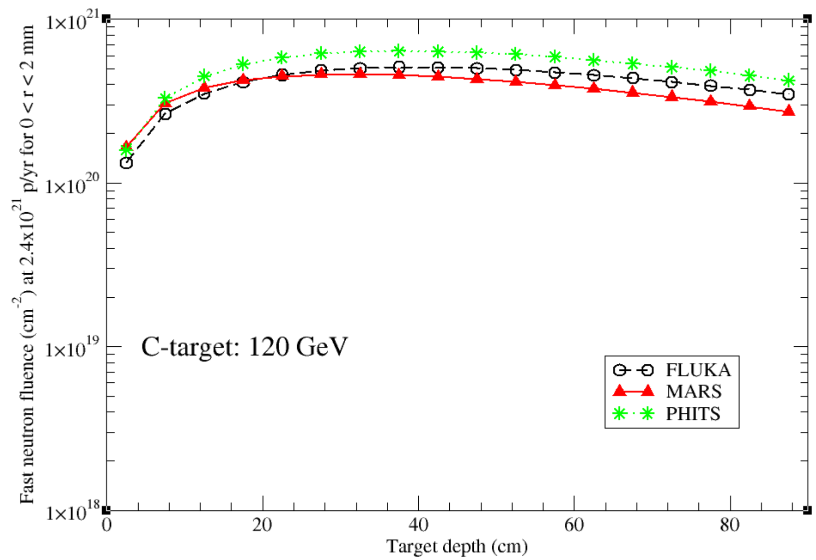


C-Target: Fast Neutrons @ 0.8, 3, 30 and 120 GeV

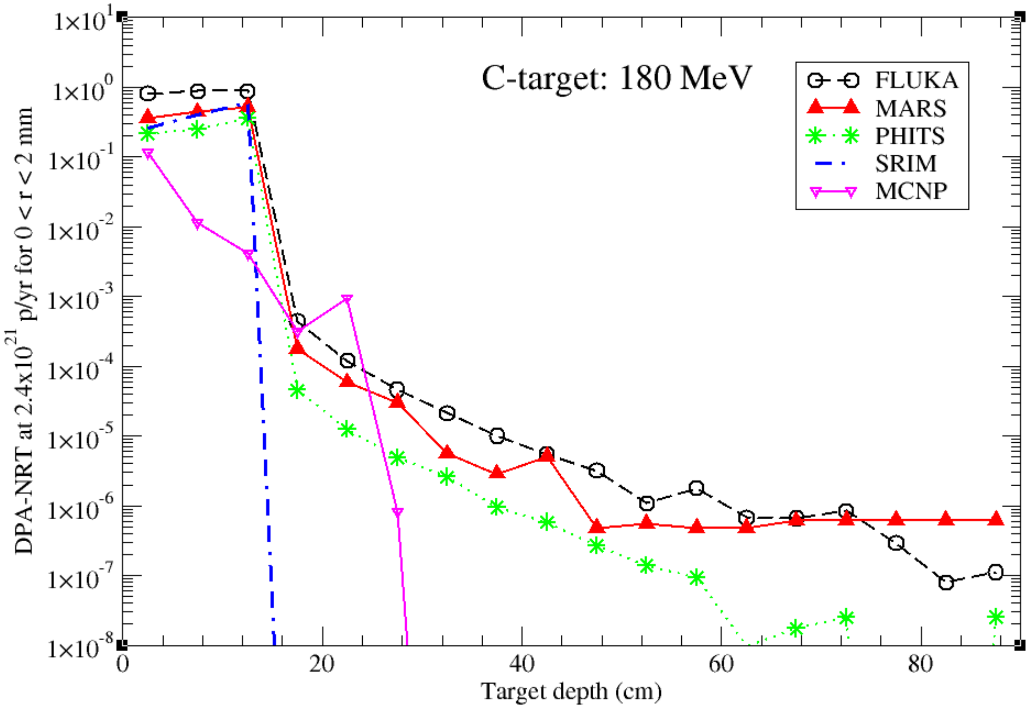


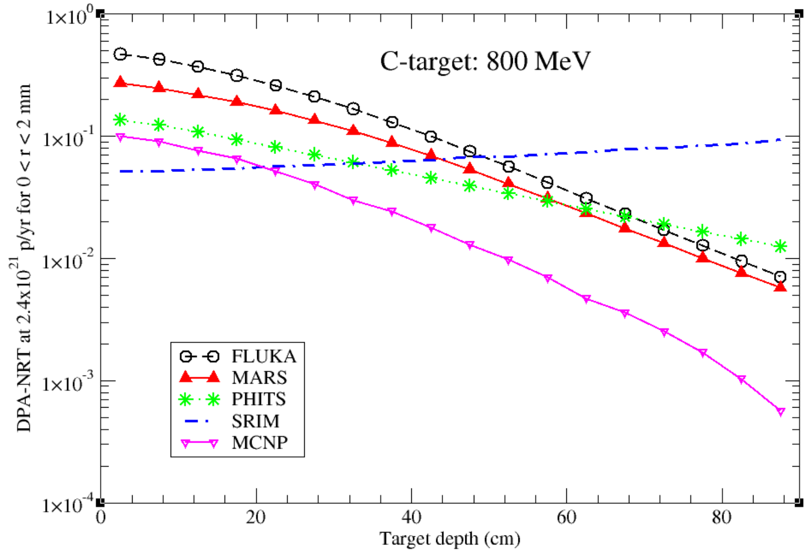


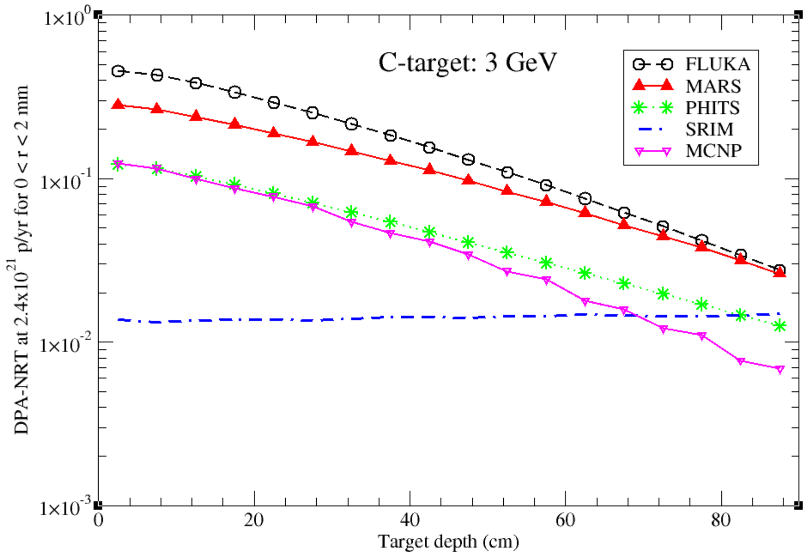




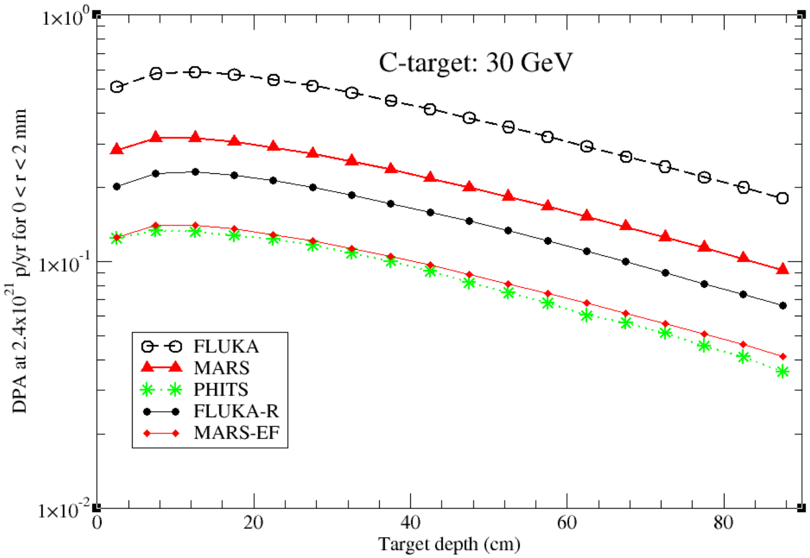
C-Target: DPA @ 180, 800 MeV and 3 GeV

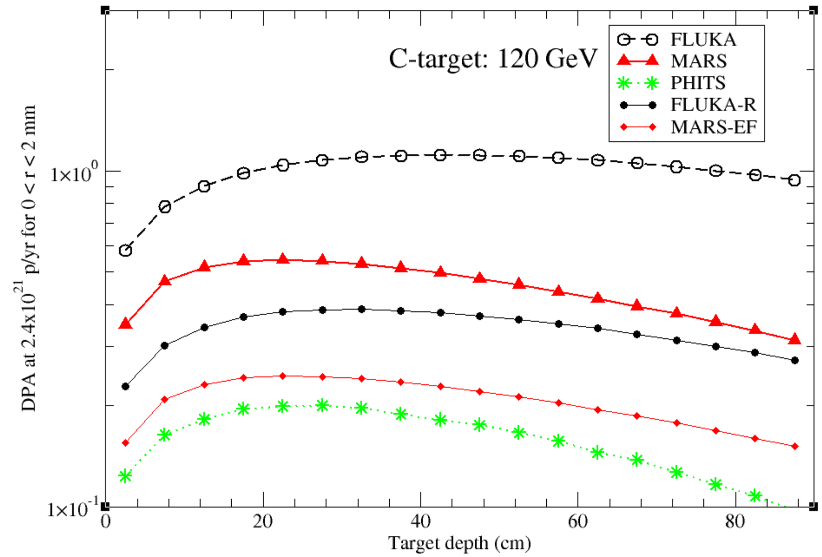


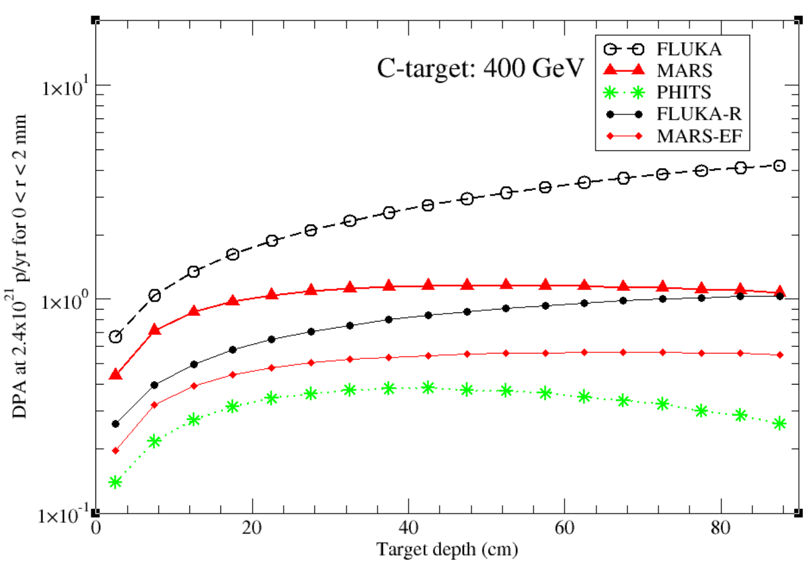


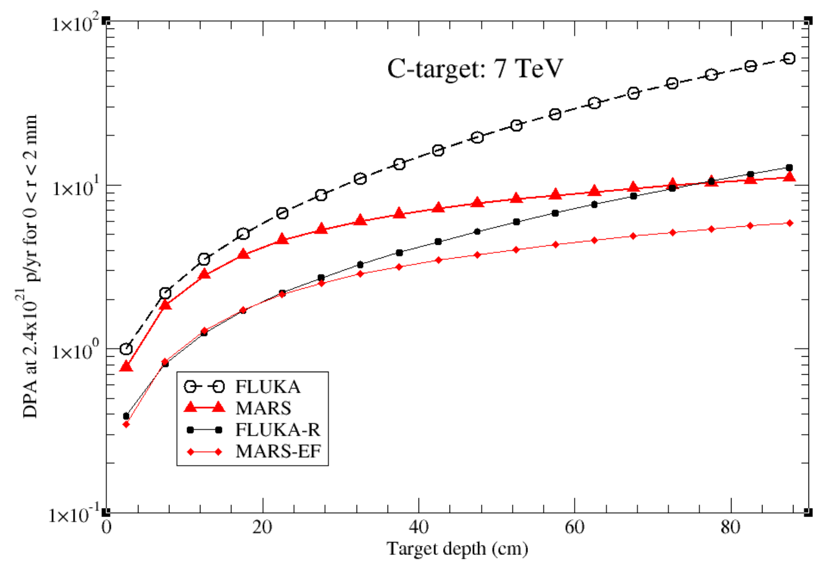


C-Target: DPA @ 30, 120, 400 and 7000 GeV





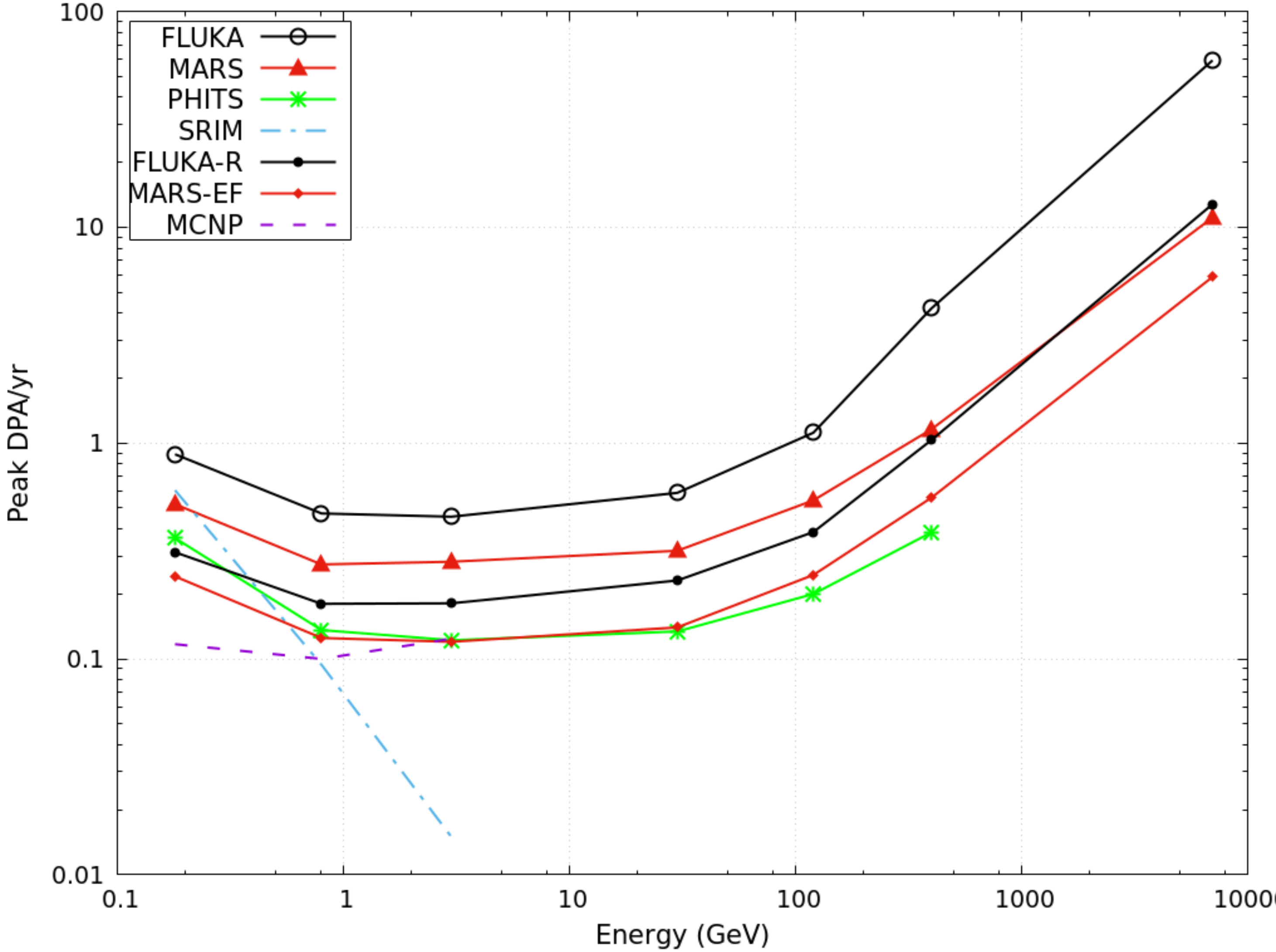




C-Target: DPA/yr at Longitudinal Peak and r<2mm

E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	SRIM	MCNP
180 MeV	0.887	0.312	0.521	0.241	0.363	0.605	0.117
800 MeV	0.472	0.180	0.274	0.125	0.136	0.094	0.100
3 GeV	0.456	0.181	0.282	0.120	0.122	0.015	0.124
30 GeV	0.588	0.231	0.317	0.140	0.134	-	-
120 GeV	1.117	0.387	0.543	0.245	0.200	-	-
400 GeV	4.214	1.034	1.160	0.559	0.386	-	-
7 TeV	59.33	12.79	11.09	5.890	-	-	-

C-Target: Peak DPA *vs* Proton Beam Energy



C-Target: H appm/DPA at r < 2 mm

E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	MCNP
180 MeV	476.	755.	835.	1711.	0.735	538.
800 MeV	528.	1398.	1087.	2330.	0.773	171.
3 GeV	632.	1568.	1180.	2816.	1.151	185.
30 GeV	512.	1376.	1569.	3481.	2.132	-
120 GeV	497.	1313.	1585.	3569.	2.724	-
400 GeV	489.	1288.	1564.	3521.	4.754	-
7 TeV	502.	1289.	1508.	3345.	-	-

The H appm/DPA ratio longitudinal distributions at r < 2mm in the target are pretty flat, therefore just maxima of the ratio are shown in the table

C-Target: He appm/DPA at r < 2 mm

E_p	FLUKA	FLUKA-R	MARS	MARS-EF	PHITS	MCNP
180 MeV	1245.	1973.	788.	1614.	7.93	1290.
800 MeV	902.	1321.	1094.	2390.	11.90	466.
3 GeV	986.	2444.	1063.	2500.	13.82	203.
30 GeV	855.	2243.	1100.	2490.	25.59	-
120 GeV	881.	2279.	1074.	2390.	35.65	-
400 GeV	860.	2265.	1074.	2355.	28.23	-
7 TeV	899.	2309.	1116.	2507.	-	-

The He appm/DPA ratio longitudinal distributions at r < 2mm in the target are pretty flat, therefore just maxima of the ratio are shown in the table

Summary (1)

- FLUKA, MARS, PHITS, SRIM and MCNP code inter-comparison exercise has been successfully undertaken for this meeting for proton beam energies from 2 MeV to 7 TeV.
- As results show, SRIM performs well at E<180 MeV, with serious issues at higher energies, large radii and thicknesses. One needs to understand these results and SRIM applicability before the final analysis. MCNP results were available at the very last moment and only up to 3 GeV.
- **Beam window**:
  - **EDEP**: all the codes are in a very good agreement over 6 orders of magnitude
  - **Fast neutron fluence**: FLUKA values were not provided since there was no a request for that in the original specs. MARS and PHITS agree at all energies.
  - **DPA:** FLUKA and MARS agree within 20% in the majority of the parameter space, with somewhat larger discrepancy at its peripheries; that is including the basic and modified DPA models. PHITS is typically lower than F&M by a factor of 1.5 to 2. MCNP (at < 3 GeV) is rather close to PHITS.
  - **Happm/DPA**: FLUKA and MARS agree within 50%; PHITS is 30-times lower
  - **Heappm/DPA**: FLUKA and MARS agree within a factor of 2.5; PHITS is typically lower than F&M by a factor of 50.

Summary (2)

- **Graphite target**
  - **EDEP:** FLUKA, MARS, MCNP (at E<3 GeV) and PHITS agree within 30%
  - **Fast neutron fluence**: FLUKA, MARS and MCNP (at E<3 GeV) are in a very good agreement; PHITS at large thicknesses is up to 30% higher.
  - **DPA:** FLUKA and MARS agree within 20% in the majority of the parameter space, with somewhat larger discrepancy at its peripheries; that is included the basic and modified DPA models. PHITS is typically lower than F&M by a factor of 1.5 to 2. MCNP (at < 3 GeV) is rather close to PHITS.
  - **Happm/DPA**: FLUKA and MARS agree within 50%; PHITS is typically lower than F&M by a factor of 30.
  - **Heappm/DPA**: FLUKA and MARS agree within a factor of 2.5; PHITS is typically lower than F&M by a factor of 50.

To Do List

Code-Specific

- SRIM: understand the applicability parameter space
- PHITS and MCNP: understand the reason for huge underestimation of gas production compared to the other codes

All Codes

- Understand noticeable variation in $_2He^4$ production
- Understand noticeable DPA underestimation by PHITS and MCNP in thick target and increasing with depth difference in DPA by FLUKA and MARS at high energies focusing on electromagnetic shower lateral modeling and leakage from the central 2-mm bin due to nuclear elastic scattering and Coulomb scattering
- Consider implementation to PHITS (just implemented!) and MCNP of defect production efficiency $\xi(T)=N_D/N_{NRT}$ to account for recombination of cascading atoms, aiming at routine use of appropriate damage efficiencies to mitigate the stringent DPA-NRT limits in high-power beam applications
- Add ion beam irradiation in future inter-comparisons