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Case Study of Decay Heat Calculations for the Spallation Neutron Source Second Target Station

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Outline

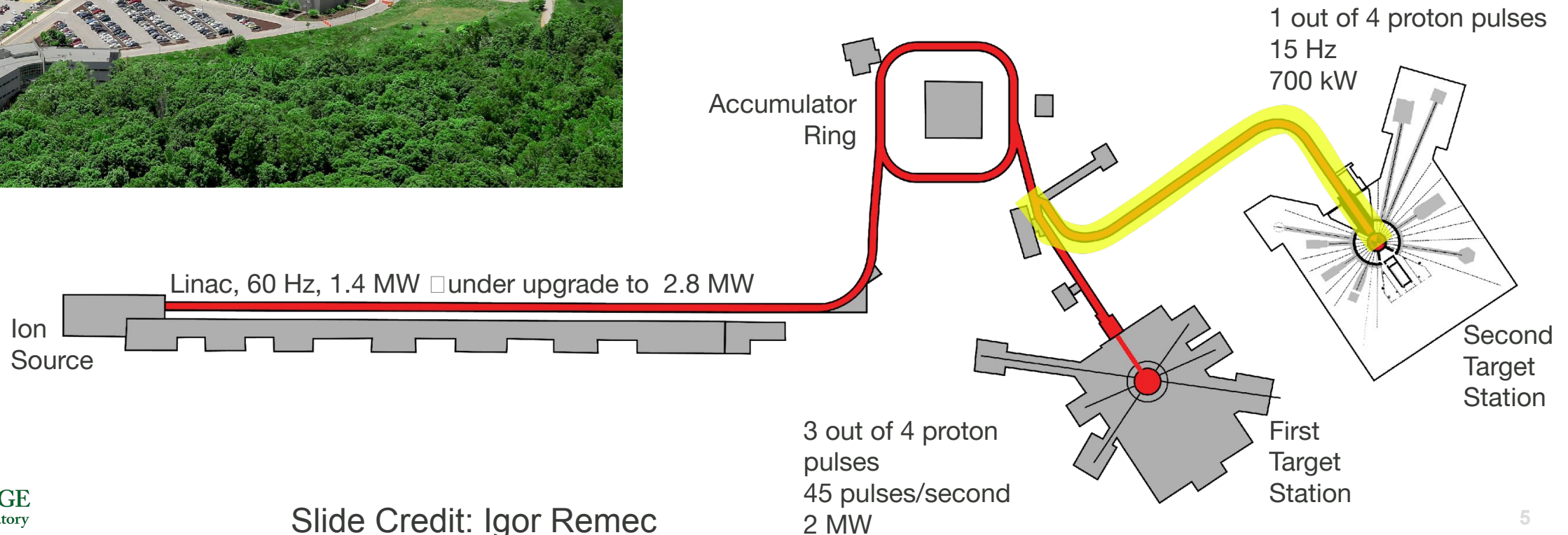
- **Second Target Station (STS) Overview**
 - Operational Overview
 - Performance metrics Overview
 - Target Overview
- **Decay Heat Case Study Overview**
 - Case Study Goals
 - Target and Operating Overview
 - Overview of Codes
- **Methodology**
 - MCNP and FLUKA Workflows
 - CINDER Comparison
- **Results**
- **Conclusions**

Second Target Station Overview

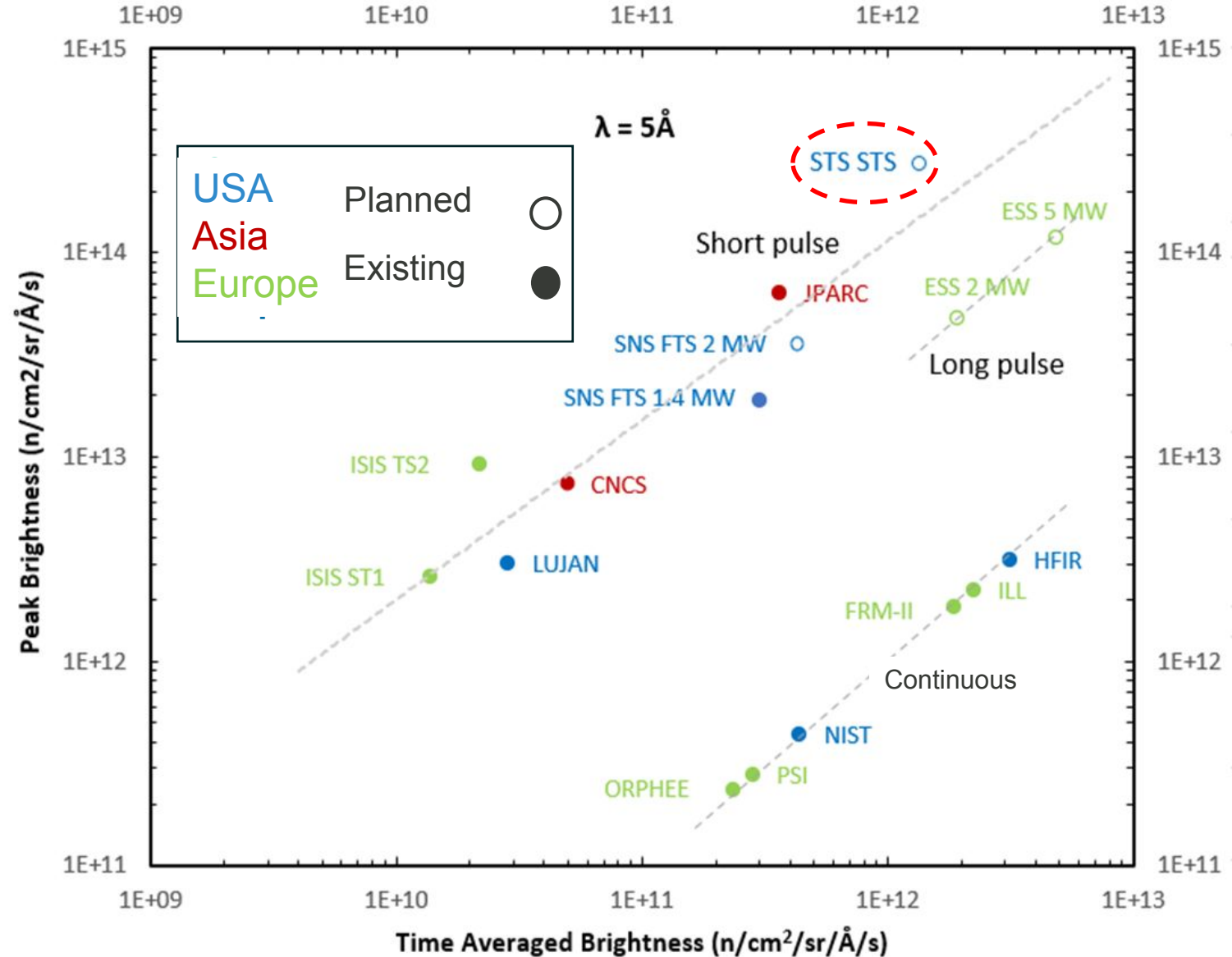
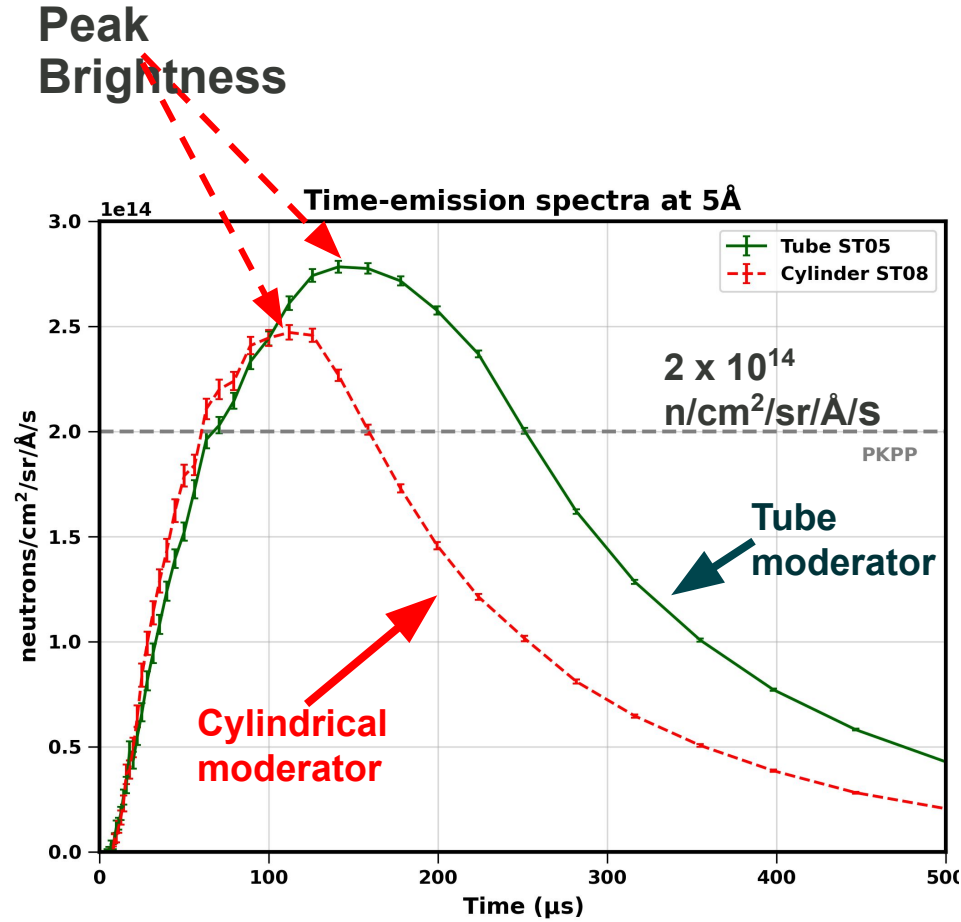
ORNL SNS and the Second Target Station (STS)



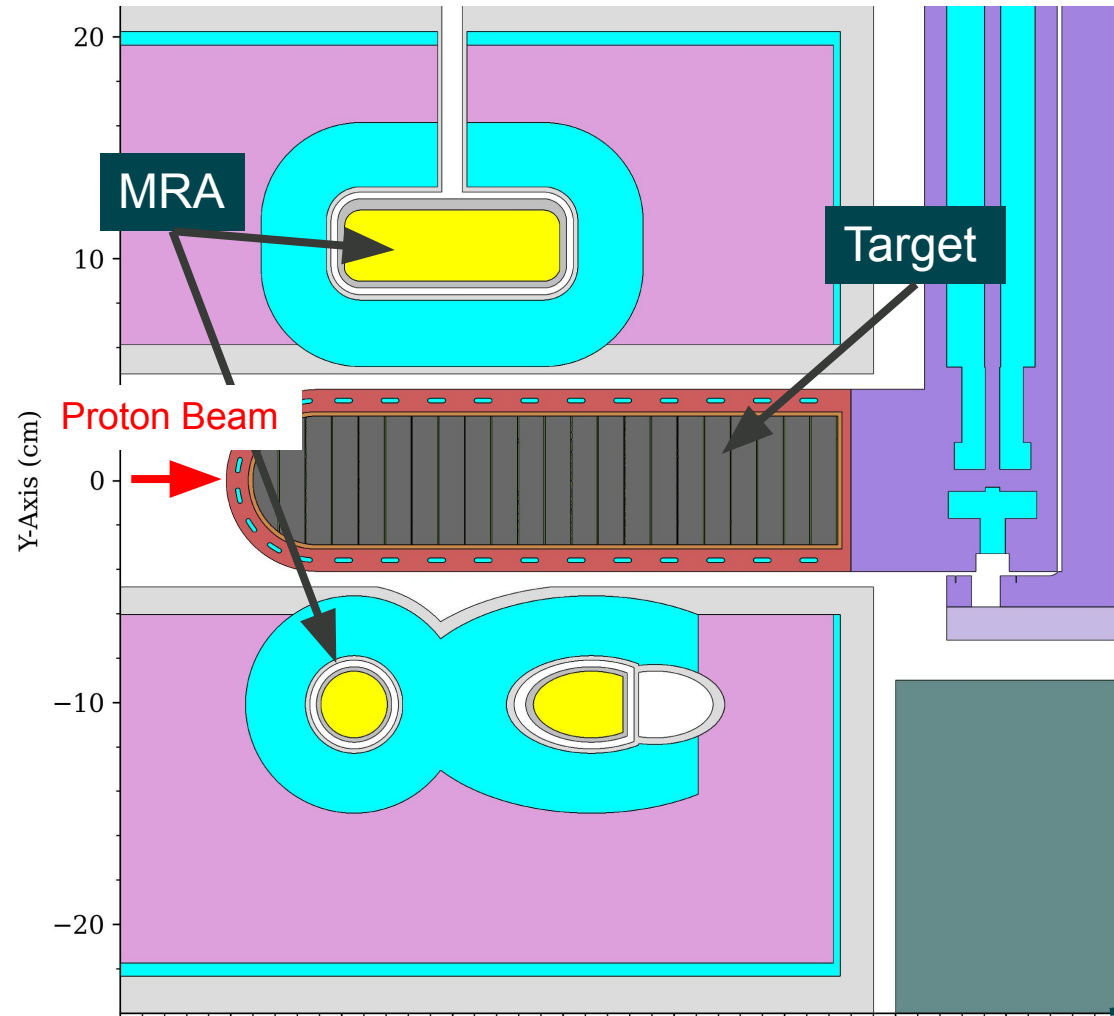
- High-brightness cold neutron source (smaller samples & shorter time)
- Supports up to 21 neutron instruments
- Sustains US/ORNL leadership in neutron sciences



The STS project objective is to become the highest peak-brightness source of cold neutrons

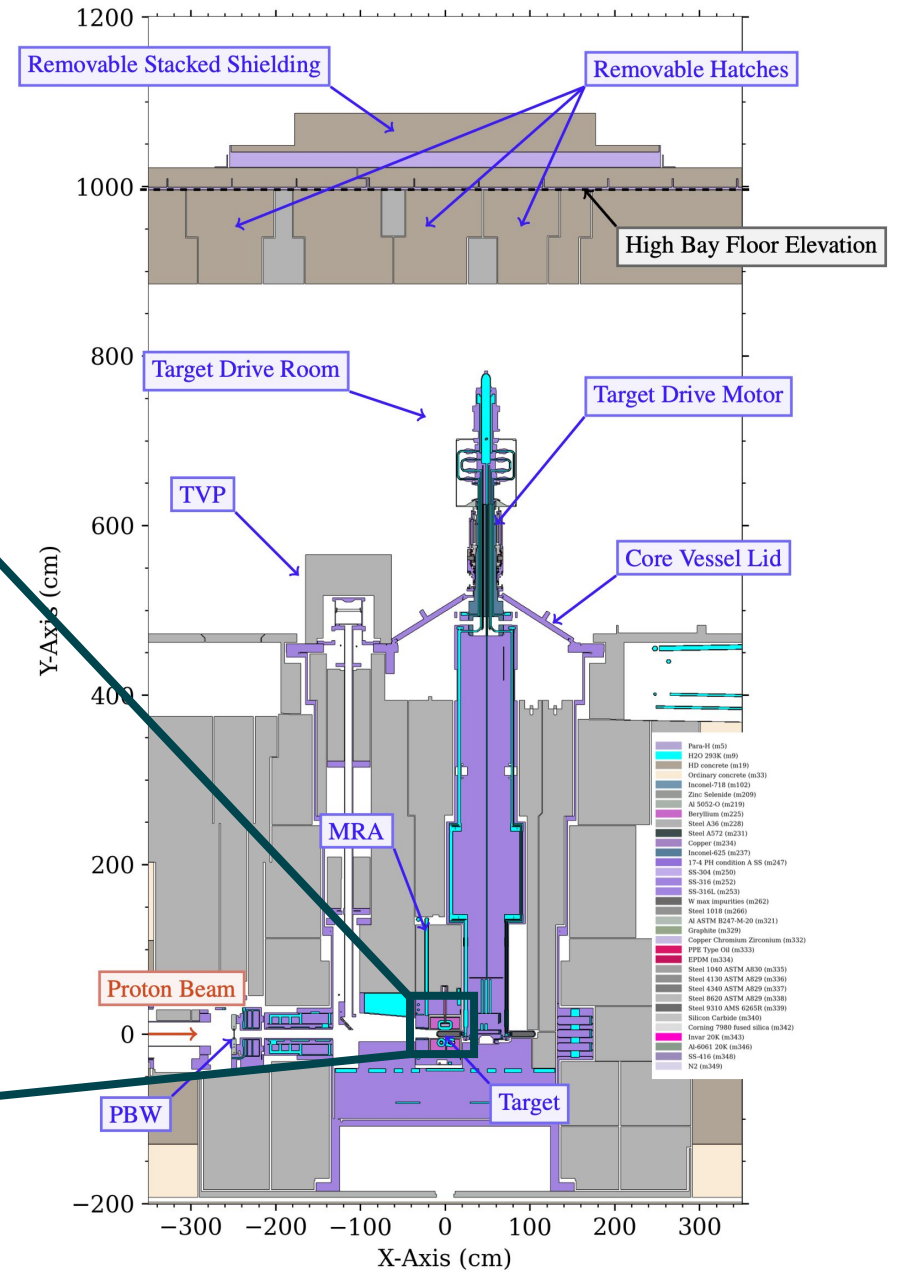


Overview of STS MCNP Geometry



Zoom Elevation View of Target Segment and Moderator Reflector Assembly

- SS-316 (m2)
- Para-H (m5)
- Al-6061 293K (m7)
- Al-6061 20K (m8)
- H2O 293K (m9)
- Be (m11)
- HD concrete (m19)
- Ordinary concrete (m33)
- Air (m69)
- Inconel-718 (m102)
- Barium fluoride (m206)
- Steel A36 (m228)
- Copper (m234)
- Invar (m238)
- SS-304 (m250)
- SS-316 (m252)
- SS-316L (m253)
- W max impurities (m262)
- SS-420 (m265)
- SS-316L/H2O_10% (m278)
- SS-316L/H2O_20% (m280)
- SS-316L/H2O_30% (m282)
- PEEK (m298)
- Al ASTM B247-M-20 (m321)
- Graphite (m329)
- Copper Chromium Zirconium (m332)



Cross Section View of the STS Geometry

Decay Heat Case Study Overview

Overview of Decay Heat Case Study

- Goal:

- Evaluate methods for calculating the decay heat of a water-cooled stationary tantalum-clad tungsten spallation target

- ^{182}Ta drives decay heat in the target

- Product of $^{181}\text{Ta} (n, \gamma) ^{182}\text{Ta}$

- 114.74 day half-life

- Emits > 1 MeV gammas

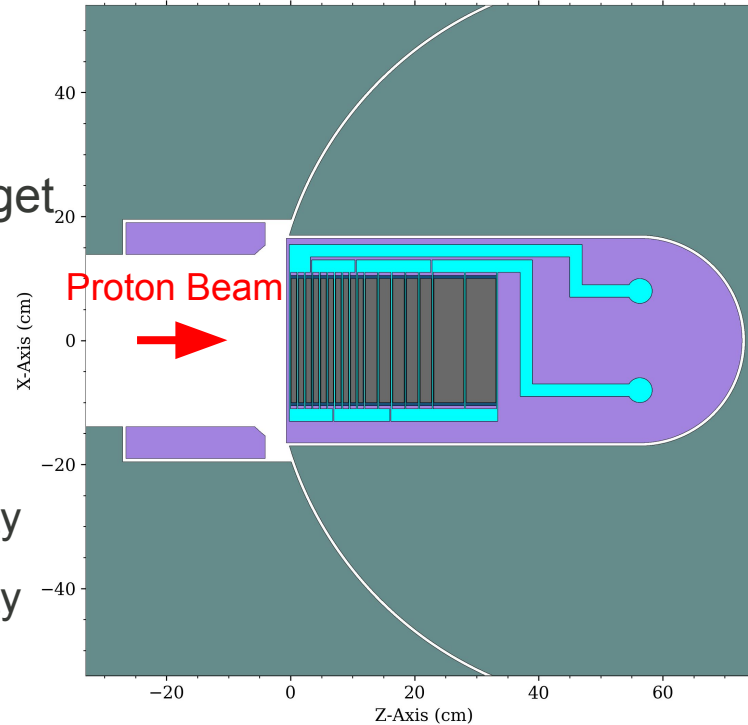
- 1.12 MeV with 35% intensity

- 1.22 MeV with 27% intensity

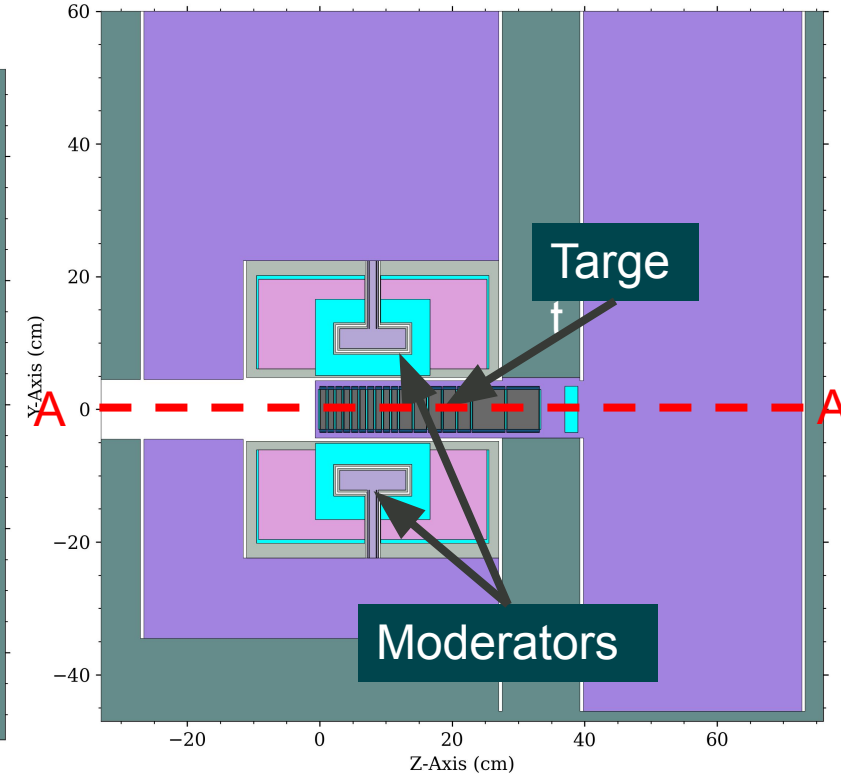
- Assumptions:

- 1.3 GeV proton beam at 700 kW with a square footprint of 125 x 48 mm²








- 5000 hours of operation



Plan View of the Case Study Geometry at A-A



Elevation View of the Case Study Geometry

	H2O 293K (m1)
	Be (m5)
	W (m23)
	Ta (m30)
	SS-316L (m31)
	SS-316L/H2O_10% (m34)
	Para-H (m37)
	Al ASTM B247-M-20 (m38)

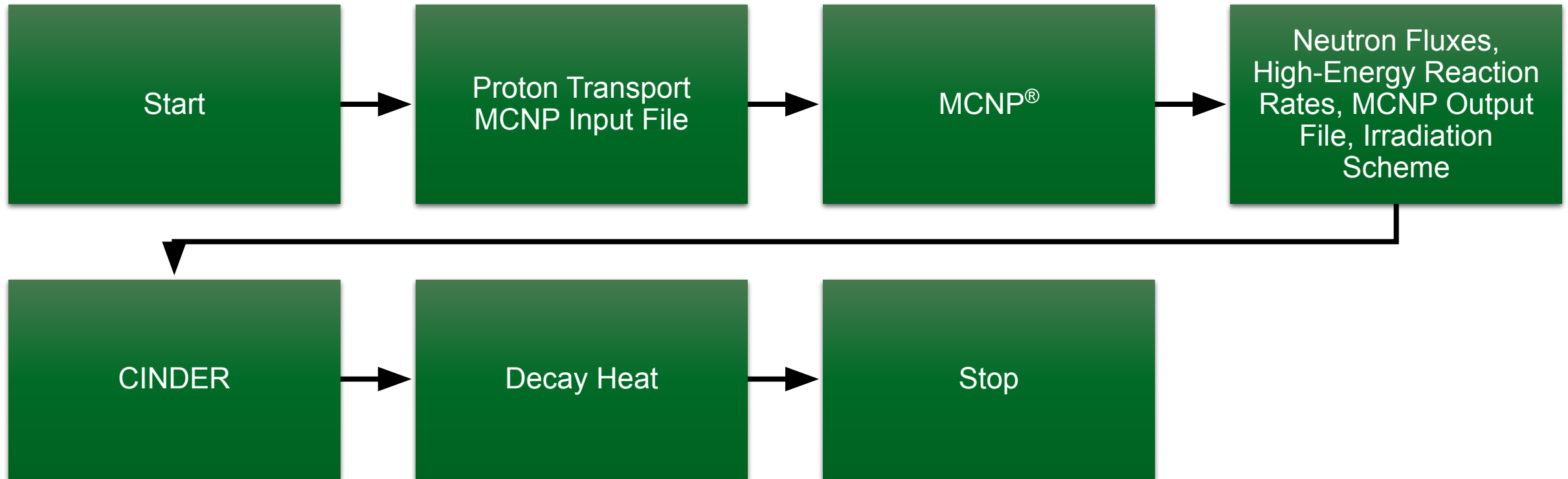
Overview of Codes and XS Evaluated in the Case Study

FLUKA	MCNPX™		MCNP® Version 6.2	
Transport and Activation XS	Transport XS	Activation XS	Transport XS	Activation XS
JEFF 3.3	ENDF/B-VII.1	CINDER90	ENDF/B-VII.1	CINDER2008
ENDF/B-VIII.0	ENDF/B-VII.1	CINDER2008	ENDF/B-VII.1	ENDF/B-VII.1*
FLUKA Multi-Group			ENDF/B-VIII.1	ENDF/B-VIII.1*
			JEFF 3.3	JEFF 3.3*

* = activation of only specific isotopes were calculated and no decay heat

Methodology

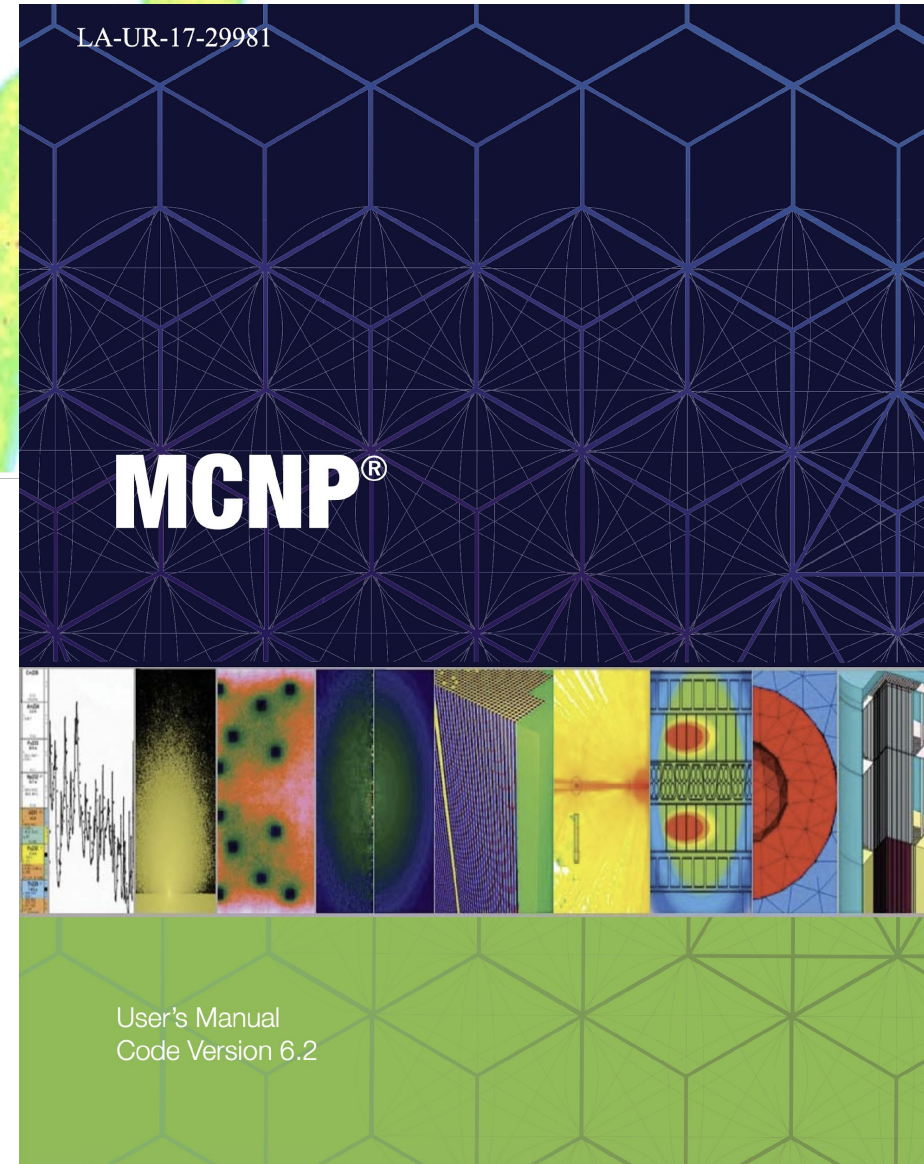
MCNP and CINDER Workflow



MCNP[®] Details

- MCNPX[™]
 - ENDF/B-VII.1 continuous energy cross sections
 - Bertini/Dresner physics model (default)
- MCNP[®] Version 6.2
 - ENDF/B-VII.1 continuous energy cross sections (unless specified otherwise)
 - CEM03.03 physics model (default)

MCNPX[™] USER'S MANUAL Version 2.7.0



CINDER Highlights

CINDER90

Cross-section Library

- 63 energy groups
- ENDF/B-VI.0-based
- No library maker

MCNPX™ Compatible

Orphan Code

Decay Heat Approximation

- Assumes all emitted energy is deposited locally

CINDER2008

Cross-section Library

- 321 energy groups
- ENDF/B-VII.0-based
- Library maker

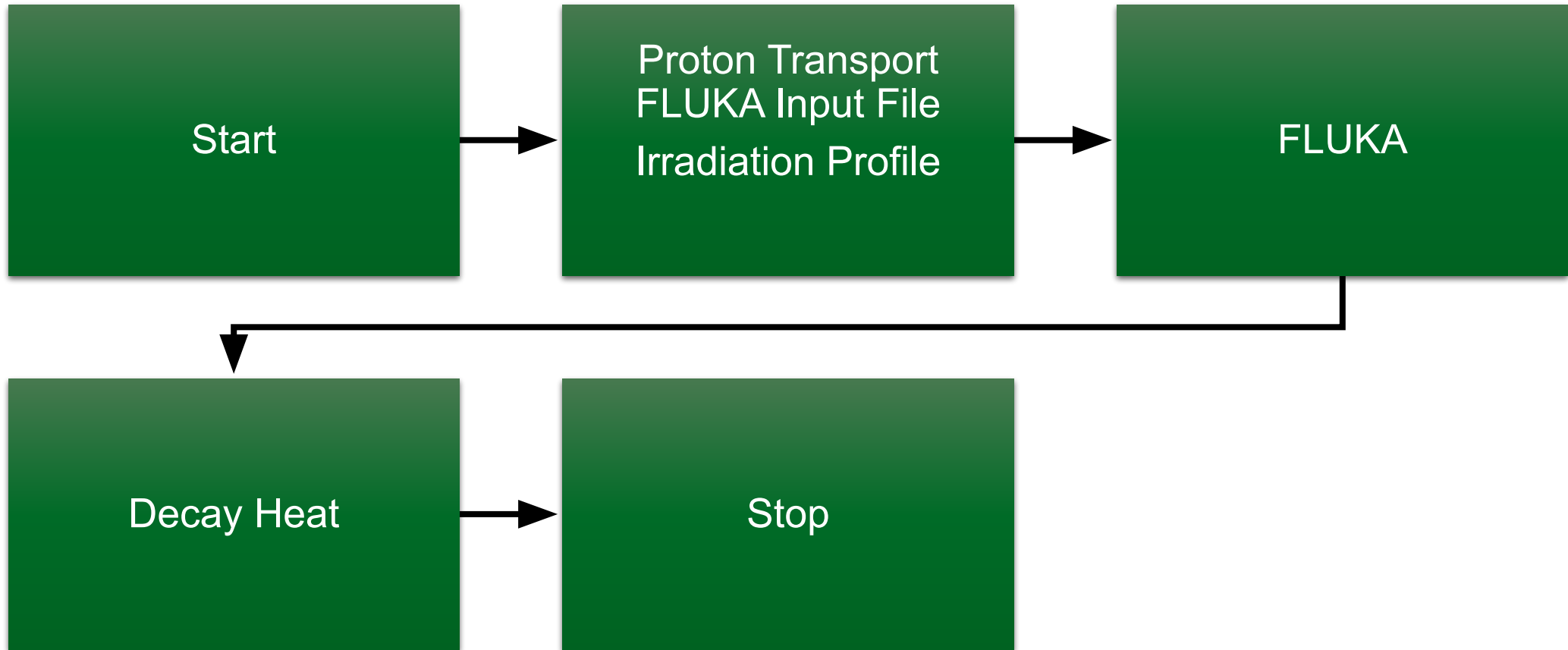
MCNP® Version 6.2 and MCNPX™ Compatible

Currently maintained by AARE developers group

Decay Heat Approximation

- Assumes all emitted energy is deposited locally

FLUKA Workflow



FLUKA Highlights

FLUKA 4-5.1

Default – PRECISION

- EMF On:
 - Transport of electrons, positrons and photons
 - Particle transport threshold set at 100 keV, except neutrons (1E-5 eV)

PHYSICS:

- COALESCence: Activate the coalescence mechanism
- EVAPORAT: Evaporation
 - New evaporation model, with heavy fragment evaporation

Low Energy Neutrons

Pointwise transport

- JEFF-3.3 (Default)
- ENDF-VIII.0

Multigroup neutron transport

- 260 groups
 - Natural W: ENDF/B-VIIR0
 - Ta-181: TENDL-13
 - Natural Fe: ENDF/B-VIR8

Results

Tantalum Cladding Decay Heat Comparison

Key Takeaways:

- CINDER90 is ~40 % more conservative than CINDER2008
- ^{182}Ta (114.74 day half-life) drives decay heat in Ta contributing between 70% to 78% over time

Mat	Decay Time	MCNP6 CINDER2008	MCNPX CINDER90 (Ratio)	MCNPX CINDER2008 (Ratio)	FLUKA (JEFF-3.3) EMF: Off (Ratio)	FLUKA (ENDFVIII.0) EMF: Off (Ratio)	FLUKA (Multi-Group) EMF: Off (Ratio)
Ta	0 sec.	5.15 kW	1.38	0.98	0.61	0.67	0.57
	1 min.	5.06 kW	1.40	0.99	0.61	0.67	0.57
	1 hour	4.80 kW	1.45	1.01	0.55	0.60	0.51
	2 hour	4.76 kW	1.45	1.01	0.55	0.59	0.51
	4 hour	4.71 kW	1.45	1.01	0.54	0.59	0.51
	8 hour	4.65 kW	1.46	1.01	0.54	0.59	0.50
	1 day	4.51 kW	1.46	1.01	0.55	0.60	0.51

Note:

- The ratios are relative to the MCNP6/CINDER2008 result
- MCNPX and MCNP6 used ENDF/B-VII.1

Tungsten Decay Heat Comparison

Key Takeaways:

- CINDER90 is ~15-20 % more conservative than CINDER2008
- ¹⁸⁷W (23.809 hour half-life) contributes 18% - 44% of the decay heat in W

Mat .	Decay Time	MCNP6 CINDER2008	MCNPX CINDER90 (Ratio)	MCNPX CINDER2008 (Ratio)	FLUKA (JEFF-3.3) EMF: Off (Ratio)	FLUKA (ENDFVIII.0) EMF: Off (Ratio)	FLUKA (Multi-Group) EMF: Off (Ratio)
Ta	0 sec.	3.26 kW	0.88	0.75	0.67	0.67	0.65
	1 min.	2.83 kW	0.88	0.82	0.61	0.61	0.60
	1 hour	2.02 kW	1.12	0.97	0.78	0.77	0.76
	2 hour	1.84 kW	1.16	0.98	0.79	0.78	0.77
	4 hour	1.65 kW	1.18	0.99	0.80	0.79	0.76
	8 hour	1.44 kW	1.18	0.99	0.79	0.77	0.75
	1 day	0.96 kW	1.16	1.00	0.78	0.77	0.76

Note:

- The ratios are relative to the MCNP6/CINDER2008 result
- MCNPX and MCNP6 used ENDF/B-VII.1

FLUKA EMF On or Off Decay Heat Comparison

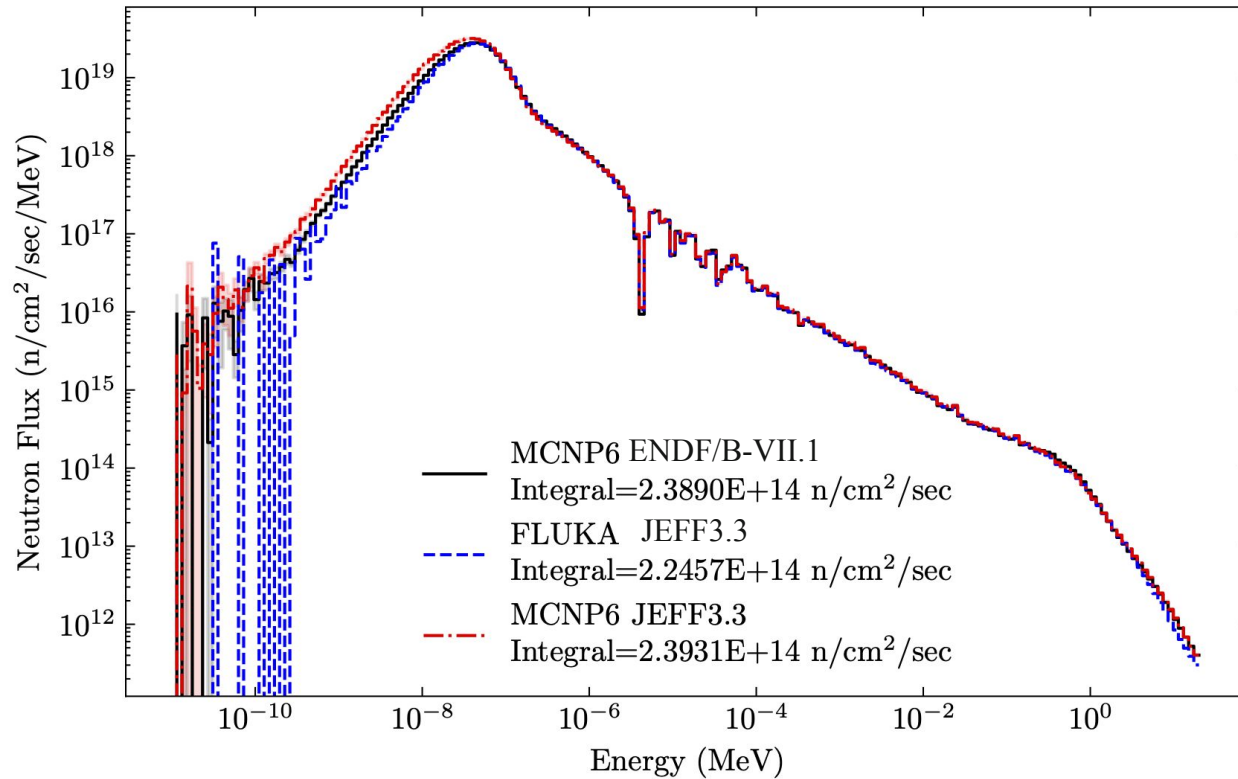
Mat.	Decay Time	FLUKA EMF On/Off Ratio	Mat.	FLUKA EMF On/Off Ratio	Mat.	FLUKA EMF On/Off Ratio	Mat.	FLUKA EMF On/Off Ratio
W	0 sec.	1.30	Ta	0.59	SS	1.33	Total	0.93
	1 min.	1.38		0.59		1.29		0.92
	1 hour	1.50		0.52		1.39		0.90
	2 hour	1.57		0.50		1.56		0.89
	4 hour	1.63		0.50		1.94		0.89
	8 hour	1.74		0.49		2.90		0.89
	1 day	2.14		0.47		4.17		0.88

Isotopic Production Comparison

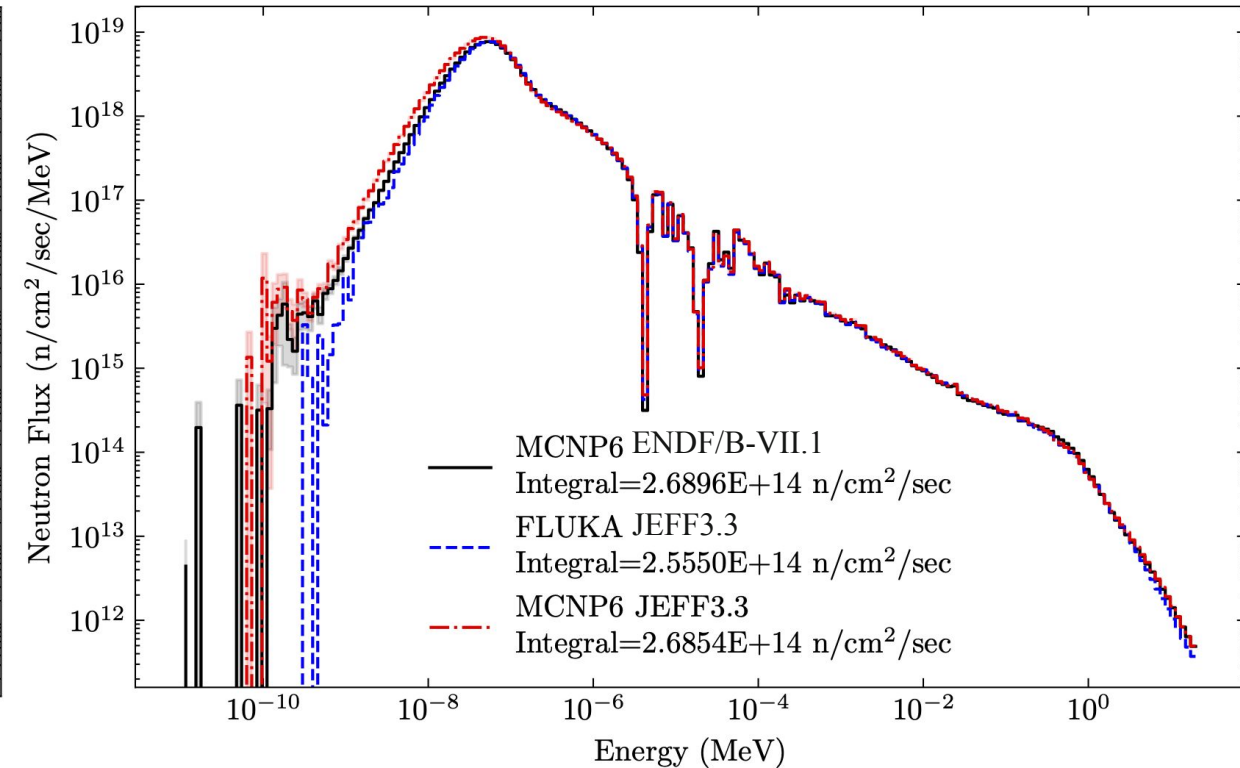
Methodology	^{187}W Activity (PBq)	^{182}Ta Activity (PBq)
MCNPX / CINDER 90	8.41	21.3
MCNPX / CINDER2008	5.77	14.9
MCNP6 / CINDER2008	5.68	14.8
MCNP6 ENDF/B-VII.1	4.049 ± 0.002	10.730 ± 0.004
MCNP6 ENDF/B-VIII.1	3.958 ± 0.002	10.773 ± 0.004
MCNP6 JEFF 3.3	3.9702 ± 0.0007	10.598 ± 0.002
FLUKA JEFF 3.3	3.743 ± 0.001	9.932 ± 0.002
FLUKA ENDF/B-VIII.0	3.563 ± 0.001	10.897 ± 0.002
FLUKA Multi-Group	3.464 ± 0.001	9.195 ± 0.002

FLUKA and MCNP[®] Version 6.2 Neutron Flux Comparison

Total Tantalum Neutron Flux Comparison



Total Tungsten Neutron Flux with Tantalum Cladding Comparison



Temperature Dependence of Activation

MCNP[®] Version 6.2 with
ENDF/B-VIII.1 Point-wise Cross
Sections

Operating Temperature: 500 K

Room Temperature: 293 K

Isotope	Room Temperature (PBq)	Operating Temperature (PBq)	Ratio (Operating/Room)
$^{187}_{74}\text{W}$	3.958 ± 0.002	3.916 ± 0.002	0.989 ± 0.003
$^{182}_{73}\text{Ta}$	10.773 ± 0.004	10.981 ± 0.004	1.019 ± 0.006

Conclusions and Future Work

- CINDER90 consistently produces higher decay heat values as compared to the other methods evaluated in this case study
 - About 40% higher for Ta compared with CINDER2008
 - 15-20% higher for W compared with CINDER2008
- FLUKA and MCNP[®] Version 6.2 with point-wise cross sections produce consistent activation results
- CINDER2008 with MCNP[®] Version 6.2 or MCNPX[™] produce statistically equivalent results (using same point-wise cross sections during proton-transport)
- Future Work
 - Calculate the net decay heat effect of transporting the betas, gammas, and positrons on the target as a whole with MCNP[®] Version 6.2
 - Better understand how much heat is deposited to the water coolant

References

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- M. B. Chadwick and et. al, “ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data,” Nuclear Data Sheets, vol. 112, no. 12, pp. 2887–2996, 2011, doi: [10.1016/j.nds.2011.11.002](https://doi.org/10.1016/j.nds.2011.11.002).
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- C. J. Werner et al., “MCNP User’s Manual Code Version 6.2,” LANL, LA–UR–17–29981, Oct. 2017.
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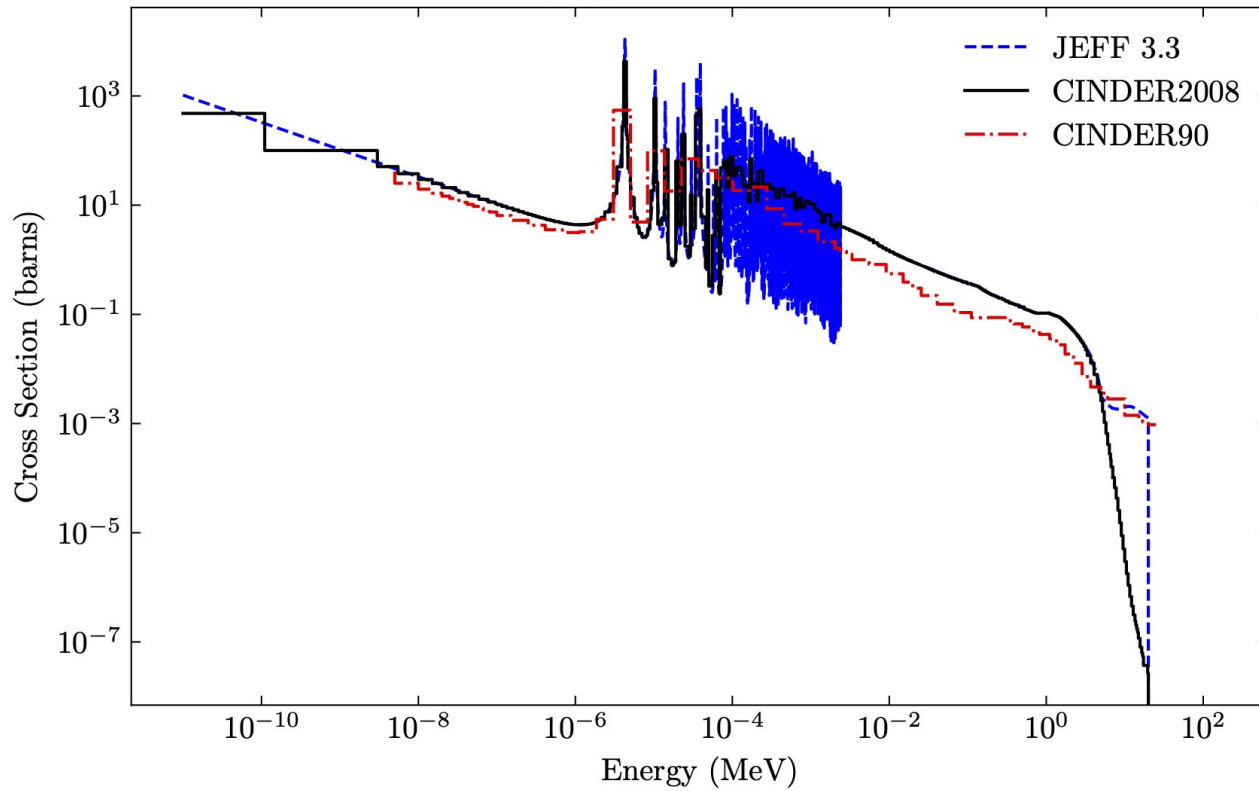


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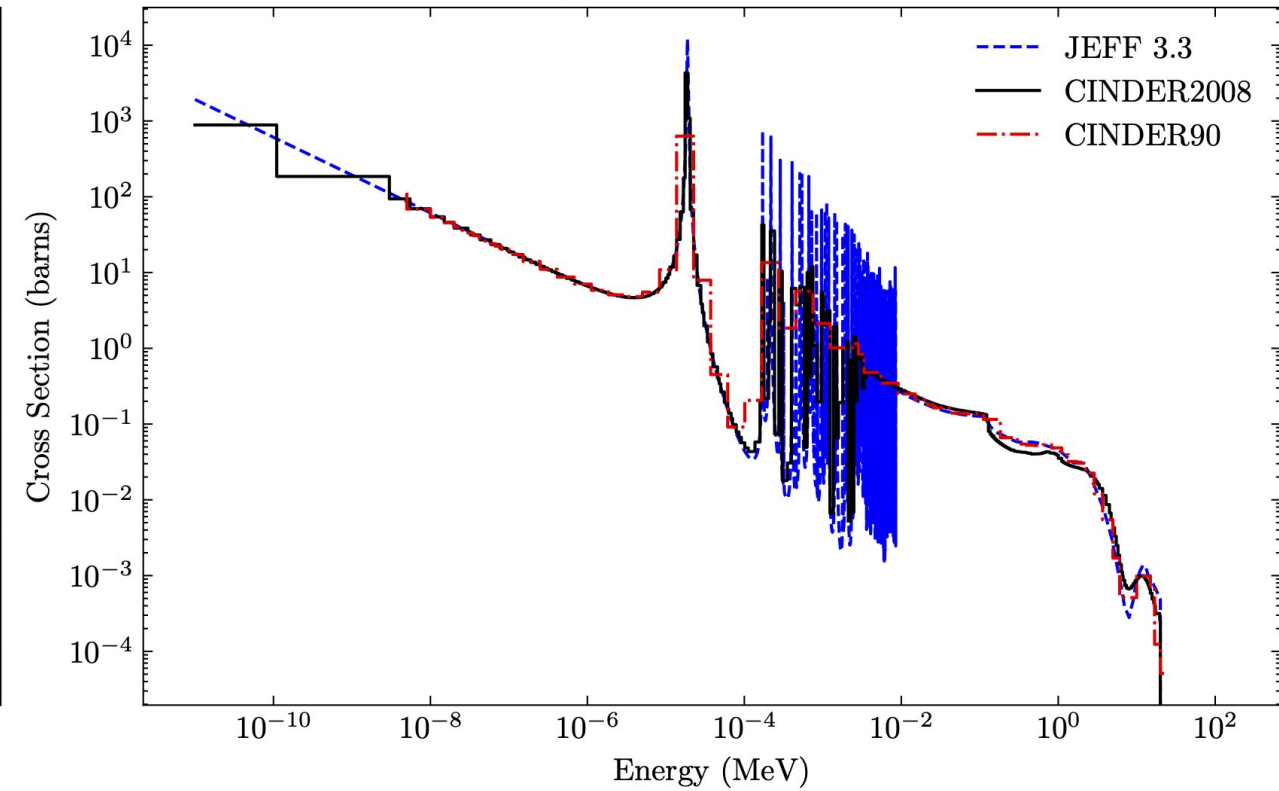
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FLUKA and CINDER Neutron Cross Section Comparison

^{181}Ta (n,γ) ^{182}Ta Cross Sections



^{186}W (n,γ) ^{187}W Cross Sections



Tantalum Cladding Decay Heat Comparison

Key Takeaways:

- CINDER90 is ~30 % more conservative than CINDER2008
- ^{182}Ta (114.74 day half-life) drives decay heat in Ta going from 70% to 78% over time

Mat	Decay Time	MCNP6 CINDER2008	MCNPX CINDER90 (Ratio)	MCNPX CINDER2008 (Ratio)	FLUKA (JEFF-3.3) EMF: Off (Ratio)	FLUKA (ENDFVIII.0) EMF: Off (Ratio)	FLUKA (Multi-Group) EMF: Off (Ratio)
Ta	0 sec.	5.15 kW	7.13 kW	5.04 kW	3.16 kW	3.43 kW	2.94 kW
	1 min.	5.06 kW	7.10 kW	5.01 kW	3.11 kW	3.38 kW	2.90 kW
	1 hour	4.80 kW	6.94 kW	4.85 kW	2.66 kW	2.89 kW	2.47 kW
	2 hour	4.76 kW	6.90 kW	4.81 kW	2.60 kW	2.83 kW	2.41 kW
	4 hour	4.71 kW	6.85 kW	4.77 kW	2.56 kW	2.79 kW	2.38 kW
	8 hour	4.65 kW	6.78 kW	4.71 kW	2.53 kW	2.76 kW	2.34 kW
	1 day	4.51 kW	6.58 kW	4.56 kW	2.47 kW	2.70 kW	2.29 kW

Note:

- The ratios are relative to the MCNP6/CINDER2008 result
- MCNPX and MCNP6 used ENDF/B-VII.1

Tungsten Decay Heat Comparison

Key Takeaways:

- CINDER90 is ~15-20 % more conservative than CINDER2008
- ¹⁸⁷W (23.809 hour half-life) contributes 18% - 44% of the decay heat in W

Mat.	Decay Time	MCNPX CINDER90	MCNPX CINDER2008	MCNP6 CINDER2008	FLUKA (JEFF-3.3) EMF: Off	FLUKA (ENDFVIII.0) EMF: Off	FLUKA (Multi Group) EMF: Off
W	0 sec.	3.26 kW	2.79 kW	3.71 kW	2.49 kW	2.47 kW	2.43 kW
	1 min.	2.83 kW	2.63 kW	3.22 kW	1.97 kW	1.96 kW	1.93 kW
	1 hour	2.02 kW	1.74 kW	1.80 kW	1.41 kW	1.39 kW	1.36 kW
	2 hour	1.84 kW	1.56 kW	1.59 kW	1.26 kW	1.24 kW	1.22 kW
	4 hour	1.65 kW	1.39 kW	1.40 kW	1.12 kW	1.10 kW	1.07 kW
	8 hour	1.44 kW	1.21 kW	1.22 kW	0.96 kW	0.94 kW	0.92 kW
	1 day	0.96 kW	0.83 kW	0.83 kW	0.65 kW	0.64 kW	0.63 kW

Note: MCNPX and MCNP6 used ENDF/B-VII.1

FLUKA EMF On or Off Decay Heat Comparison

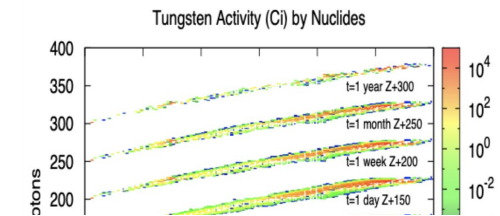
Mat.	Decay Time	FLUKA EMF: Off (kW)	FLUKA EMF: On (kW)	Mat.	FLUKA EMF: Off (kW)	FLUKA EMF: On (kW)	Mat.	FLUKA EMF: Off (kW)	FLUKA EMF: On (kW)	Mat.	FLUKA EMF: Off (kW)	FLUKA EMF: On (kW)
W	0 sec.	2.49	3.23	Ta	3.16	1.88	SS	0.42	0.56	Total	6.07	5.67
	1 min.	1.97	2.71		3.11	1.82		0.41	0.53		5.49	5.06
	1 hour	1.41	2.12		2.66	1.37		0.31	0.43		4.37	3.92
	2 hour	1.26	1.98		2.60	1.31		0.25	0.39		4.11	3.67
	4 hour	1.12	1.83		2.56	1.27		0.17	0.33		3.85	3.43
	8 hour	0.96	1.67		2.53	1.23		0.10	0.29		3.59	3.19
	1 day	0.65	1.39		2.47	1.17		0.06	0.25		3.19	2.81

CINDER2008 Details

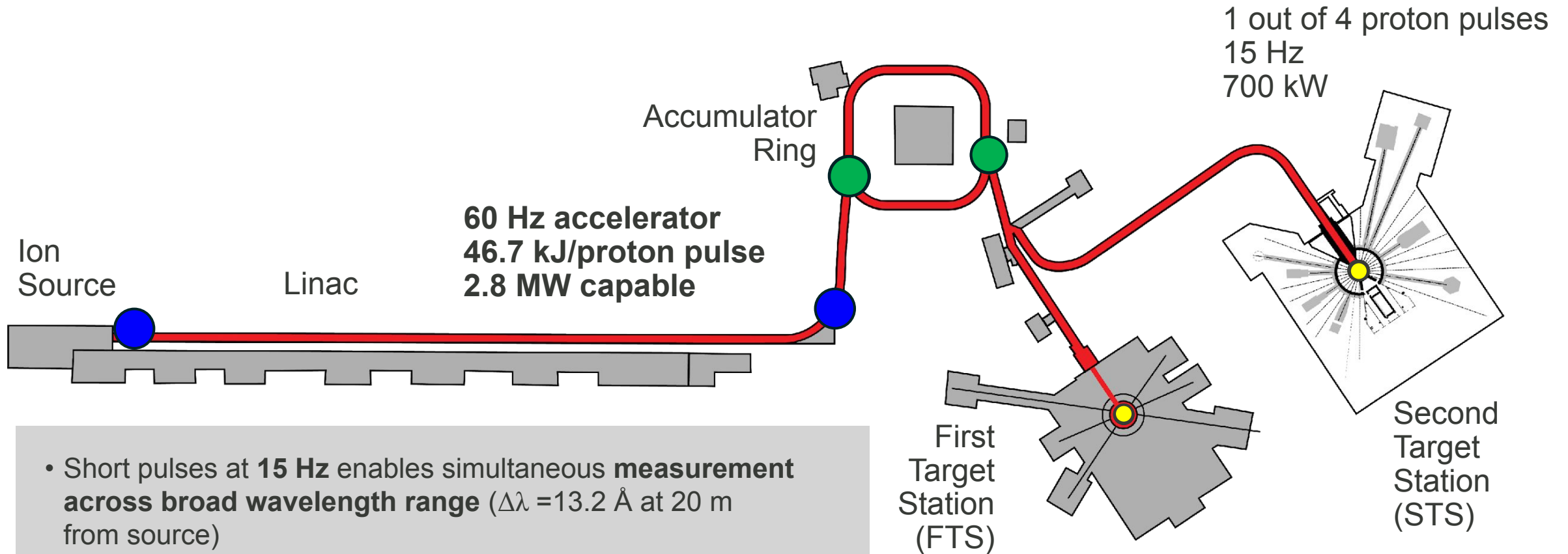
- AARE Package
 - Perl-based wrappers for CINDER2008
 - Cell-based activation
 - Single-core compatible
 - RNUCS Patch
 - Tally high-energy physics production/destruction rates
 - 321-group flat spectrum ENDF/B-VII-based multigroup cross-section library

- ACTIUM Package
 - Python wrappers for CINDER2008
 - UM and Cell-based activation
 - Multi-core compatible

AARE_ACTIVATION Script Version 2.0 User Guide



Overview of SNS and STS Operations



- Short pulses at **15 Hz** enables simultaneous **measurement across broad wavelength range** ($\Delta\lambda = 13.2 \text{ \AA}$ at 20 m from source)
- Complementarity with FTS – **uses all available accelerator capability provided by PPU**
- **Flexibility** will be provided to **operate** both FTS and STS at the same time or separately if either is shutdown

3 out of 4 proton pulses
45 pulses/sec
2 MW

1 out of 4 proton pulses
15 Hz
700 kW

ORNL SNS and the Second Target Station (STS)

- High-brightness cold neutron source (smaller samples & shorter time)
- Supports up to 22 neutron instruments
- Sustains US/ORNL leadership in neutron sciences



STS project: Build the second target station with initial suite of beam lines

- Optimized for cold neutrons
- World-leading peak brightness
- Provide new science capabilities for measurements across broader ranges of temporal and length scales, real-time, and smaller samples