

Conceptual Neutronics Design of a Coupled Solid Methane – Supercritical Parahydrogen Moderator and the Importance of Neutron Data Selection

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Historical excursion to the STS



- From the beginning, the capacity for a second target station (STS) to generate neutrons with longer wavelengths has been included in the SNS project
- STS uses the same SNS accelerator
- High-power target (lower than first target station (FTS), 440 - 880 kW, not Hg)
- Lower repetition rate (10 – 20 Hz)
- Coldest possible moderators
- Originally high-flux source (> factor of 3 FTS)
- Broaden the scientific program with more beamlines available
- More room for SNS suite optimization
- Expected at 25% of the SNS capital cost



Longer wavelengths (cold neutrons)

A long-wavelength target station for the spallation neutron source[☆]

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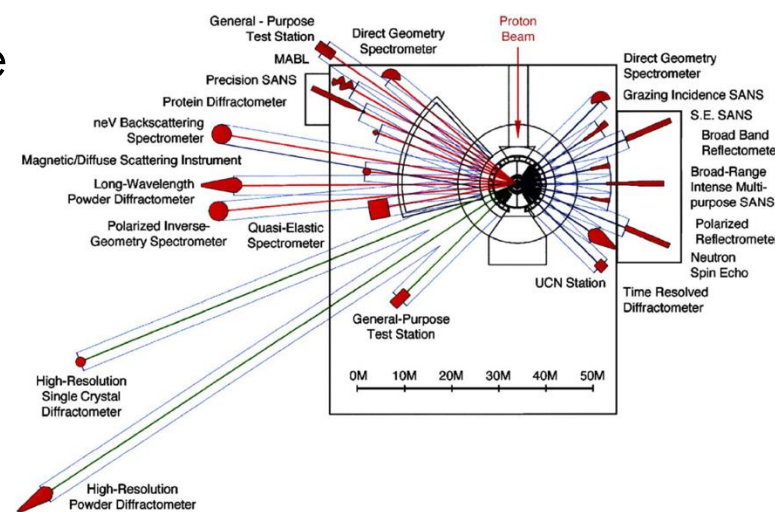


Fig. 1. Preliminary layout of target, guides, and instruments in the LWTS.

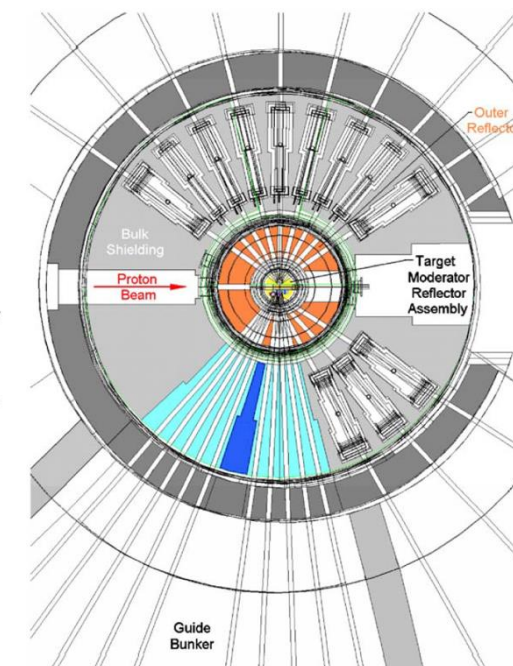


Fig. 4. Shield and beam transport arrangements in the LWTS.

Historical excursion to the STS

- Three proposed cryogenic moderators:
 - 20 K pelletized solid methane cooled by supercritical hydrogen
 - **20 K supercritical hydrogen**
 - 100 K circulating liquid methane
- Long beamlines for high resolution
- Extensive use of neutron optics
- Wide accessible wavelength band

STS selection

- Low dimensional [refs.] 20 K parahydrogen for high-brightness beams of cold neutrons
- Coupled, water pre-moderated
- Rotating W target for better passive cooling & decay heat removal

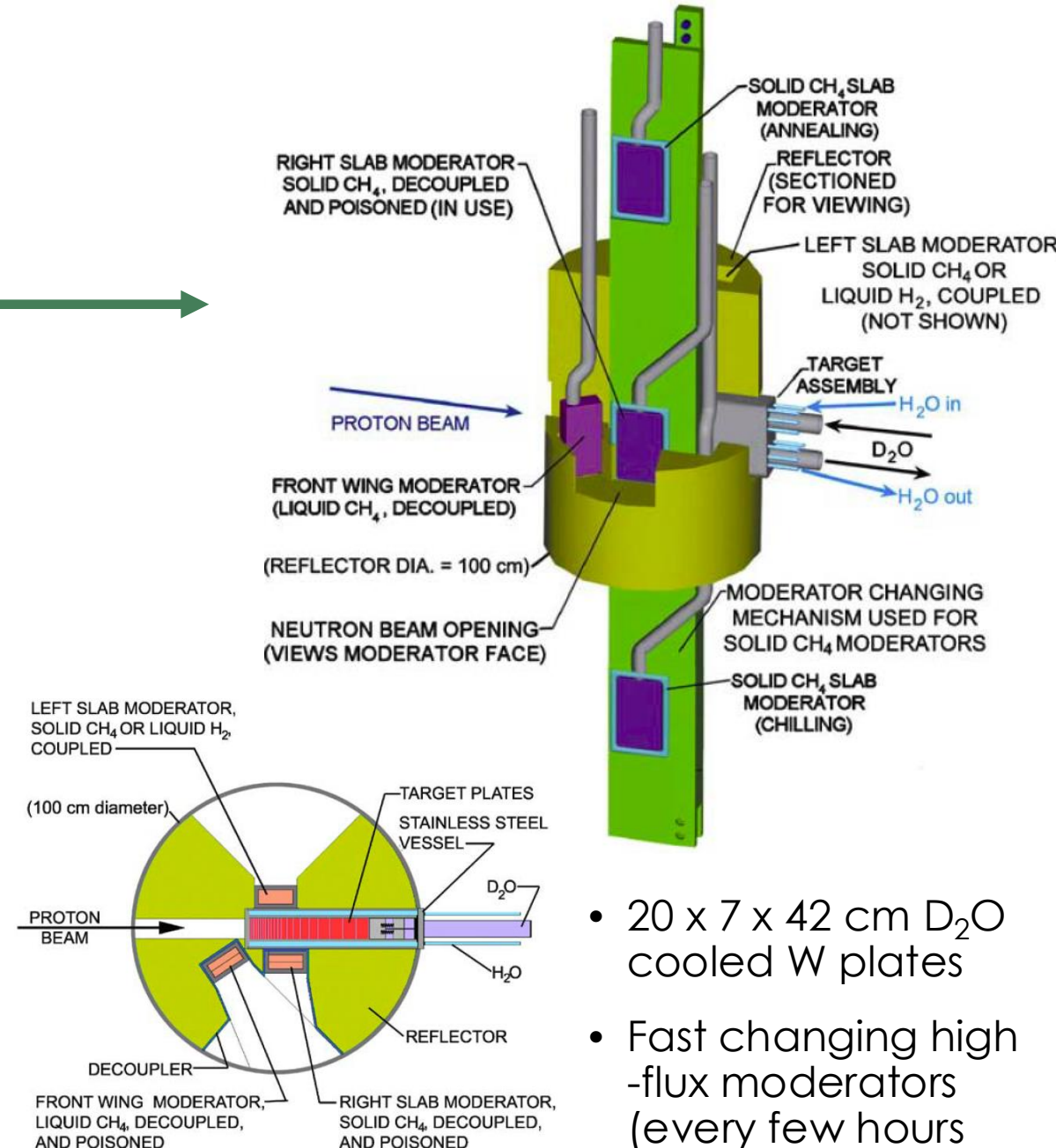
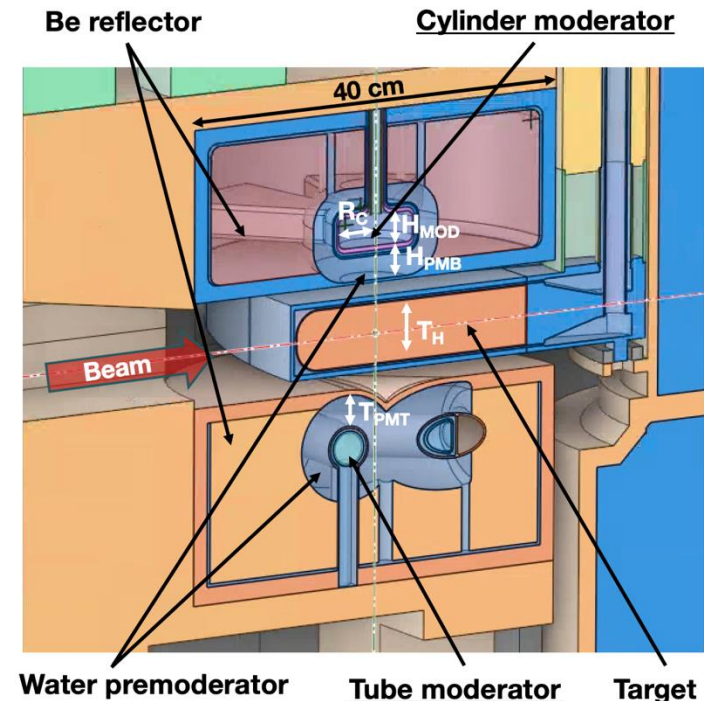
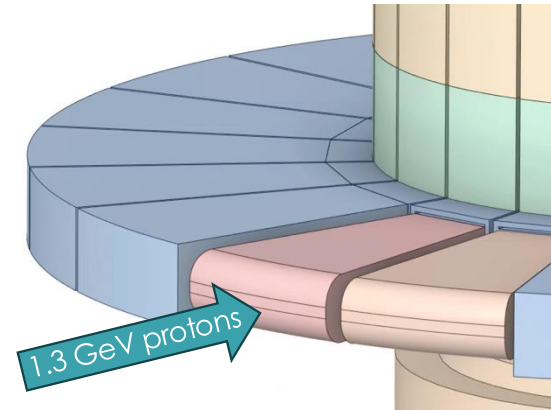
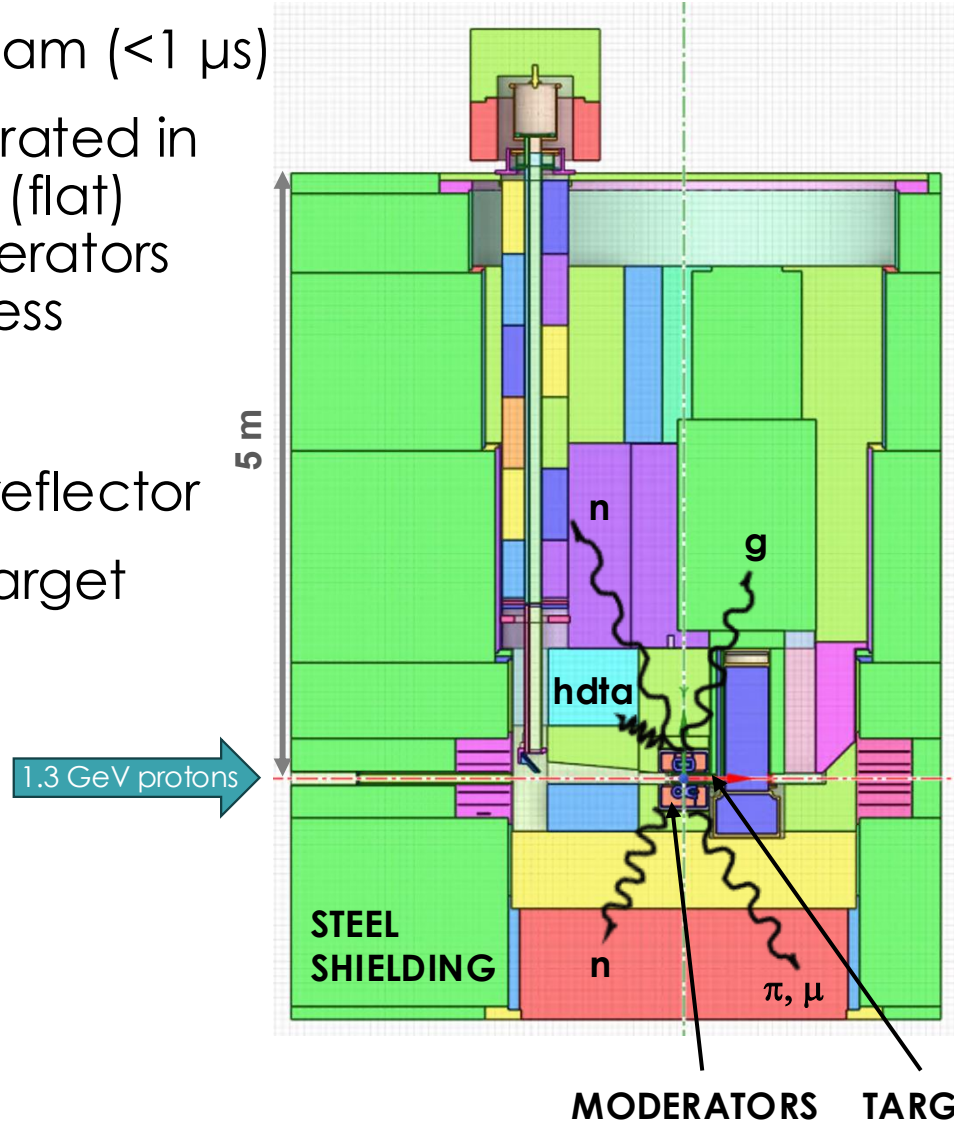
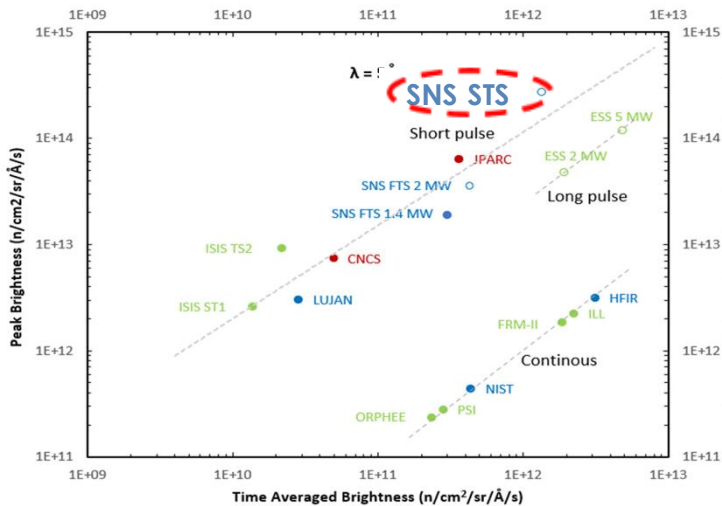


Fig. 2. A cross-sectional view taken at the horizontal midplane of the target and showing the relative positions of the target-moderator-reflector components.

- 20 x 7 x 42 cm D₂O cooled W plates
- Fast changing high-flux moderators (every few hours CH₄ annealing)

SNS Second Target Station (STS)

- Rotating W target
- 1.3 GeV 700kW proton beam (<math><1 \mu\text{s}</math>)
- Spallation neutrons moderated in coupled low-dimensional (flat) cylindrical and tube moderators designed for high brightness
- Para-hydrogen at 20 K
- Water premoderator, Be reflector
- Tightly coupled with the target

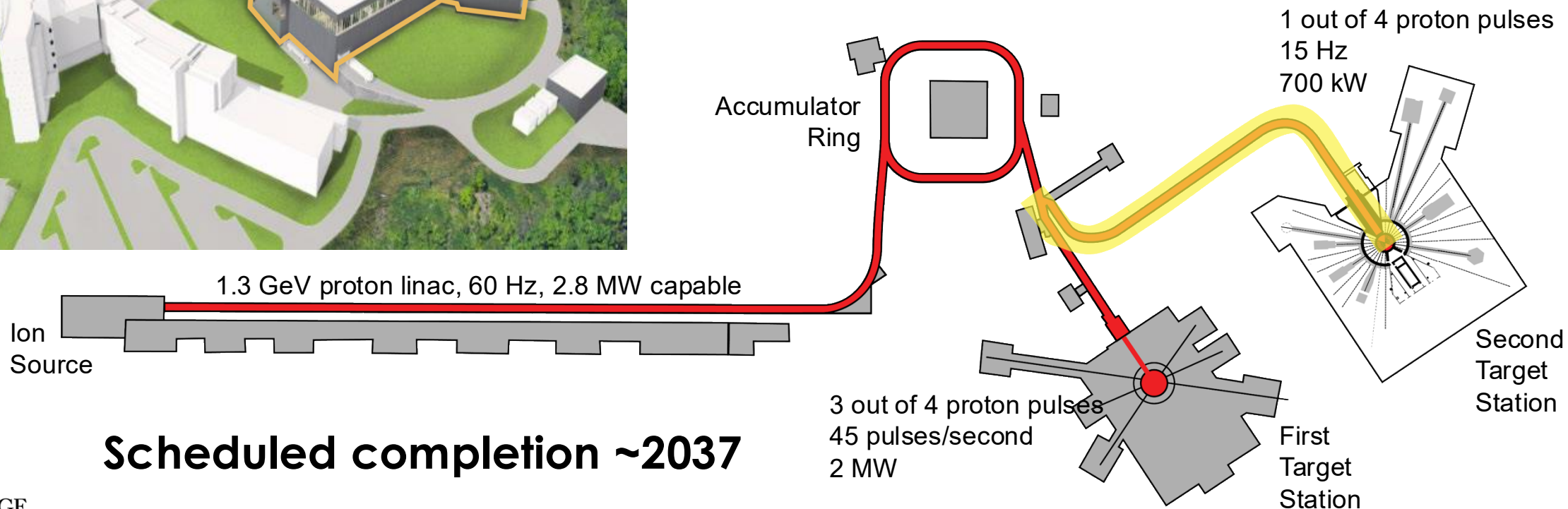
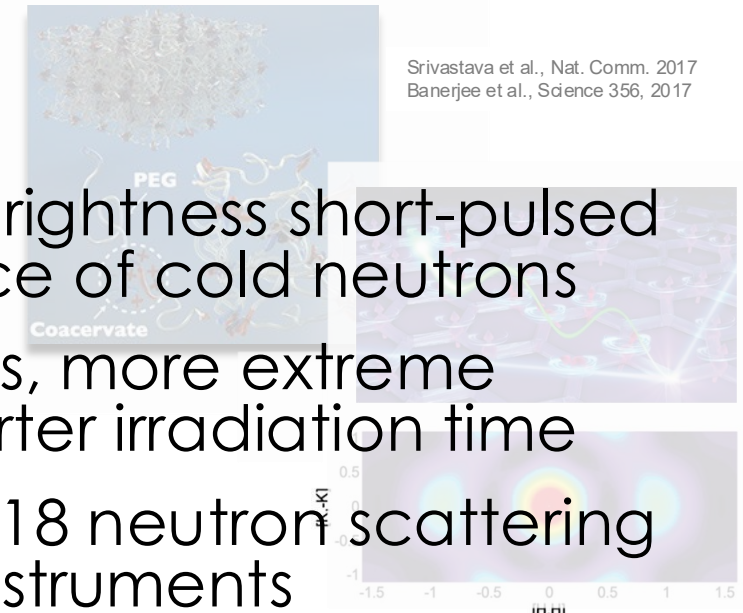


SNS Second Target Station (STS)

Srivastava et al., Nat. Comm. 2017
Banerjee et al., Science 356, 2017



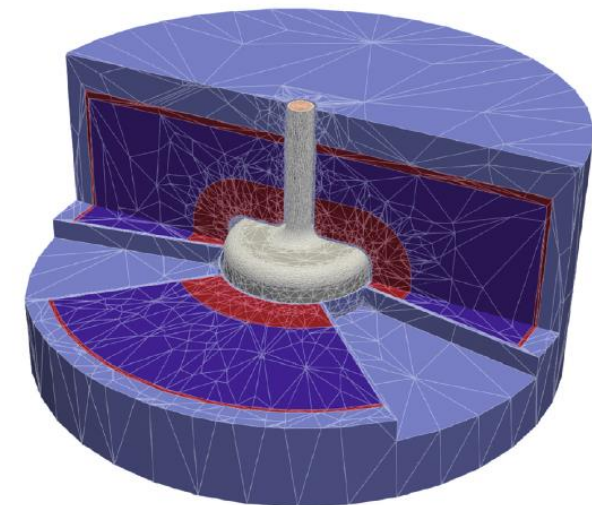
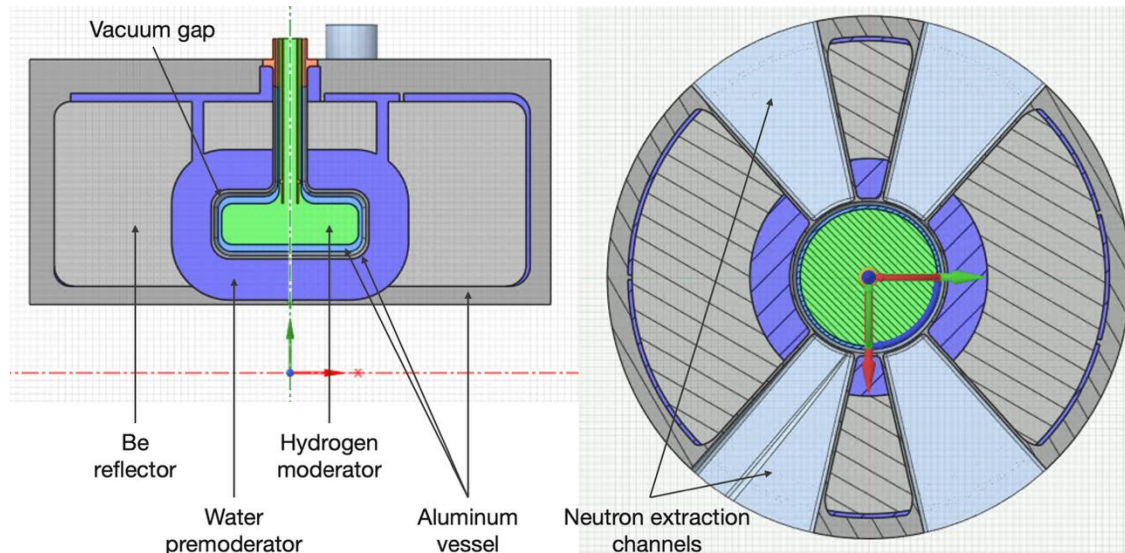
- Highest peak-brightness short-pulsed spallation source of cold neutrons
- Smaller samples, more extreme conditions, shorter irradiation time
- Supports up to 18 neutron scattering and imaging instruments



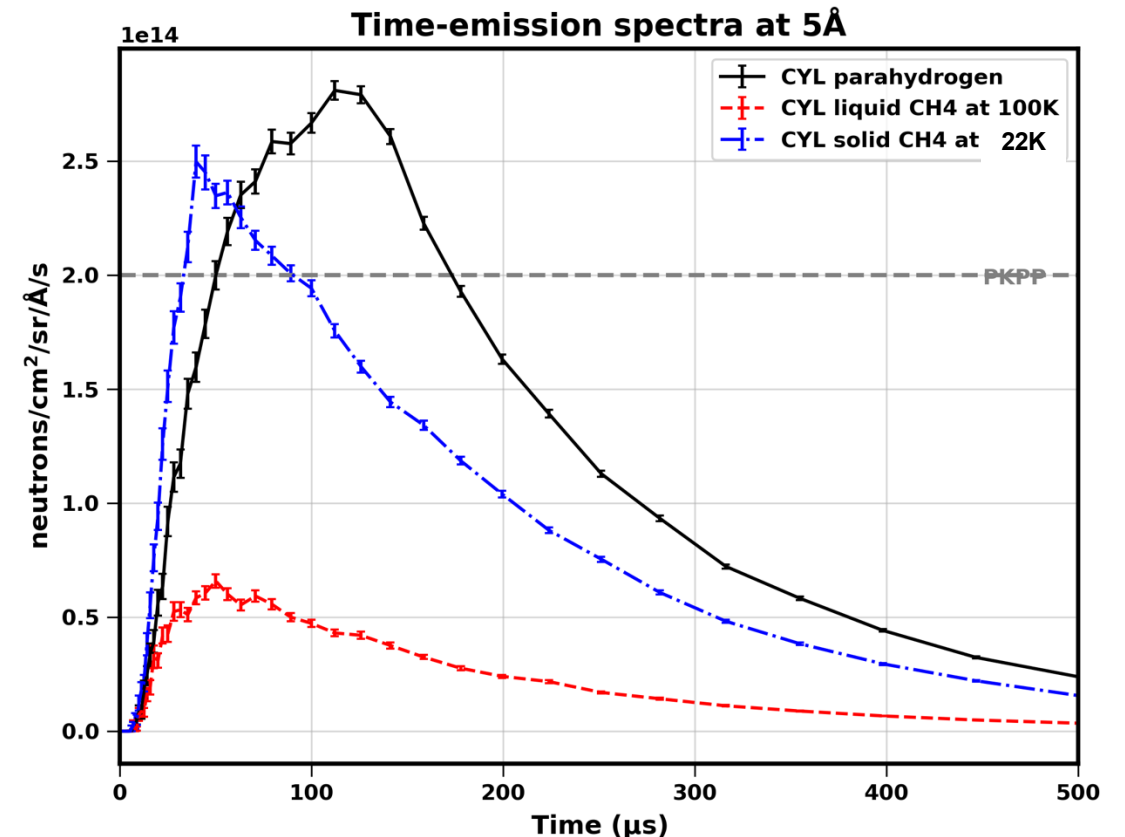
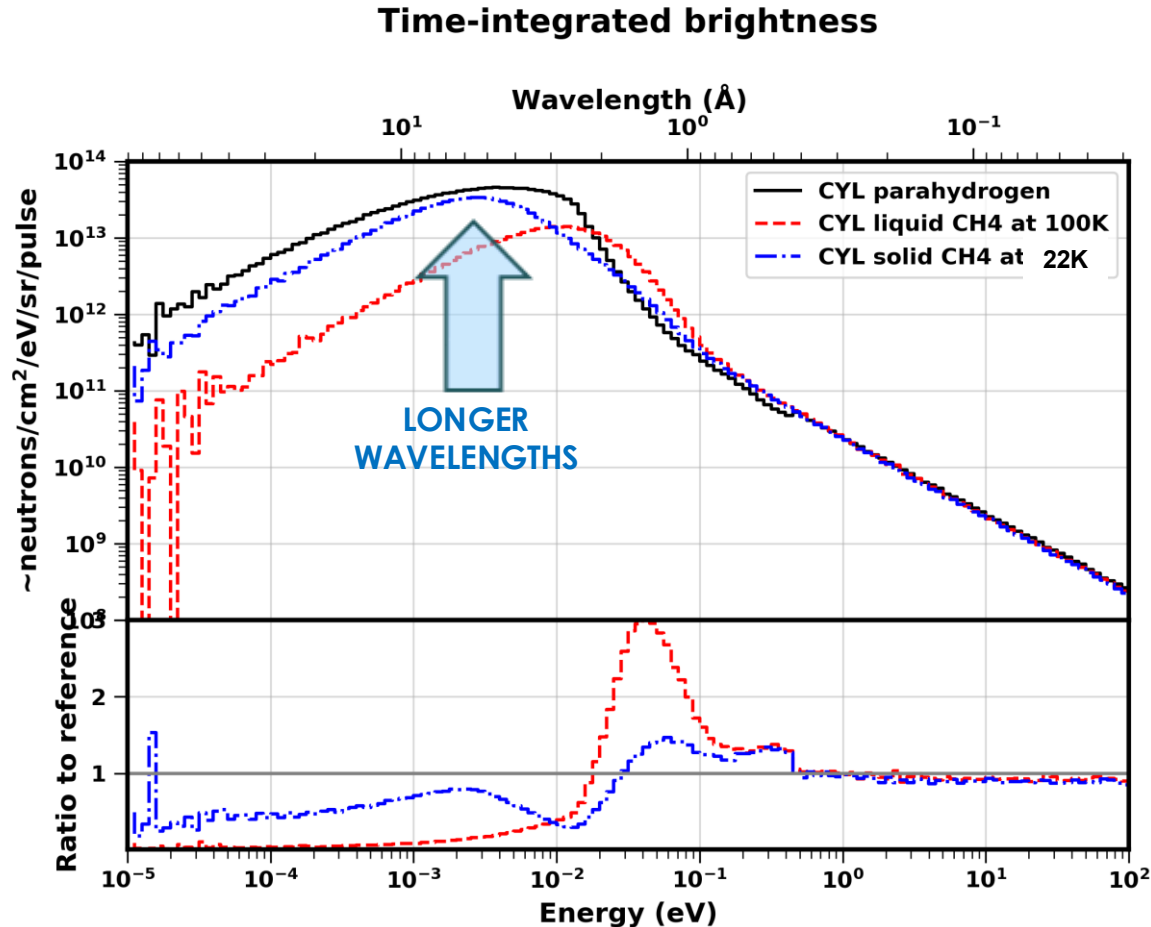
Scheduled completion ~2037

Revisiting alternative moderator designs for STS

- Alternative design study for STS revisited in 2024
- Goal: to find more efficient moderator designs for the production of cold neutrons
- Three candidate materials: liquid hydrogen LH_2 at 20 K and solid methane CH_4 at 20 K and liquid methane CH_4 at 100K
- STS cylinder moderator design chosen as a starting point



Revisiting alternative moderator designs for STS



- Neither solid nor liquid CH₄ performs better than the current LH₂ design
- Solid methane chosen as the best candidate material for longer wavelengths

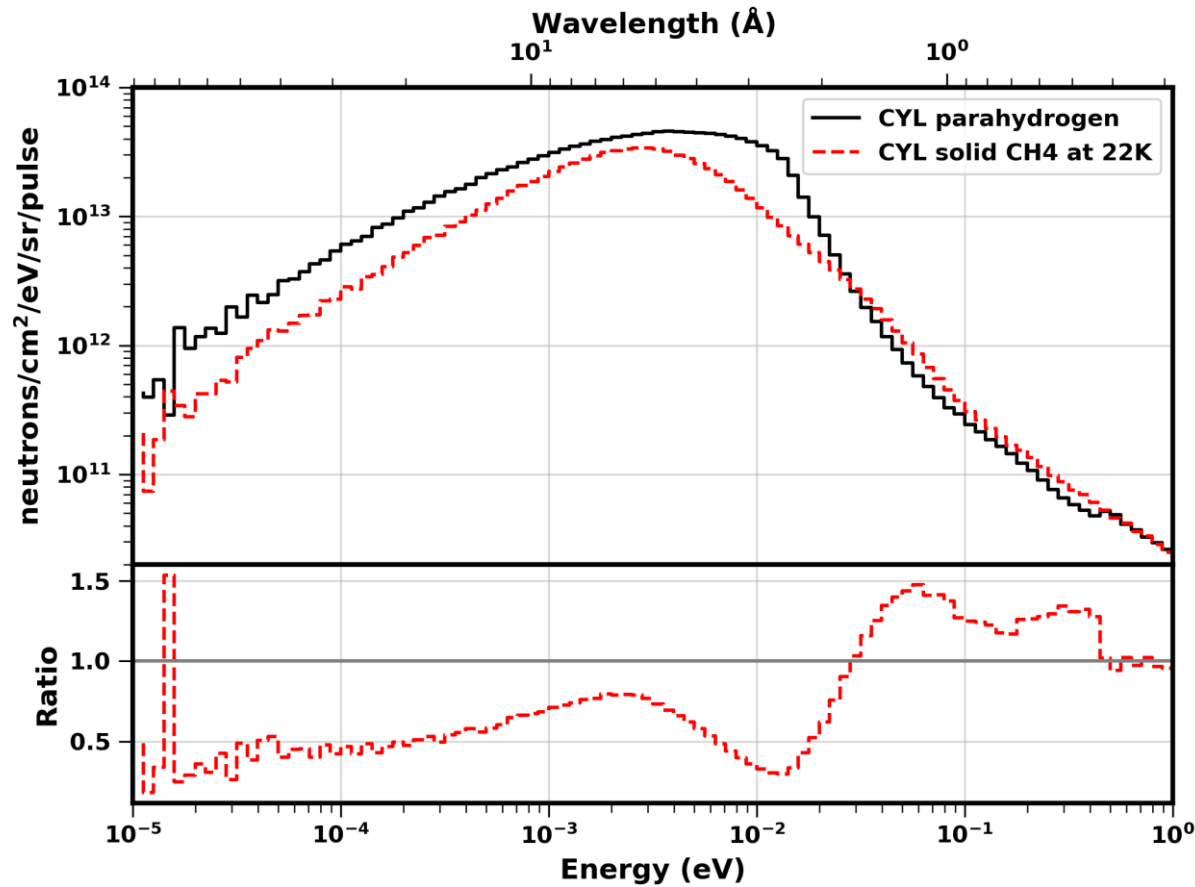
Solid methane CH₄

- PROS: High proton density compared to LH₂
- CONS: Burping effect at high powers, needs annealing
- Exists in three phases at low temperatures
 - Phase II (< 20.4 K) partially ordered, used in neutron moderators
 - Distinct nuclear spin modifications
- Development ongoing
 - Geometry: Grooved/slab designs
 - Form: pellets cooled by flowing He/LH₂ ([ACoM coll.]
- ENDF/B-VIII.0 has scattering kernels for 22K

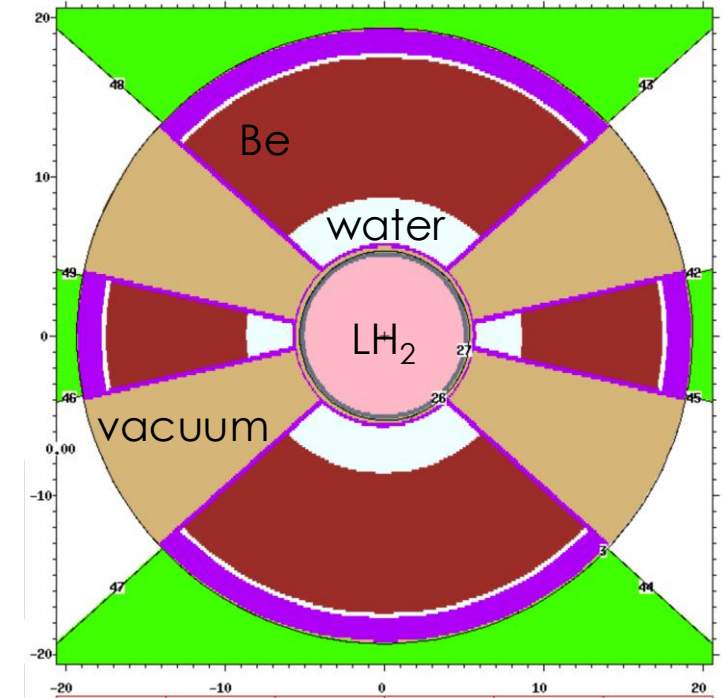
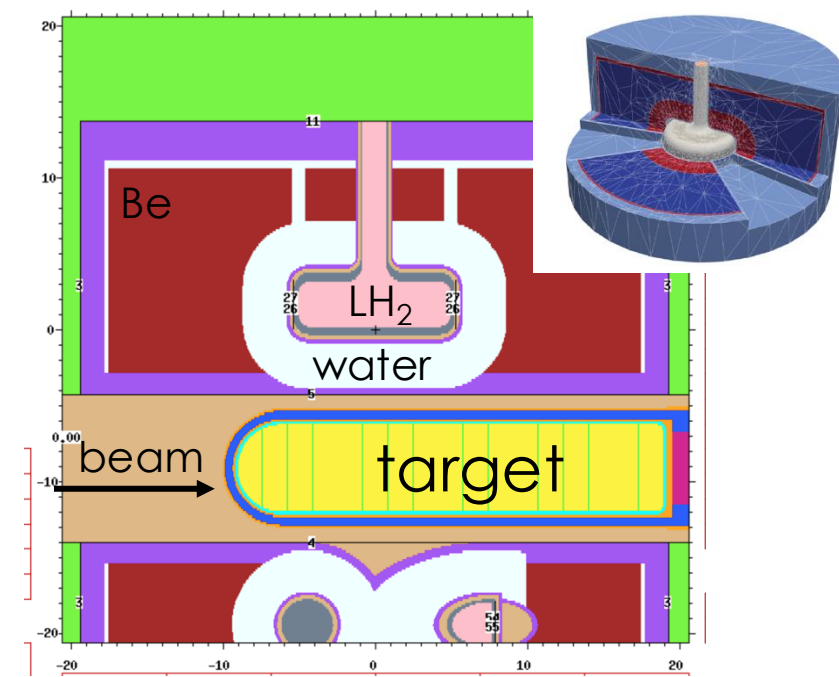
Solid methane CH₄

Current STS cylinder design with LH₂ with a radius of 5 cm:

Time-integrated brightness

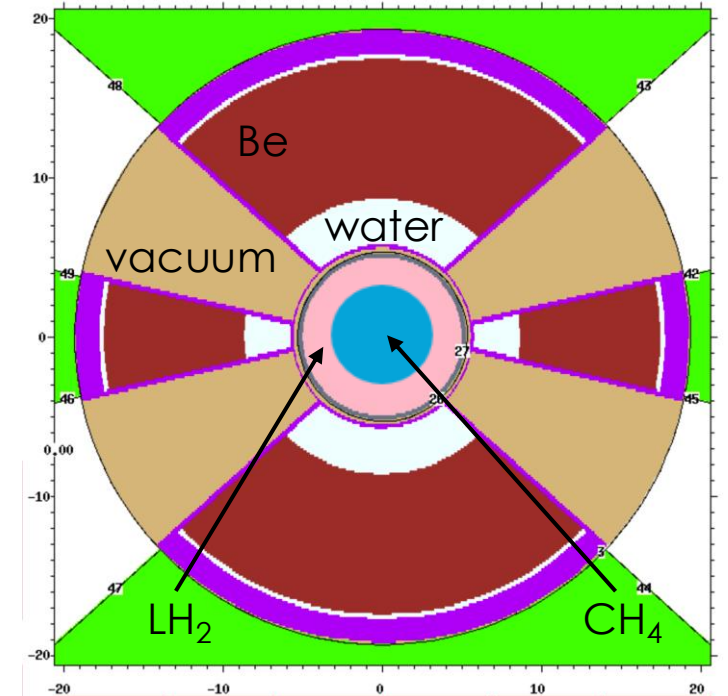
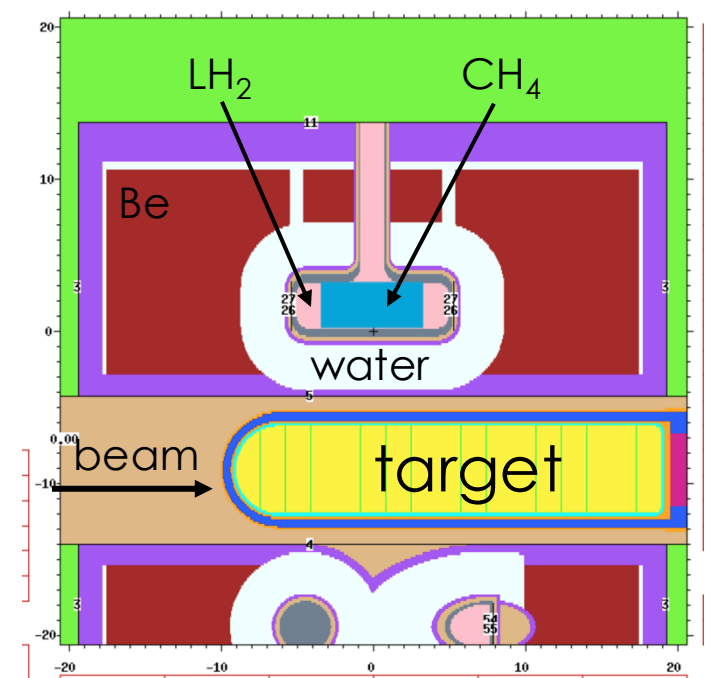
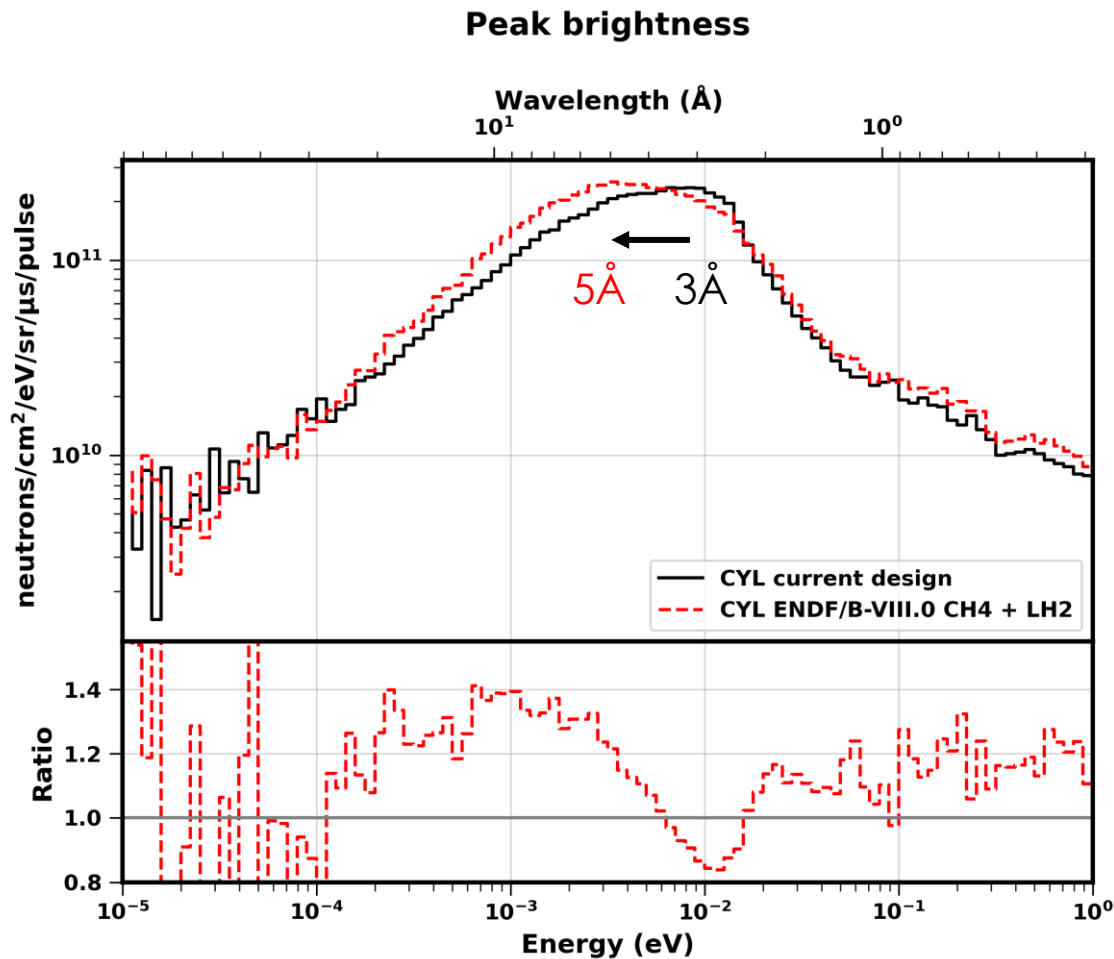


Solid CH₄ does not perform better than the current LH₂ design, however...



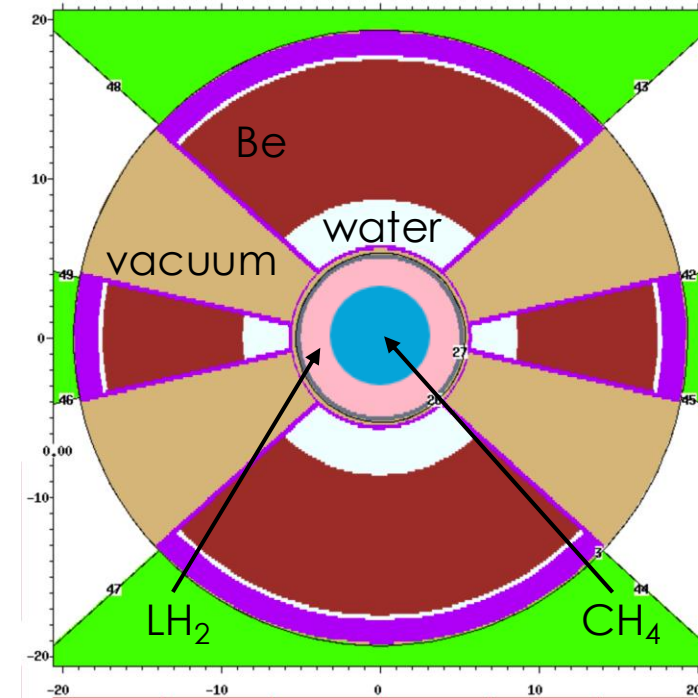
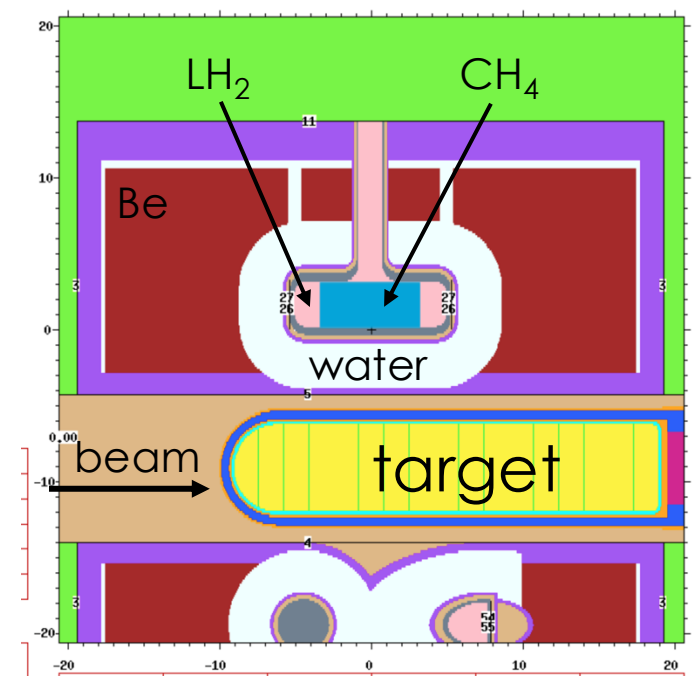
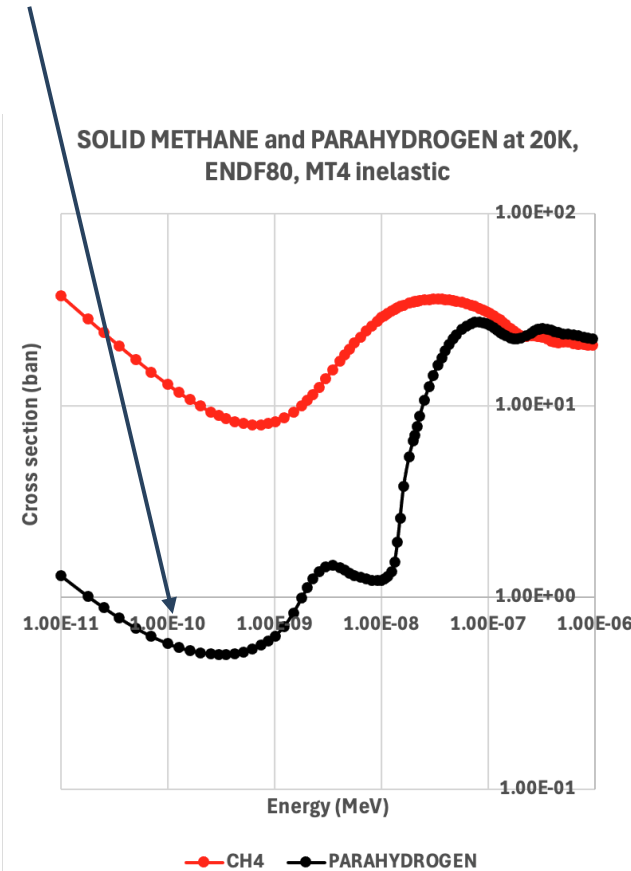
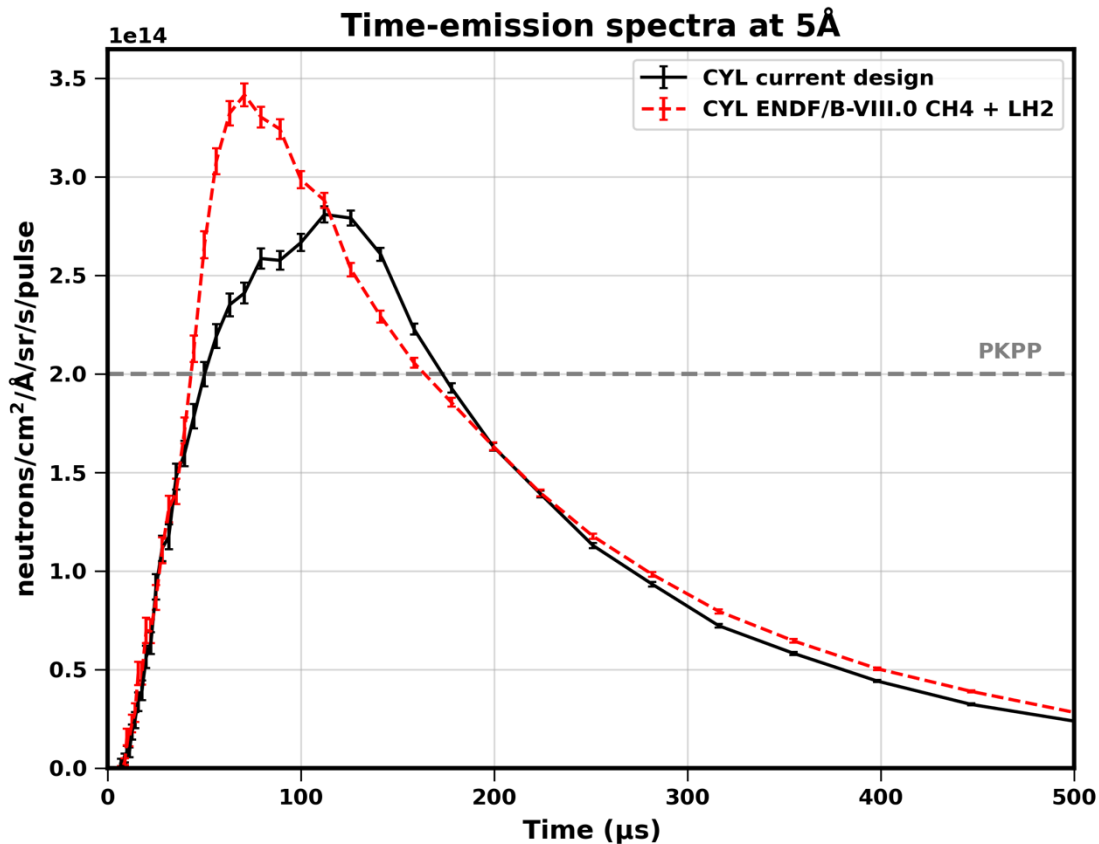
Solid methane CH₄

A combination of central region (radius of 3 cm) of CH₄ at 22K surrounded with parahydrogen at 20 K (2 cm) shows 40% gain in peak brightness at longer wavelengths



Solid methane CH₄

Taller & sharper pulses with 20% better time resolution due to a high-proton density core and a relatively transparent outer layer



Based on ENDF/B-VIII.0 scattering kernel smeth.40t at 22K

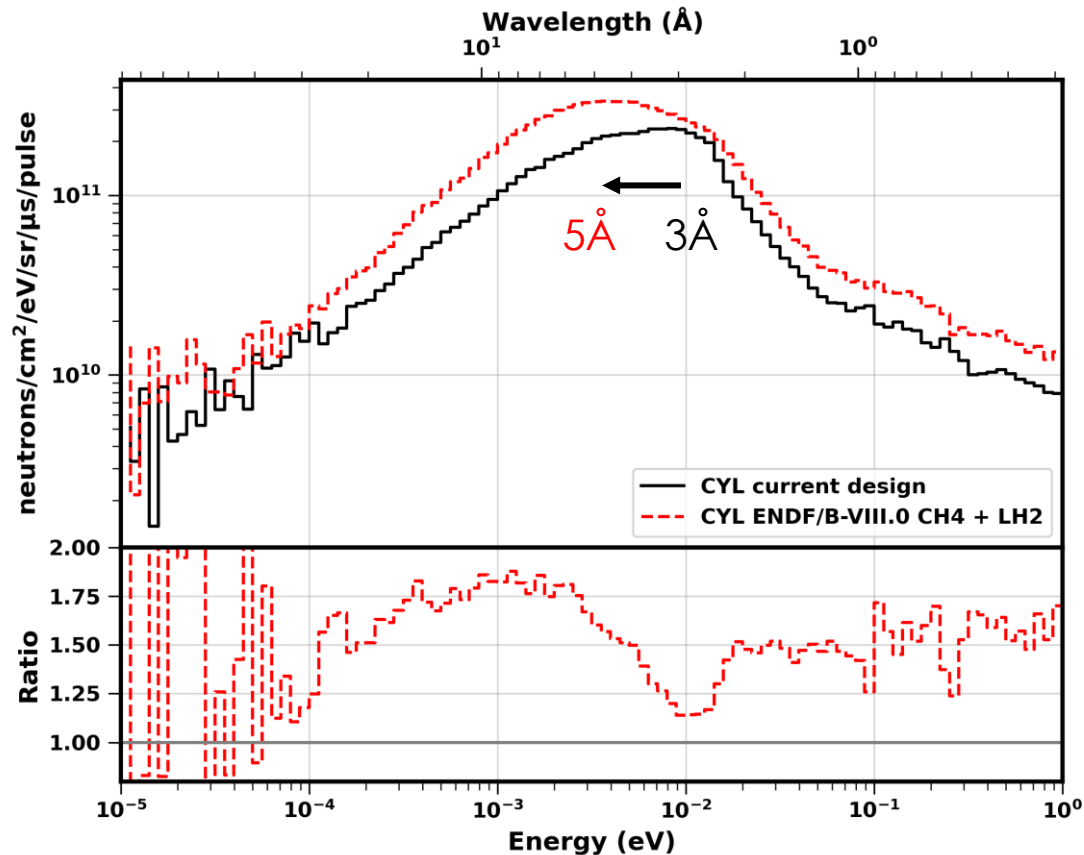
Solid methane CH₄ with additional STS upgrades

A factor of 2 improvement in peak brightness can be achieved with additional STS upgrades:

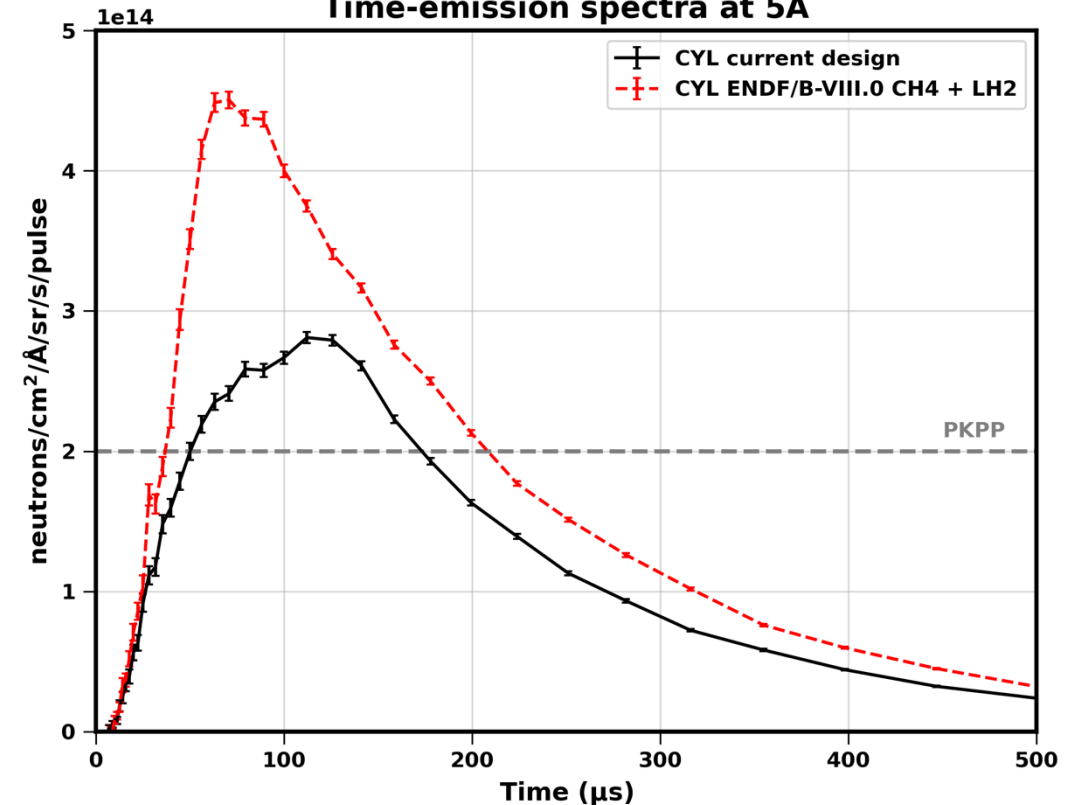
- +5% Increased premoderator temperature
- +5% D₂O cooling of the target and shielding
- +10% More focused proton beam on target

- +5% Increased target height
- +5% Reduced number of target segments
- +XYZ % Optimized design

Peak brightness

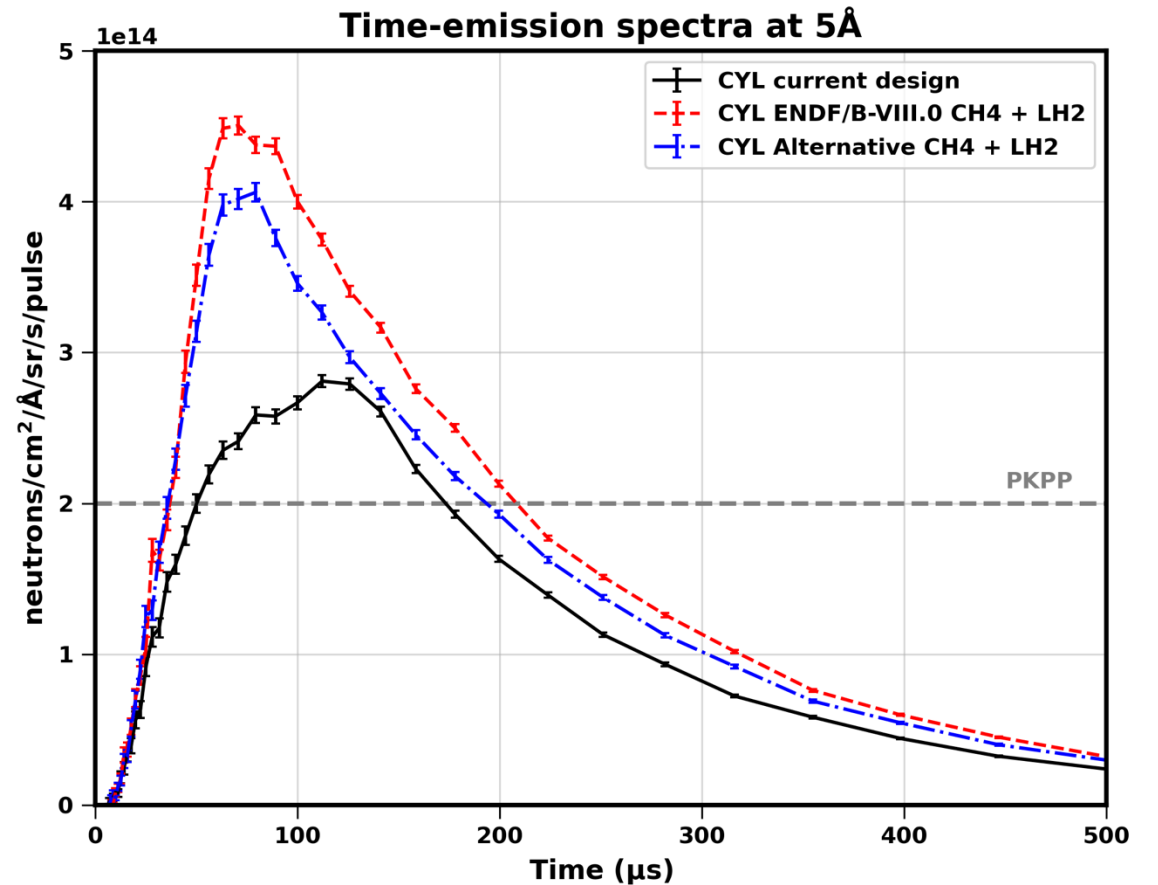
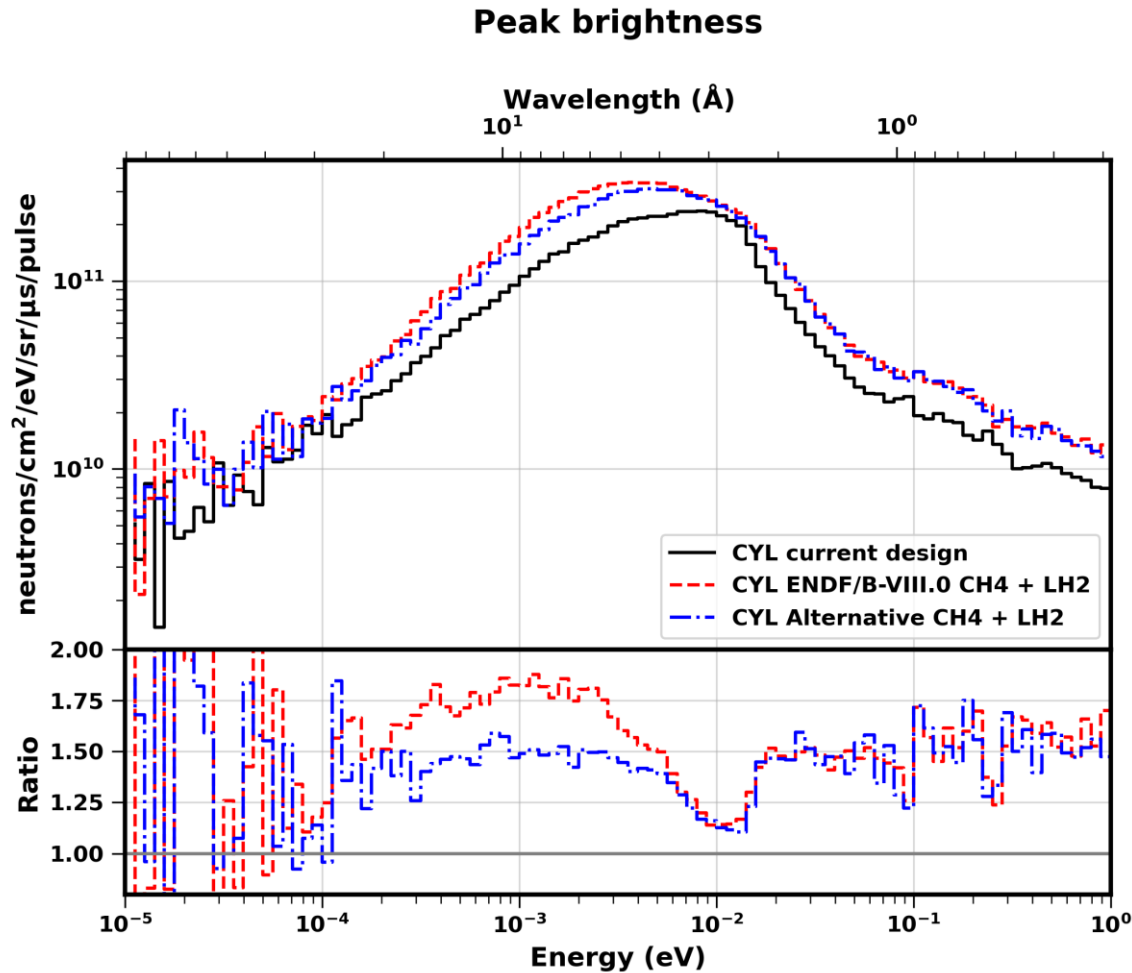


Time-emission spectra at 5 Å



Alternative scattering kernels

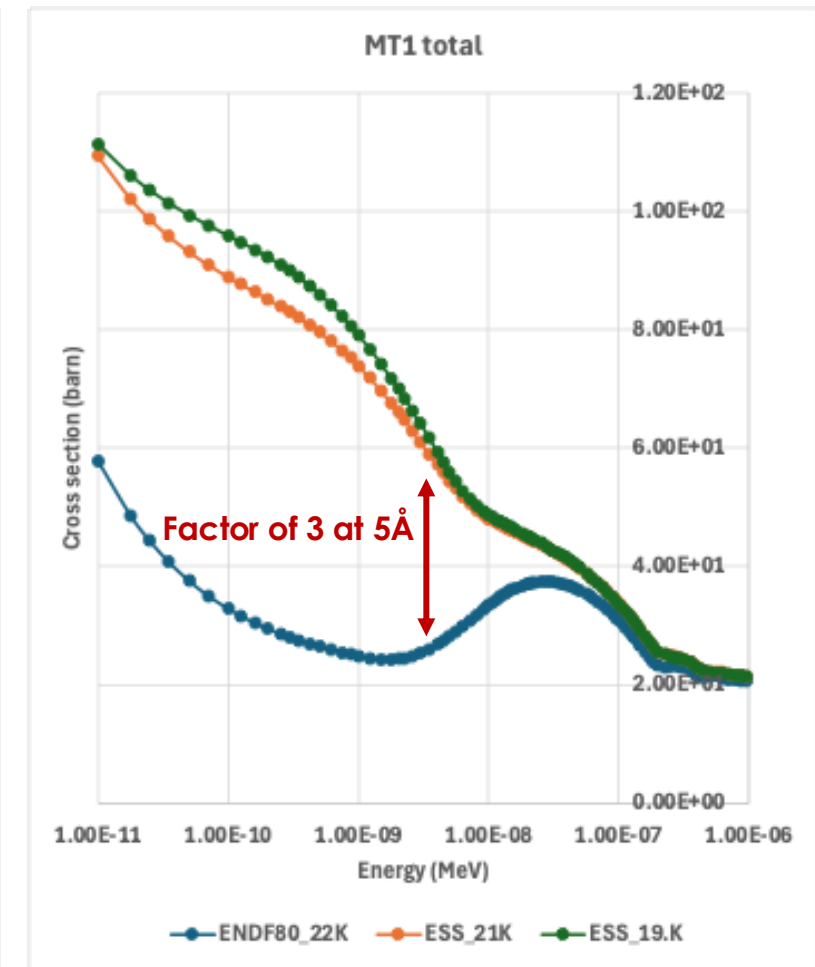
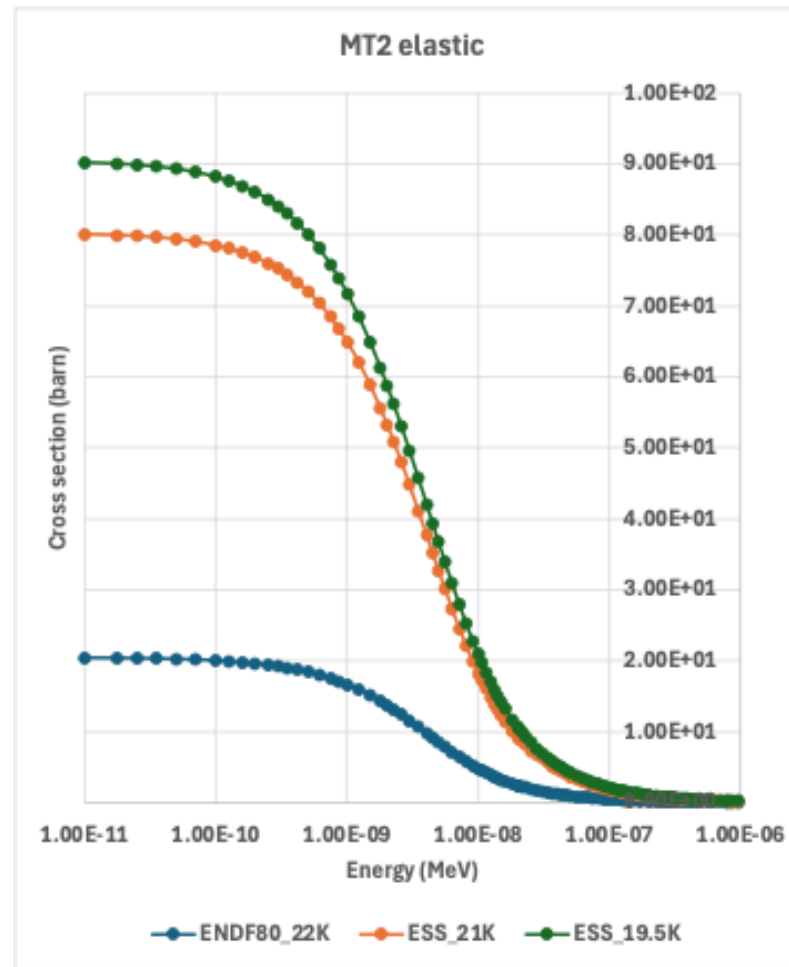
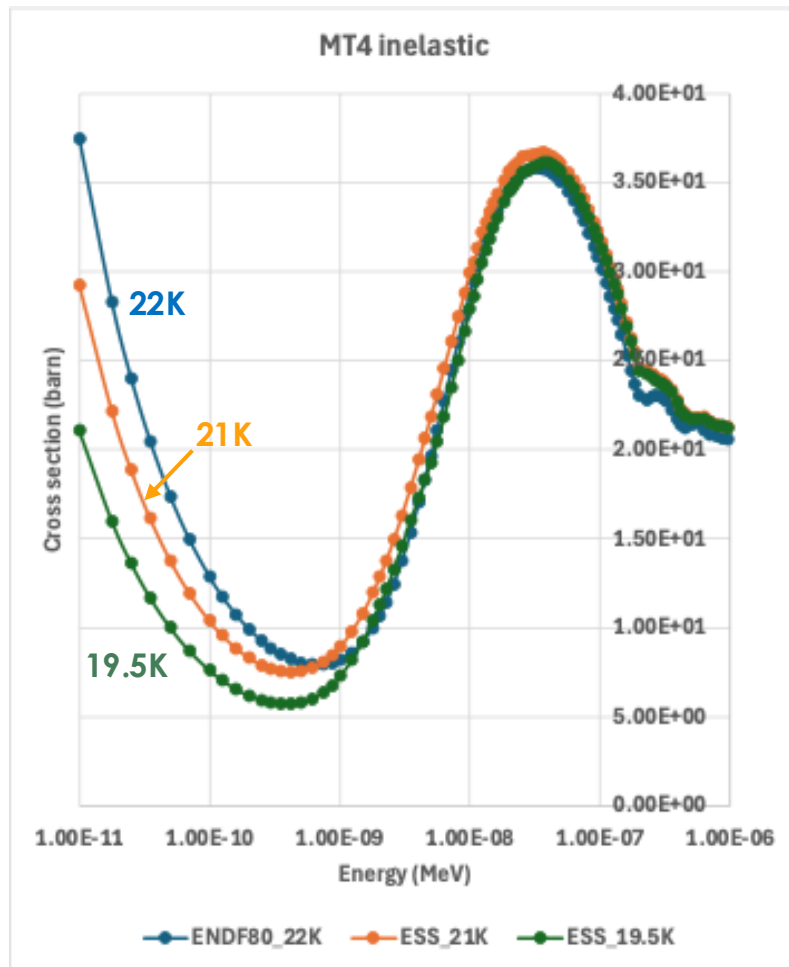
- Smaller performance gains with alternative scattering kernels (21K)



Alternative scattering kernels

- A newer set of scattering kernels for solid methane at 21K (phase I) and 19.5K (phase II) available at ESS GitHub, as of March 24, 2026:

https://git.ess.dk/spallation-physics-group/methane-tsl-libraries/-/blob/main/ace_files



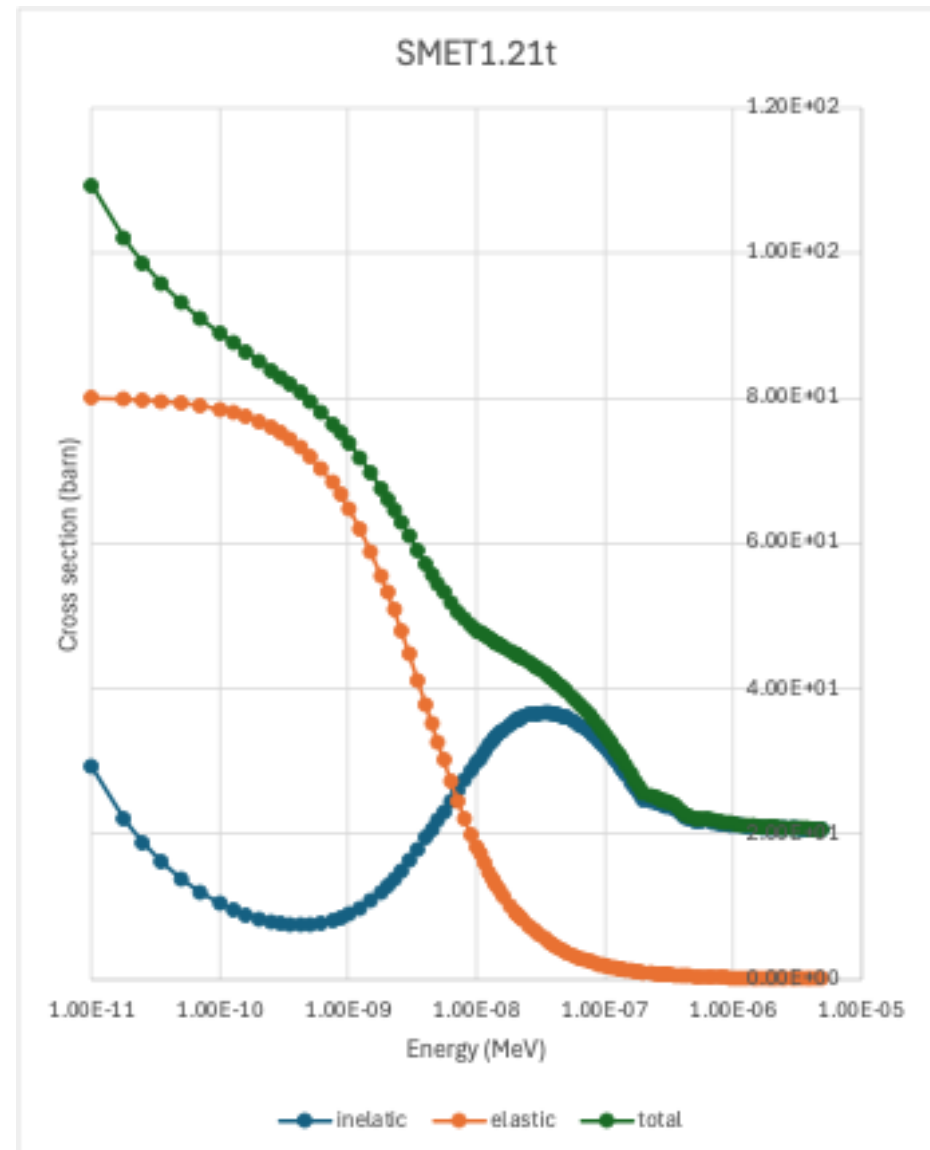
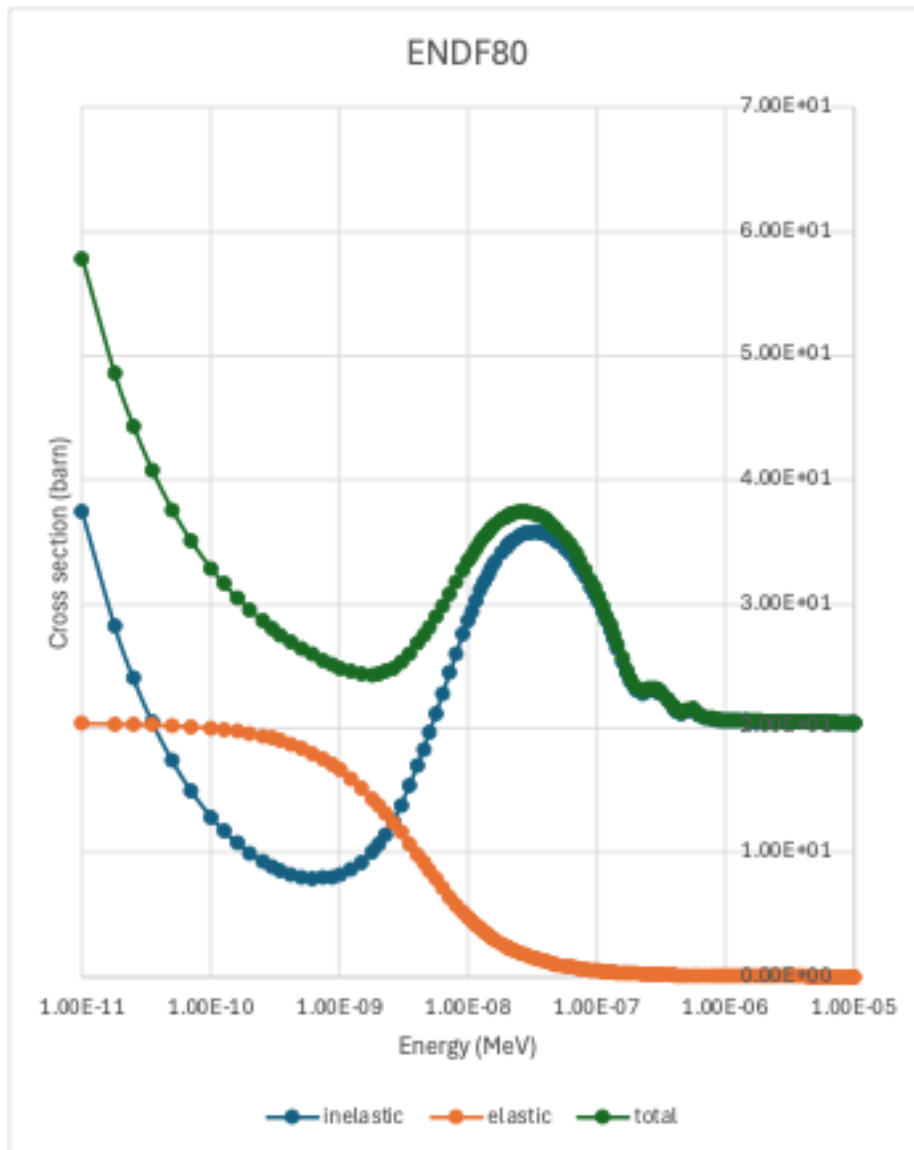
Conclusion

- A promising design of solid methane CH_4 / supercritical parahydrogen LH_2 moderator design presented
- Based on ENDF/B-VIII.0
 - Non-optimized CH_4/LH_2 moderator design provides up to 40% higher peak brightness at longer wavelengths with sharper pulses and 20% better time resolution
 - Optimized CH_4/LH_2 moderator design with other upgrades could potentially lead up to a factor of 2 gain at 5 Å
- Gains are smaller with alternative CH_4 scattering kernels
- Difference in elastic cross sections needs to be clarified
- This study represents an excellent case for moderator test stations



Thank you for your attention

Alternative scattering kernels

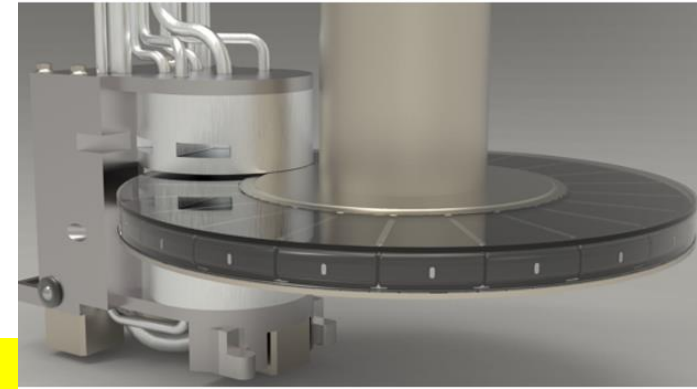


FTS and STS



FTS (upgraded)

- Short ($<1 \mu\text{s}$) proton pulses
- 1.3 GeV protons
- 45 pulses/second
- 1.8 MW, ramping up to 2 MW beam power
- 44.4 kJ per proton pulse
- Hg target
- Large beam footprint (140 cm²)
- 4 moderators (water & hydrogen)
- Moderator viewed area 10 x 12 cm²
- Coupled & decoupled moderators
- In operation since 2006

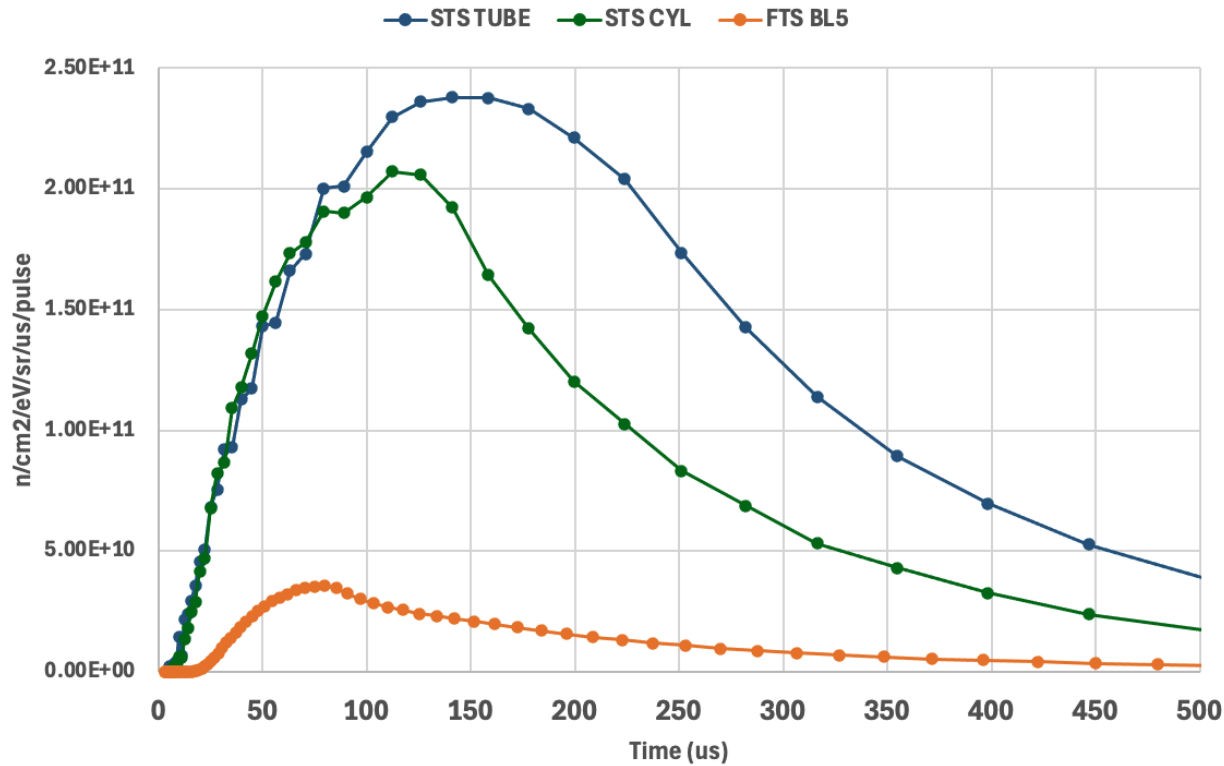


STS

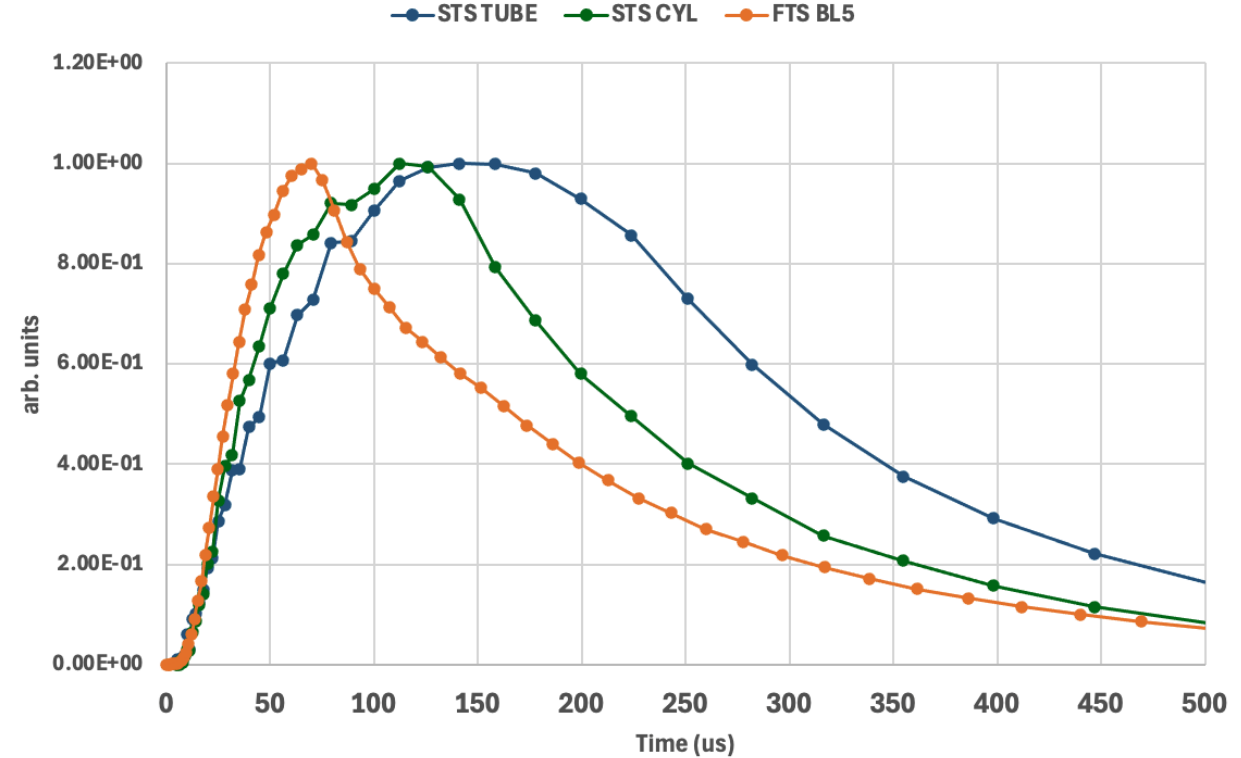
- Short ($<1 \mu\text{s}$) proton pulses
- 1.3 GeV protons
- 15 pulses/second
- 700 kW beam power
- 46.7 kJ per proton pulse
- Rotating W target (Inconel shroud, water cooled)
- Smaller beam footprint ($\sim 60 \text{ cm}^2$)
- 2 coupled moderators (para-hydrogen)
- Moderator viewed area 3 x 3 cm²
- Start of operation $\sim 2037-2039$

STS (0.7 MW) / FTS (2 MW)

Time-emission spectra at 5A



Time-emission spectra at 5A



FWHM at 5 A:

FTS = 145 us

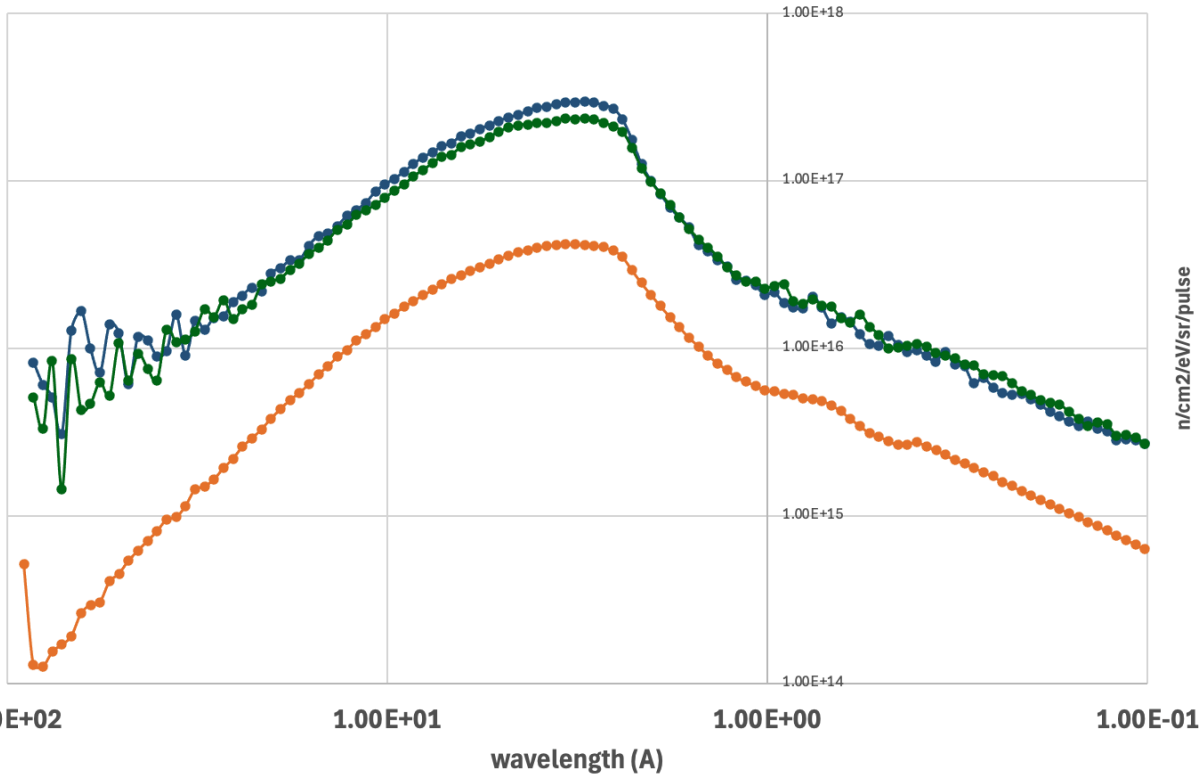
STS TUBE = 270 us

STS CYL = 200 us

STS (0.7 MW) / FTS (2 MW)

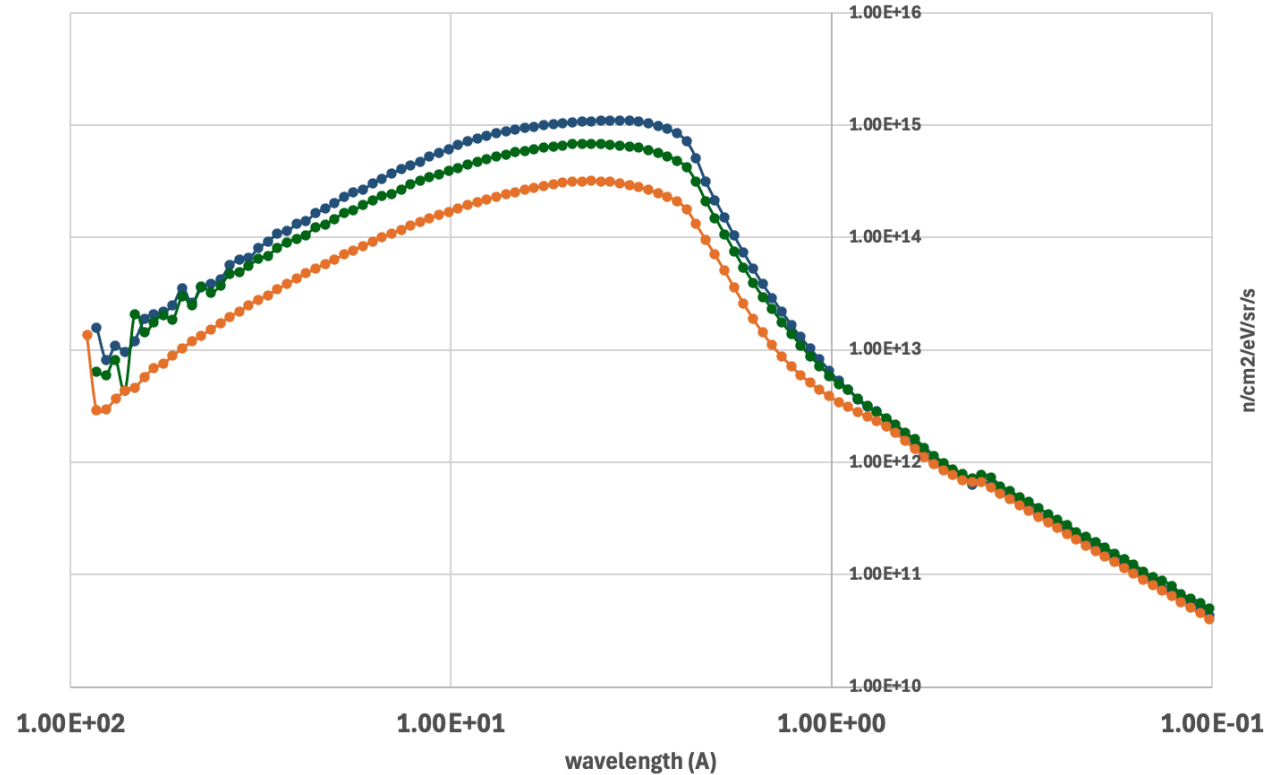
PEAK per pulse

— STSTUBE — STS CYL — FTS BL5



TINT per second

— STSTUBE — STS CYL — FTS BL5

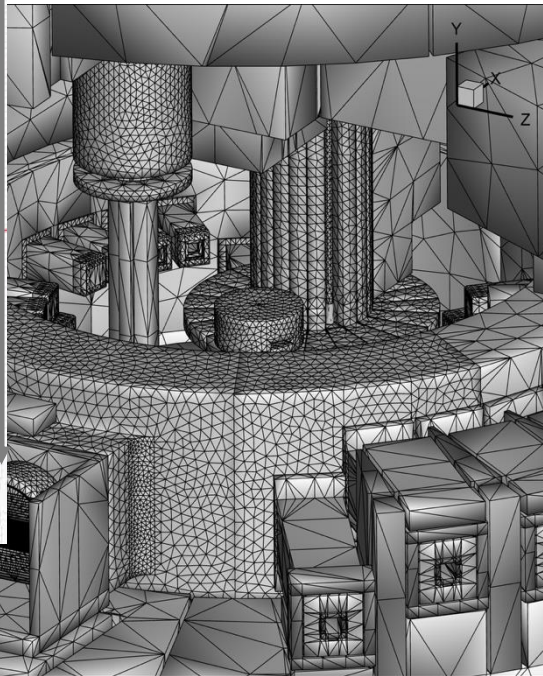
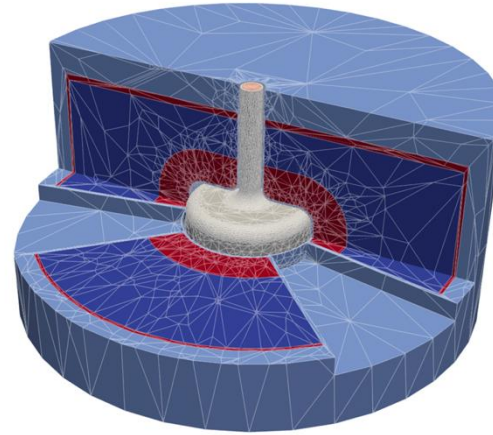
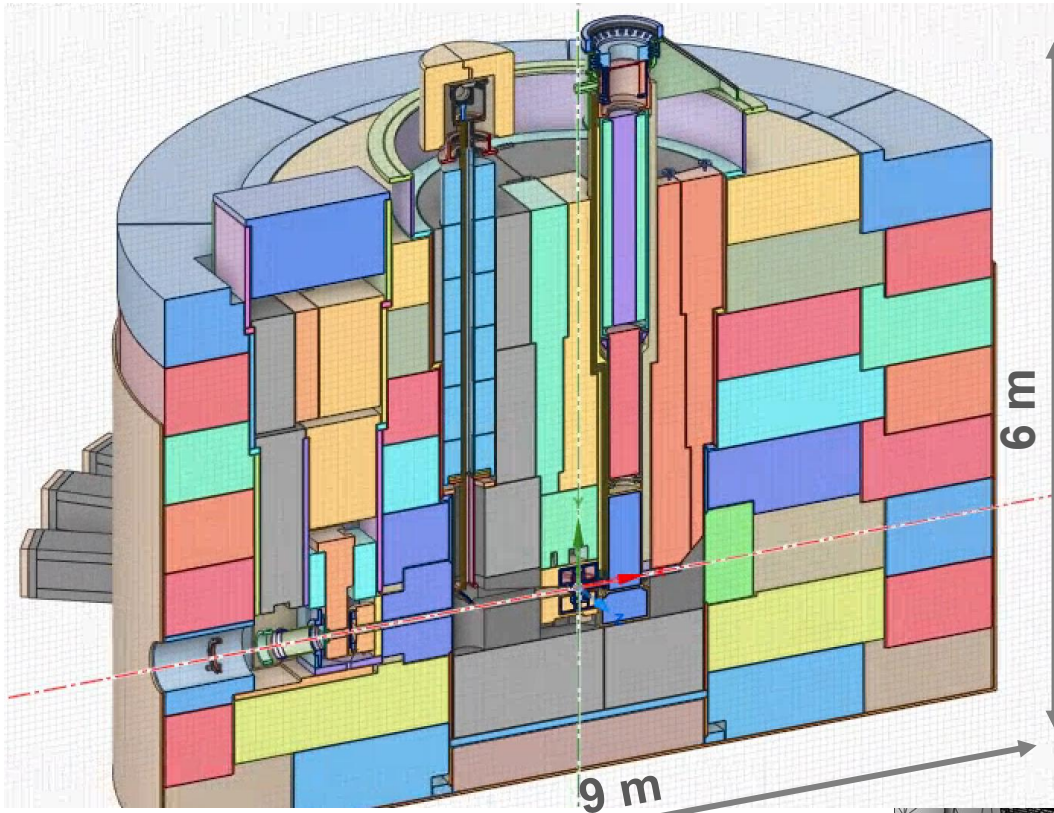


STS TUBE/FTS: PEAK per pulse at 5 Å = 6.7

STS TUBE/FTS: TINT per second at 5 Å = 3.4

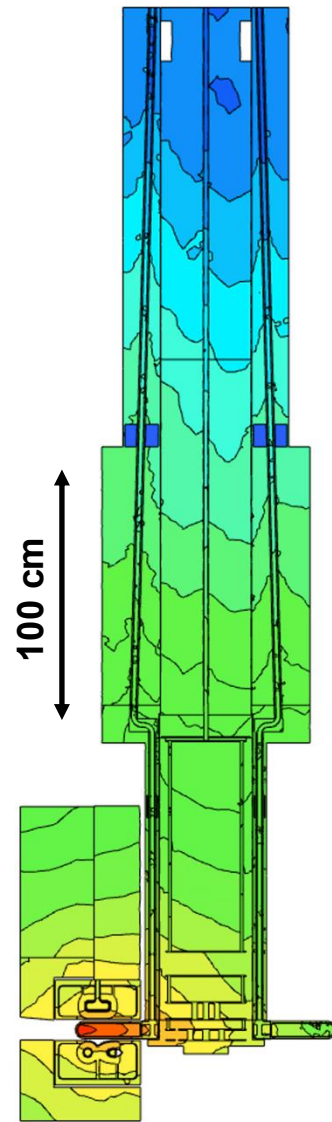
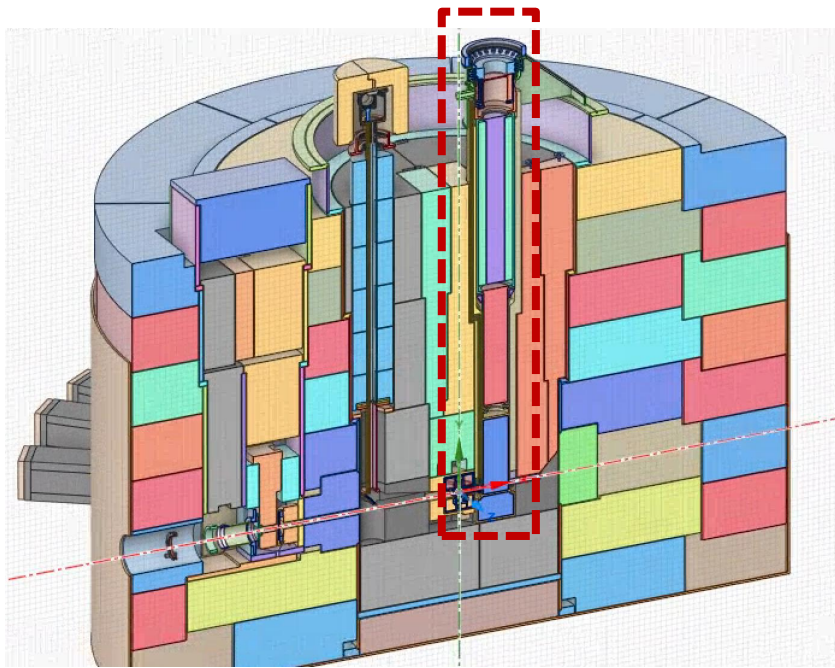
Extensive use of Unstructured Mesh (UM) at STS

- Modern radiation transport tools
- Automated CAD to MCNP conversion with Attila4MC
- Advanced & coupled optimization
- CADIS/FW-CADIS variance reduction



Case study II: Target Shaft

- Energy deposition



Cooling pipes and narrow streaming gaps



Starts with 1.3 GeV protons