Automating the coupled neutronics-structural stress optimization at ORNL's Second Target Station (STS)
-neutronics aspects

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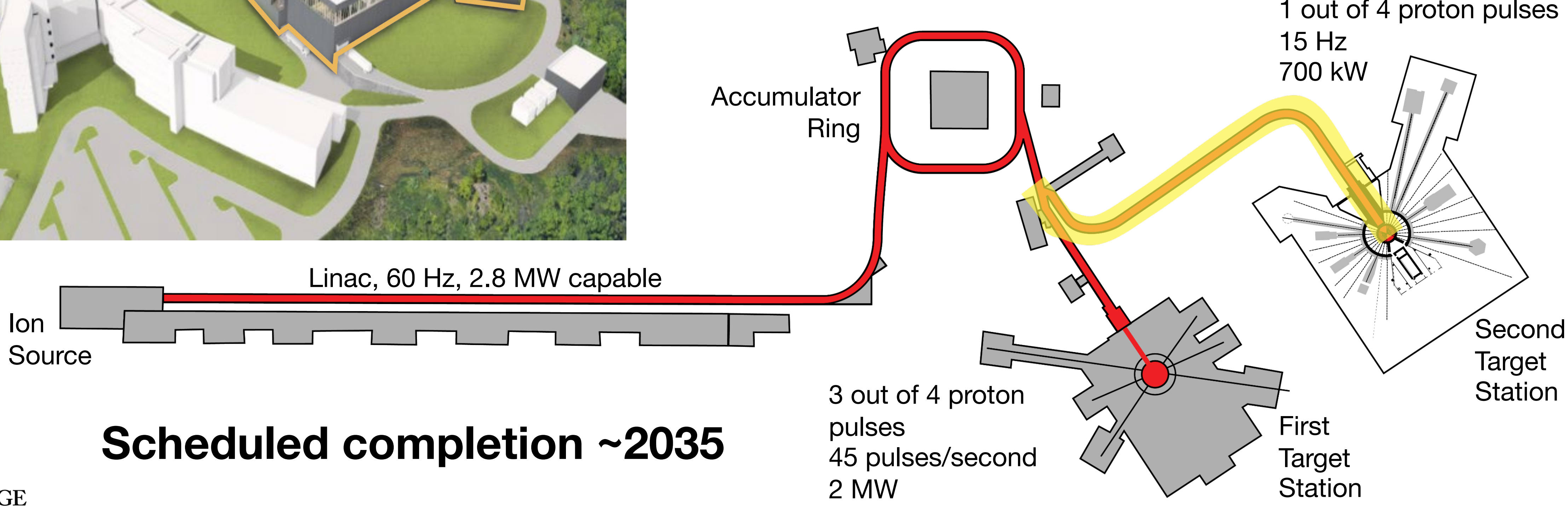
ORNL Second Target Station (STS)

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 ~2035

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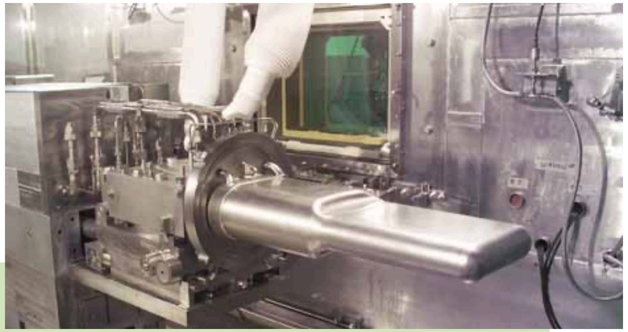
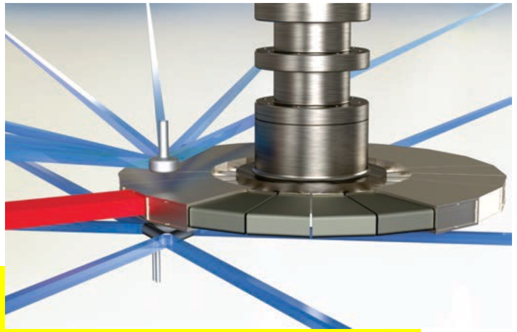
STS vs. FTS



FTS (upgraded)

- Short (<1 μs) 1.3 GeV proton pulses
- 45 pulses/second
- 2 MW beam power
- 44.4 kJ per proton pulse
- Large beam footprint (140 cm^2)
- Hg target
- 4 moderators (water & hydrogen)
- Moderator viewed area 10 x 12 cm
- Coupled & decoupled moderators
- In operation since 2006

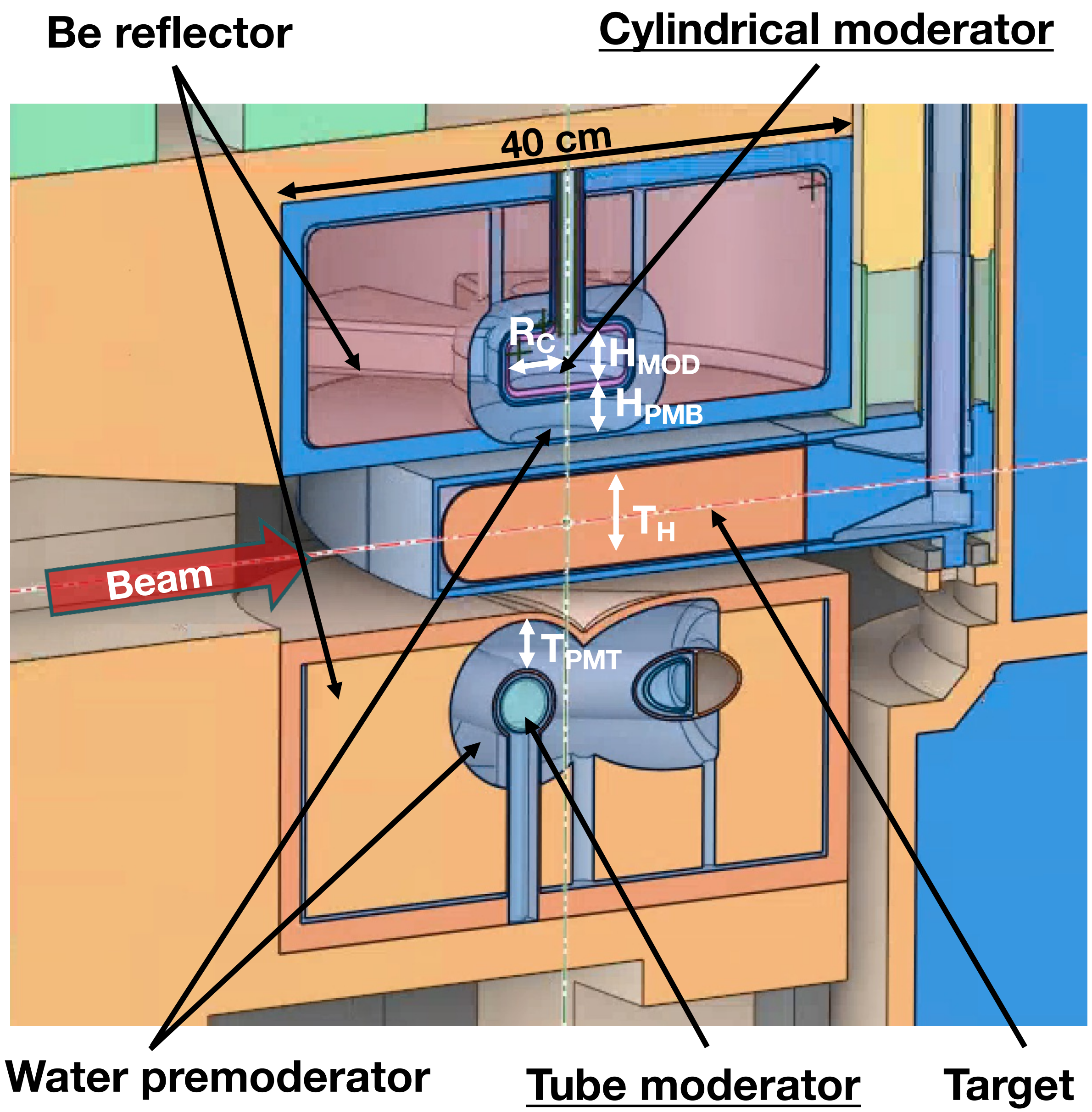


STS

- Short (<1 μs) 1.3 GeV proton pulses
- 15 pulses/second
- 700 kW beam power
- 46.7 kJ per proton pulse
- Smaller beam footprint (30-90 cm^2)
- W target (water cooled)
- 2 moderators (hydrogen)
- Moderator viewed area 3 x 3 cm
- Coupled moderators
- Scheduled commissioning ~2035
- **MODERN SIMULATION AND OPTIMIZATION TOOLS**

Target & Moderator-Reflector Assembly (MRA)

- Rotating W target
- 1.3 GeV proton beam (<1 μs)
- 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 (10 mm gap)
- Serve 12 + 6 instruments



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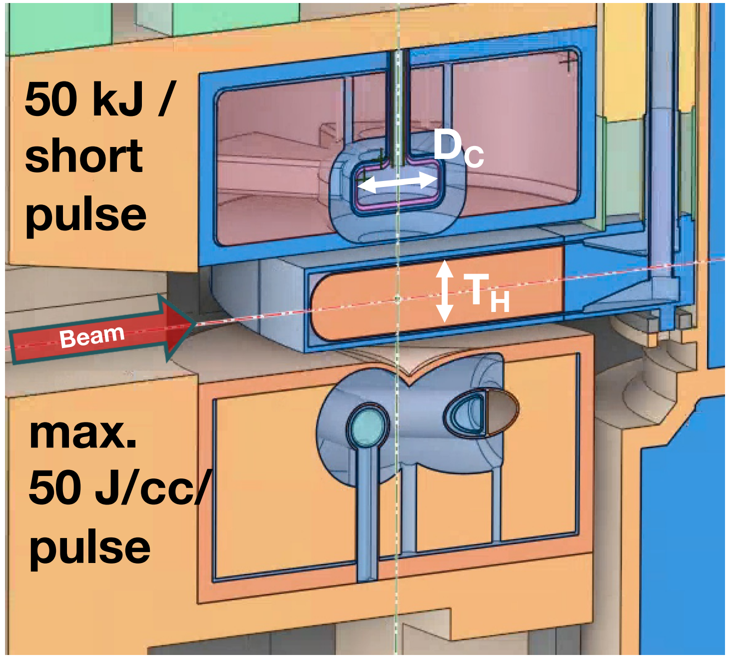
Goal of the STS design optimization

- **Maximize neutron brightness while maintaining structural integrity**
- **Multi-physics multi-parameter study**
- **Coupled neutronics and structural stress optimization**
  - Optimal parameters for separate neutronics and structural analyses can differ greatly
  - Improved structural integrity reduces neutronics performance
- **Problems with many design parameters**
  - Target and moderator dimensions
  - Beam footprint on target
- **Quantities span broad ranges in *E, t, L,* etc.**
- **Limited resources for such studies in the past**
- **Modern tools necessary for efficient optimization**



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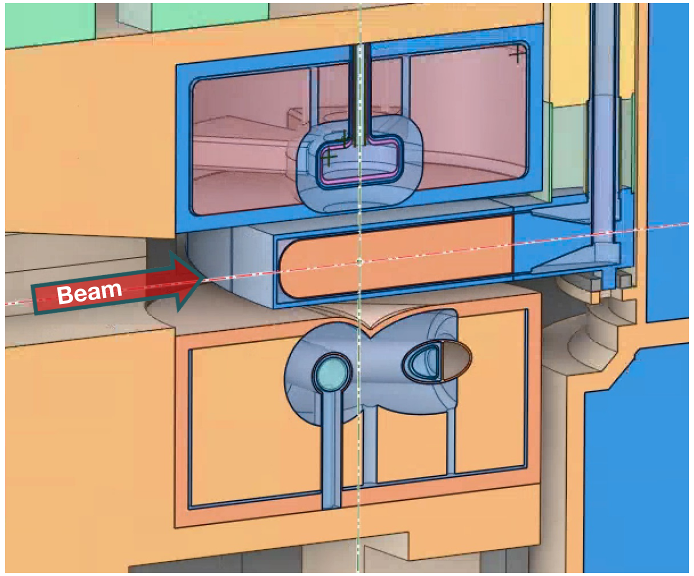
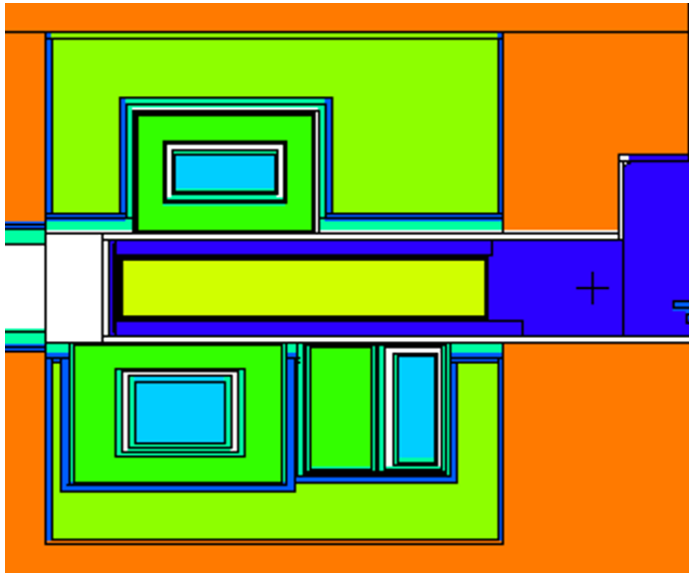
Once upon a time…



Solid CAD model

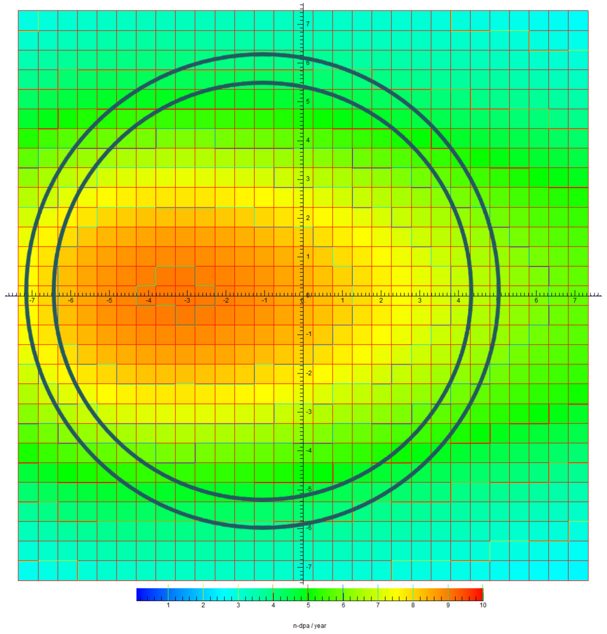


Neutronics MCNP model

Constructive Solid Geometry (CSG)
Simplified geometry
Details omitted
Manual model conversion
Time demanding
Prone to human errors

Cartesian mesh tallies

Low spatial distribution
Mixed materials at boundaries



Manual import for FEA
Data mapping
FEA

“optimization”

Maybe 2-3 iterations with a limited number of design parameters

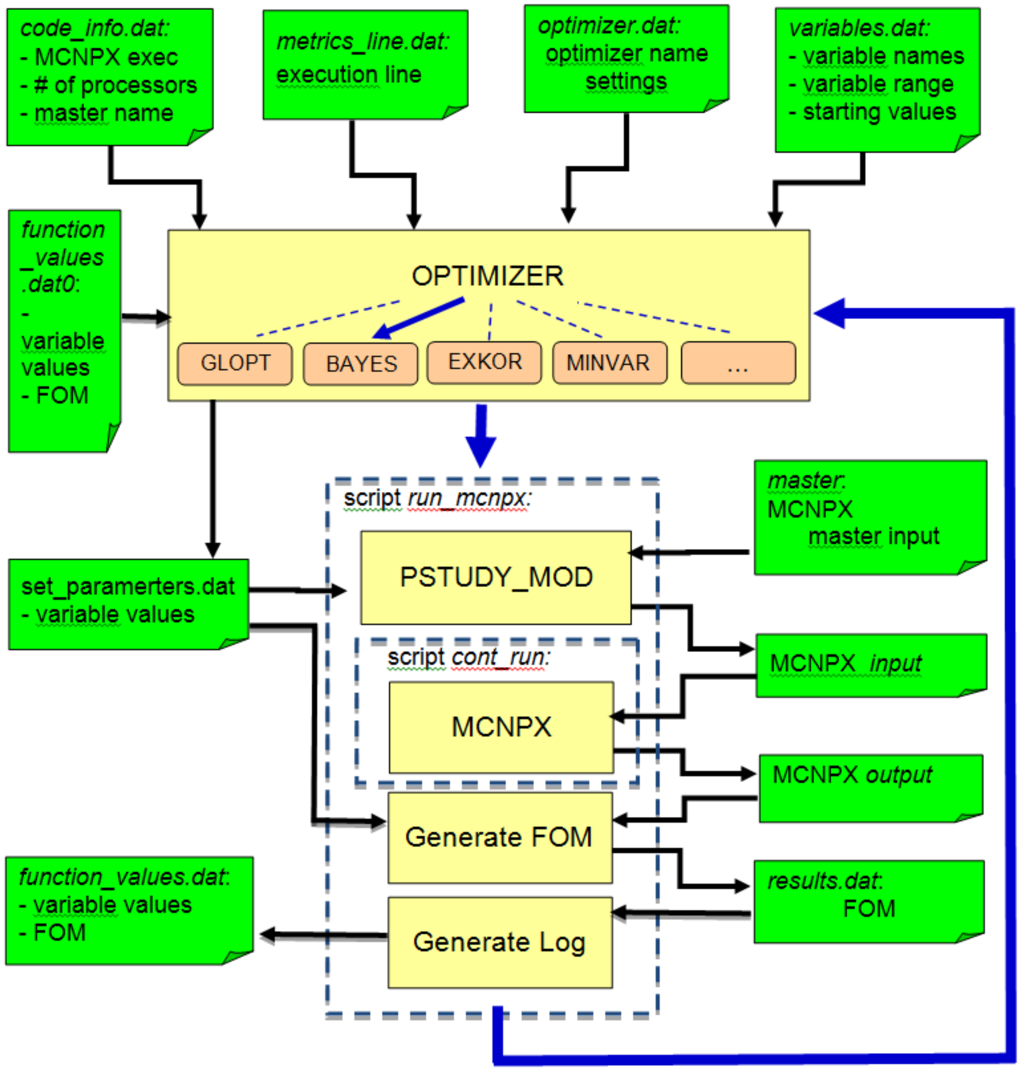
WEEKS AND MONTHS

Analysts working on different projects

Still actual???

Once upon a time…

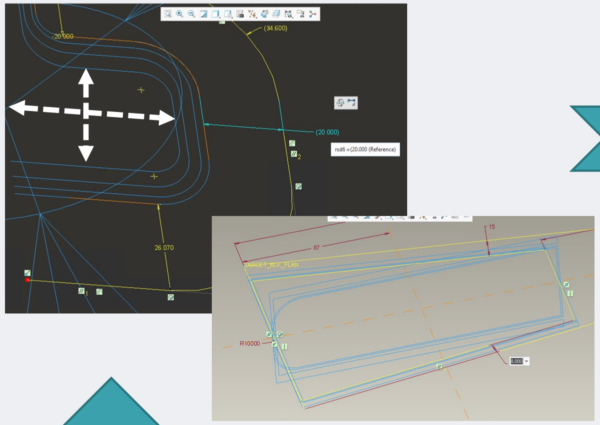
- **Different components often optimized separately**
- **Optimized component "A" rarely re-optimized after the design of a component "B" has changed**
- **Powerful tools, nevertheless!**
- **STS needs new tools**



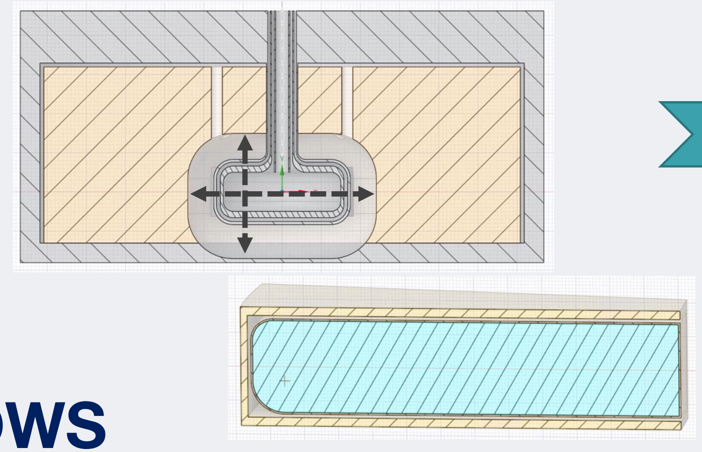
[1] F. B. Brown et al., Monte Carlo Parameter Studies and Uncertainty Analysis with MCNP5, PHYSOR-2004, *American Nuclear Society Reactor Physics Topical Meeting*, Chicago, IL, April 25-29 (2004)
[2] J. Mockus et al, *Bayesian Heuristic Approach to discrete and Global Optimization*, Kluwer Academic Publishers, Boston/London/Dordrecht (1996).

Unstructured mesh based automatic optimization workflow

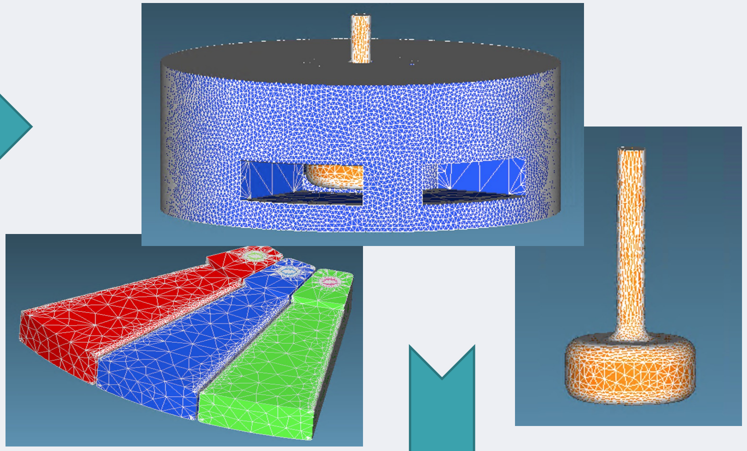
Parametrization with CREO



Filling volumes with SpaceClaim

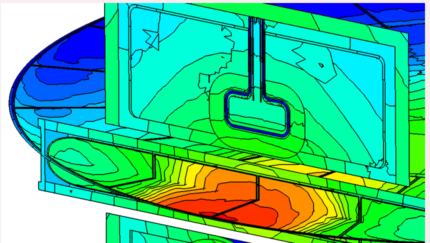


Unstructured Mesh (UM) generation with Attila4MC

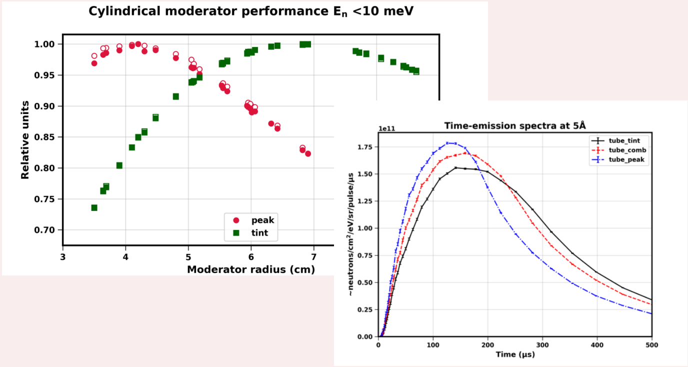


WINDOWS

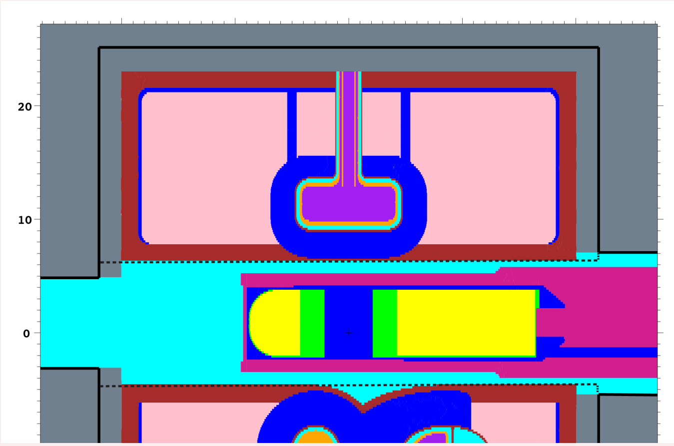
LINUX



Sierra & Cubit



Hybrid UM/CSG MCNP model



DAKOTA
Optimization

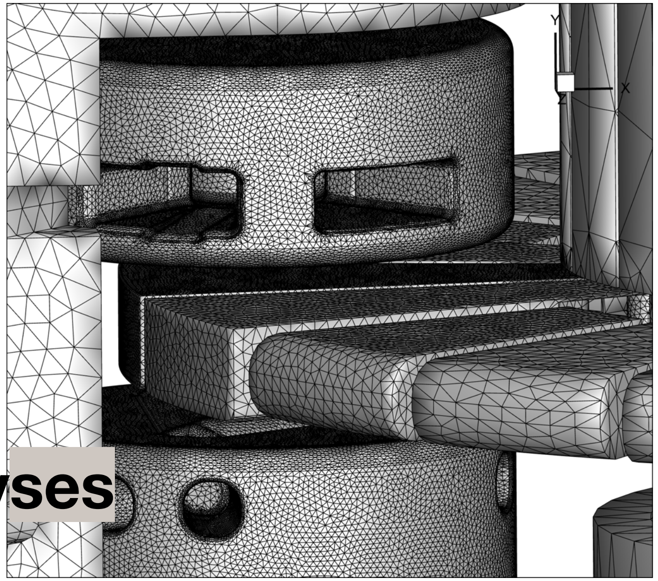
OPTIONAL **Structural analysis**

Neutronics analysis

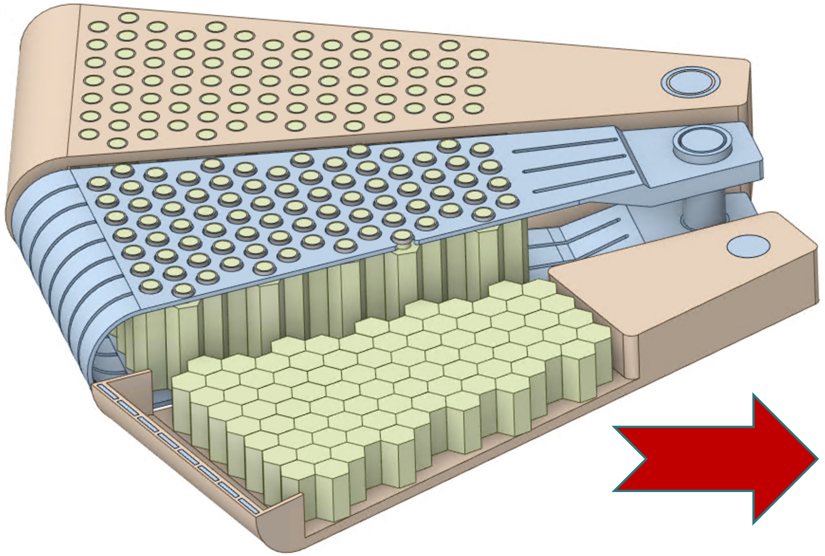
MCNP6

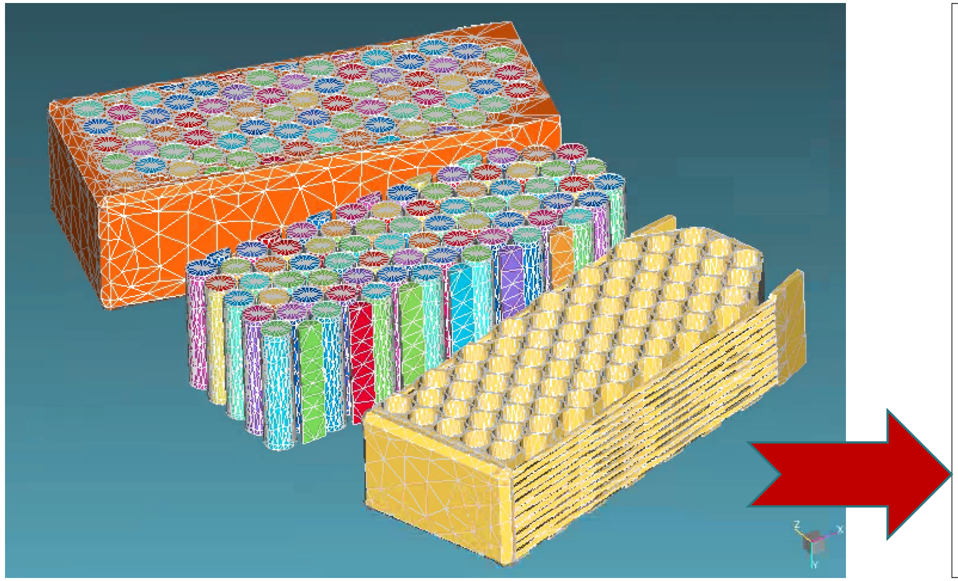
L. Zavorka et al., An unstructured mesh based neutronics optimization workflow, NIM A 1052 (2023) 168252.

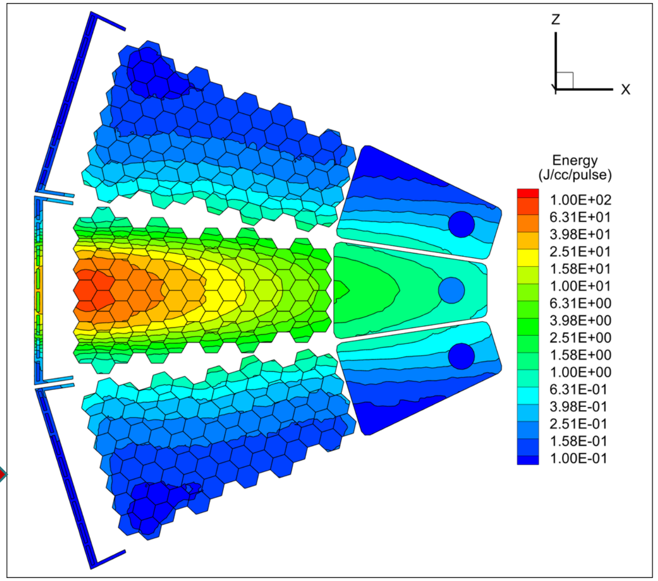
Unstructured mesh based automatic optimization workflow



- **Direct CAD to MCNP model conversion**
  - Fast, efficient, reduces potential for introducing errors
- **High-fidelity neutronics models**
  - High-quality data with high spatial resolution
- **Results (heating, dpa, …) available for subsequent analyses**
  - Direct export/import for structural stress/dynamic FEA

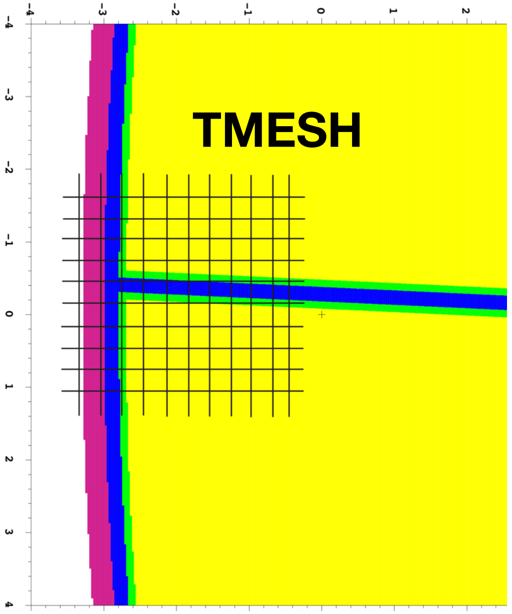


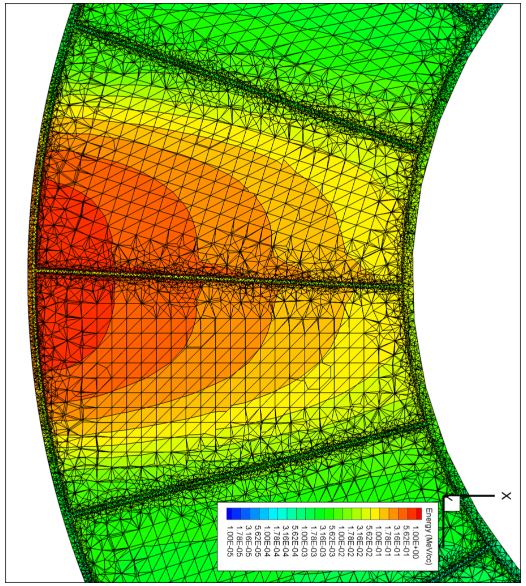


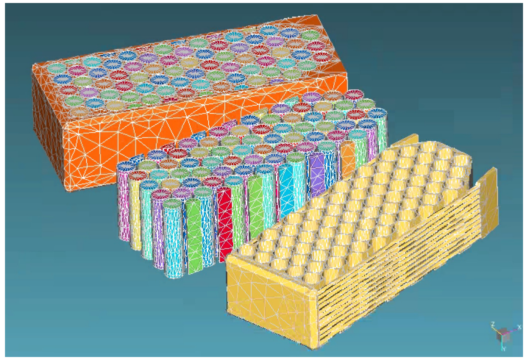


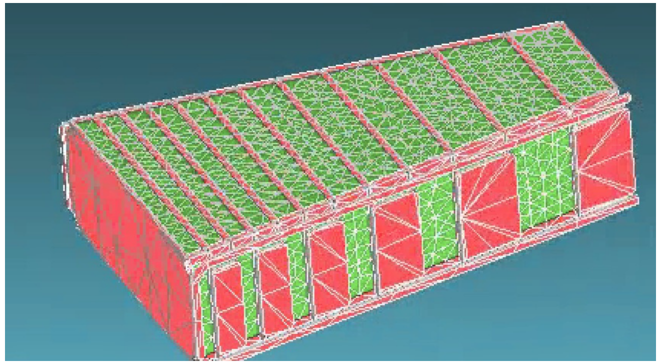
Unstructured mesh based automatic optimization workflow

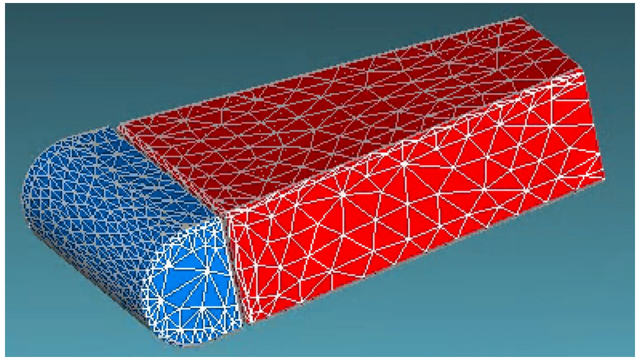
- **Departure from the cartesian mesh tallies**
  - UM serves as a mesh tally for energy deposition
- **Time to explore many more alternative target designs**
  - Quick throughput and decision to accept/reject

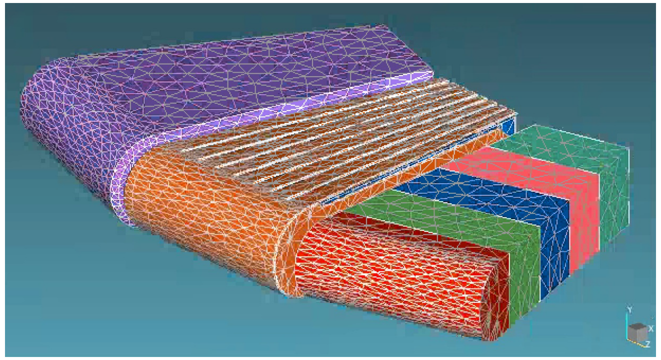


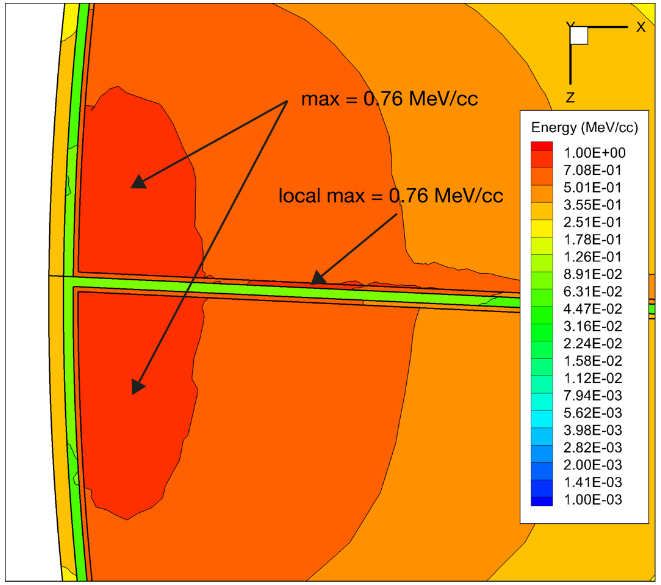




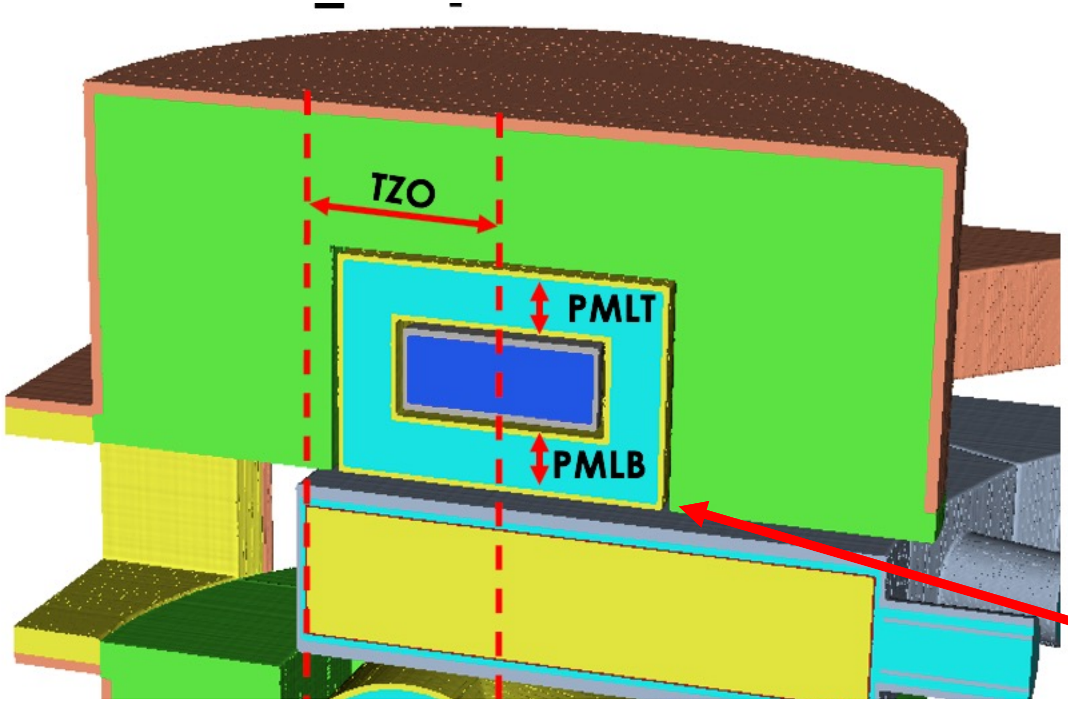


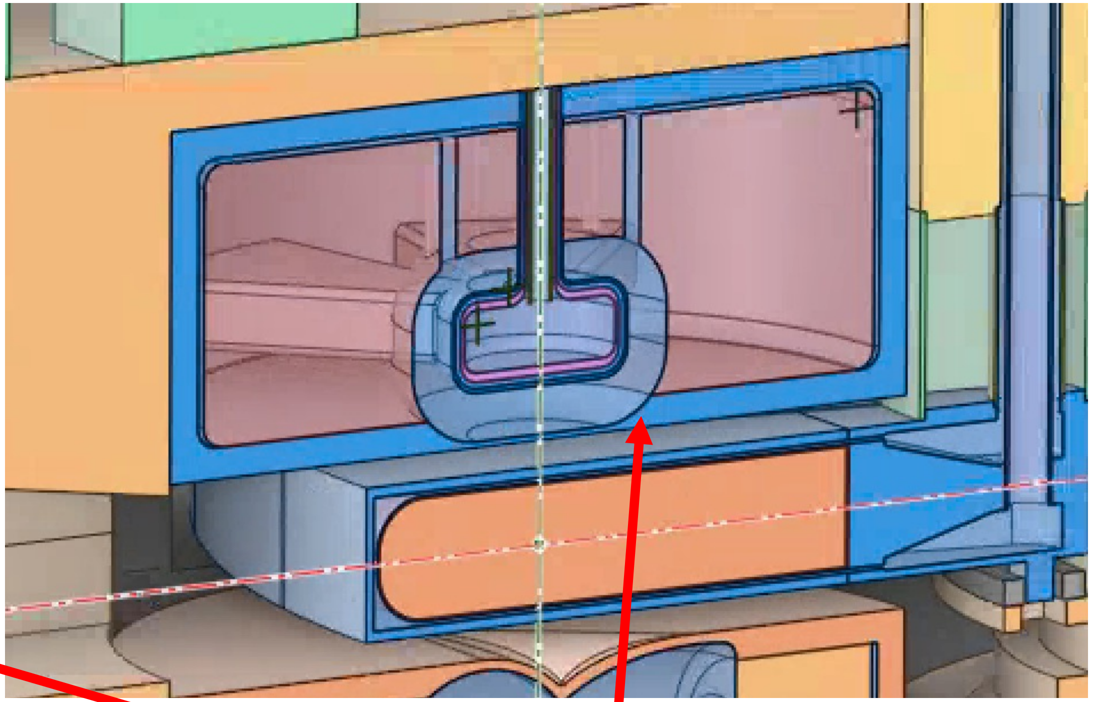






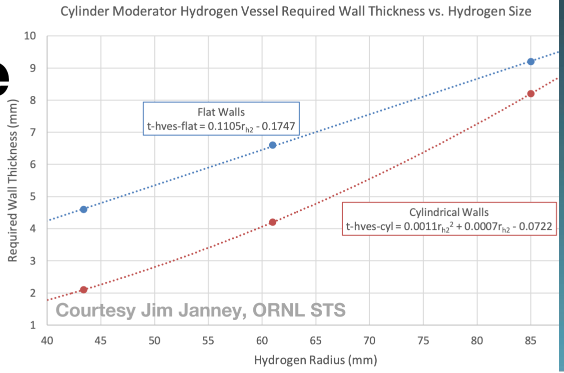
Original MCNP PSTUDY vs novel UM based optimization

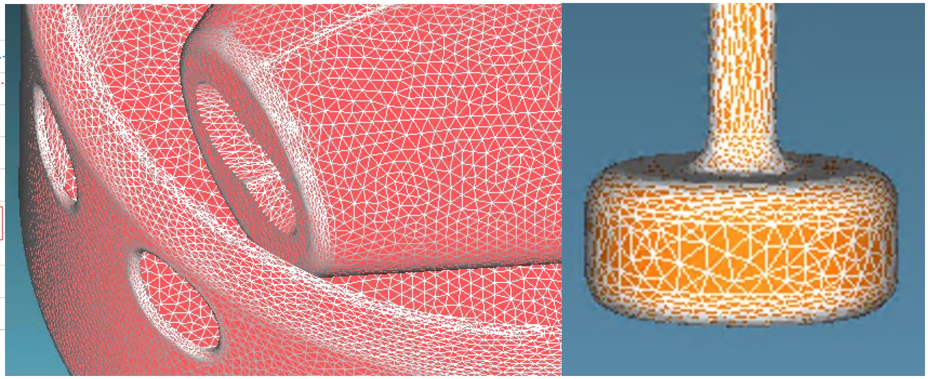




~10% performance difference when using a simple vs. high-fidelity model

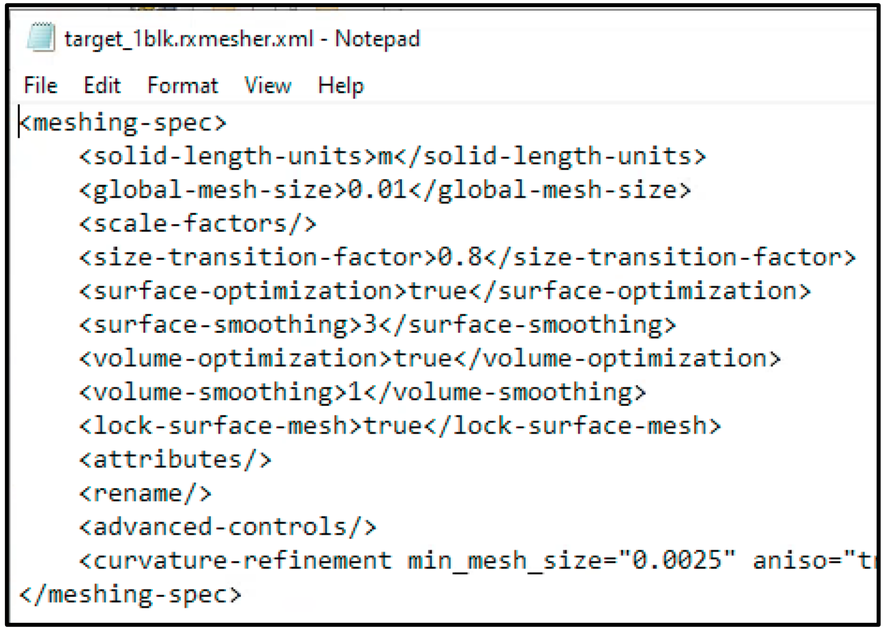
UM models contain variable thicknesses of the walls to withstand H_2/H_2O pressure





Unstructured mesh based automatic optimization workflow

- **Scripted model re-generation, conversion to UM, MCNP input generation**
  - CREO/Solidworks, SpaceClaim, Attila4MC, MCNP, Sierra, Dakota run from a command line
- **Controlled by in-house bat/bash scripts on Win/Linux**
- **On-line data analysis**
- **Captures errors, restarts if necessary**

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    <attributes/>
    <rename/>
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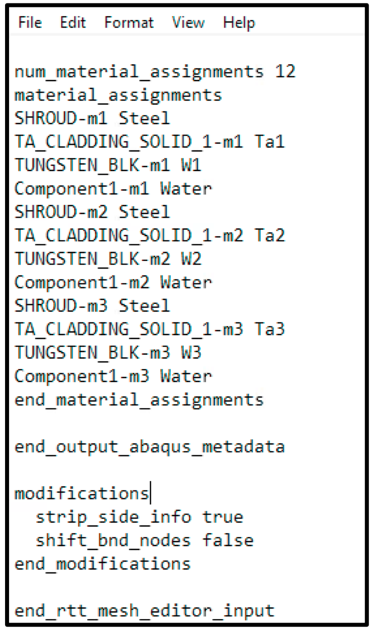
```




```
num_material_assignments 12
material_assignments
SHROUD-m1 Steel
TA_CLADDING_SOLID_1-m1 Ta1
TUNGSTEN_BLK-m1 W1
Component1-m1 Water
SHROUD-m2 Steel
TA_CLADDING_SOLID_1-m2 Ta2
TUNGSTEN_BLK-m2 W2
Component1-m2 Water
SHROUD-m3 Steel
TA_CLADDING_SOLID_1-m3 Ta3
TUNGSTEN_BLK-m3 W3
Component1-m3 Water
end_material_assignments

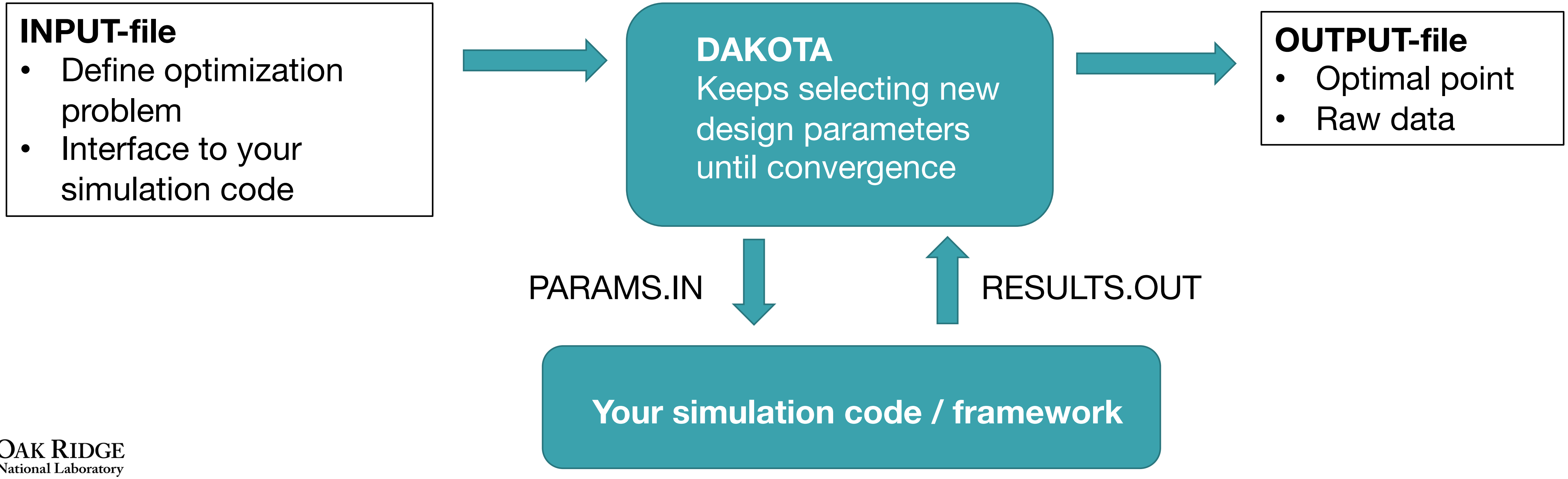
end_output_abaqus_metadata

modifications
  strip_side_info true
  shift_bnd_nodes false
end_modifications

end_rtt_mesh_editor_input
```

Unstructured mesh based automatic optimization workflow

- **Controlled by Dakota Software Toolkit**
- **State-of-the-art optimization methods (efficient global, …)**
  - Optimal solution found faster
- **Parameter and sensitivity study**

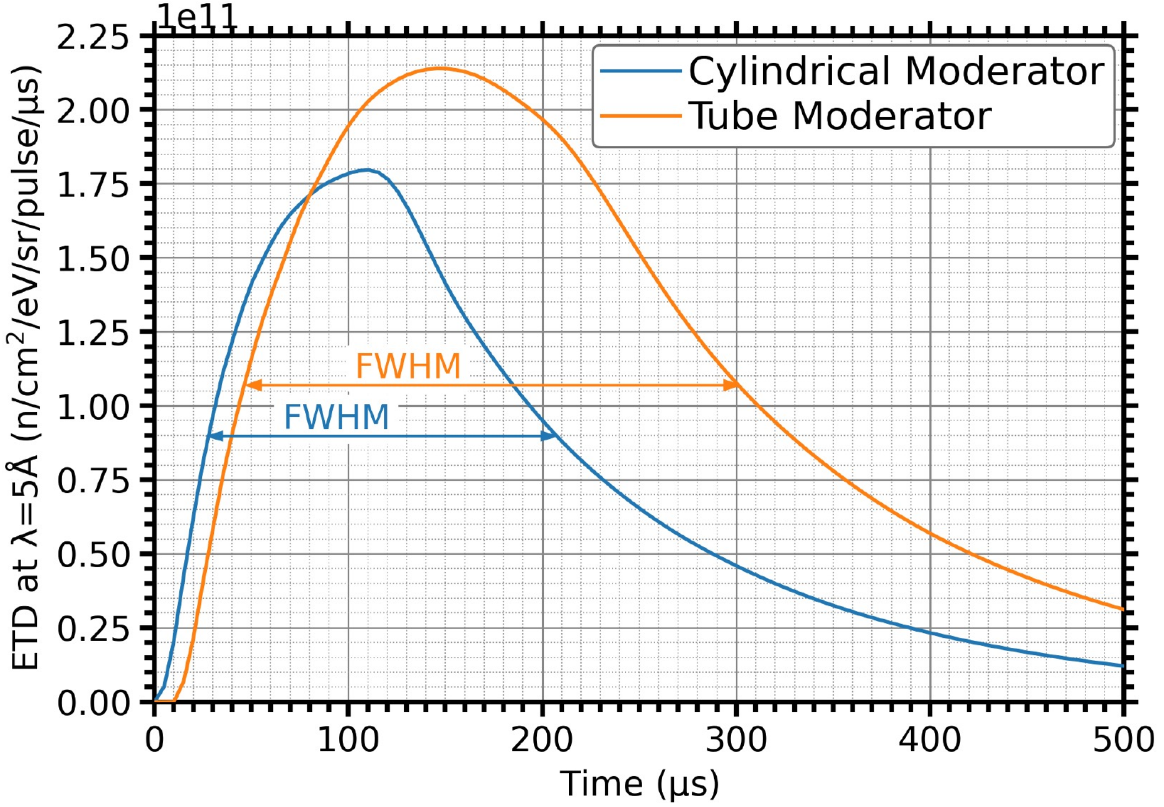


Key features

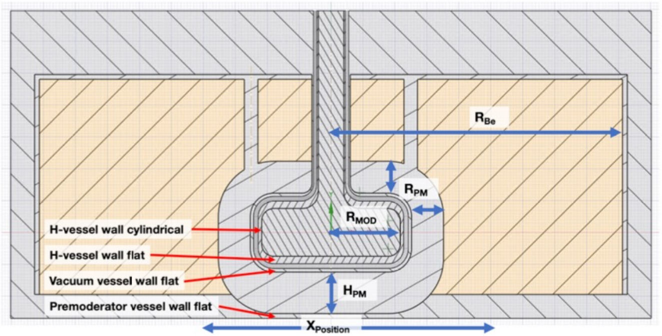
- **Only one parametric solid CAD engineering model is necessary**
  - Contains all the details + provides detailed results
  - The same CAD model is used both for neutronics and FEA
  - No manual conversion to an MCNP model (potential error reduction)
- **Coupled multi-physics multi-parameter optimization**
- **Reduction of the time per one iteration from weeks/months to hours**
- **Many more design options can be explored and analyzed**
- **Efficient optimization of the coupled problems with a large number of design parameters (>10)**

Applications

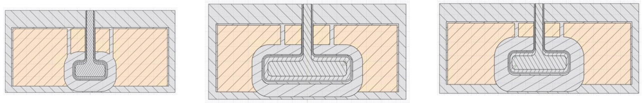
- **Neutronics optimization of the moderator-reflector assembly**
  - 10 geometry parameters
- **Neutronics and structural optimization of the target**
  - 6 geometry parameters
- **Coupled Target + Moderator + + Beam optimization**
  - 10 geometry parameters for the moderator
  - 12 geometry parameters for the target
  - 4 parameters for the beam on target

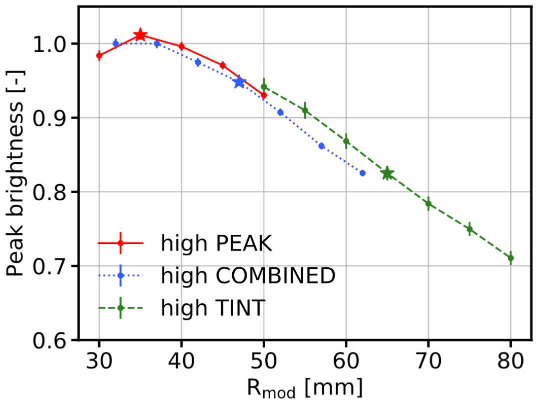


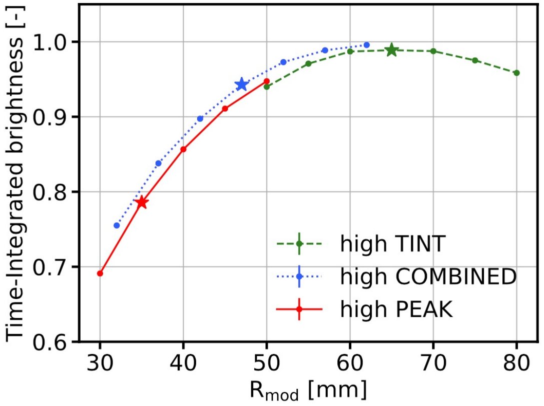
Neutronics optimization of the moderator-reflector

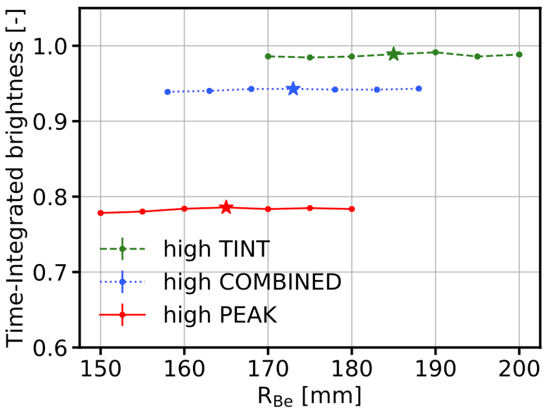


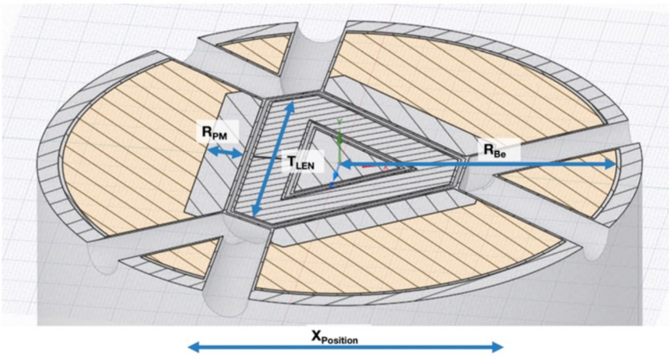
(a) Cylindrical moderator



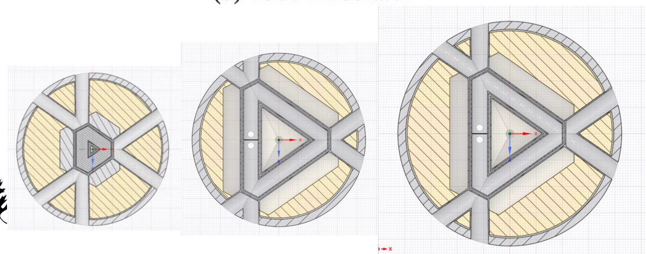


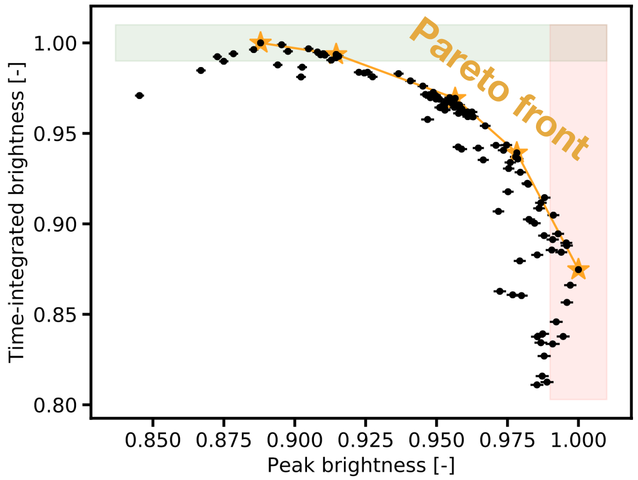


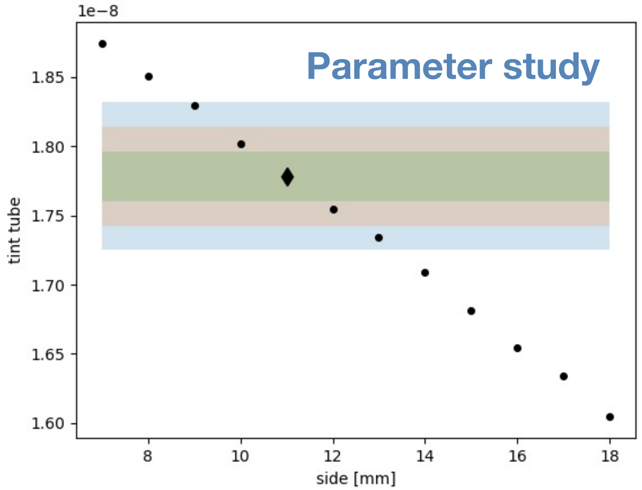




(b) Tube moderator





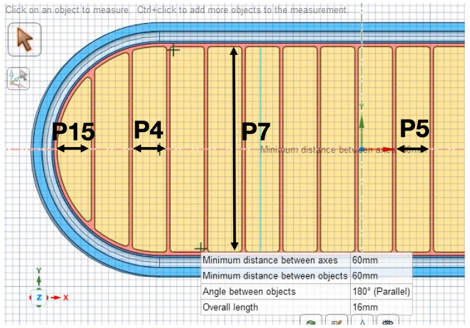


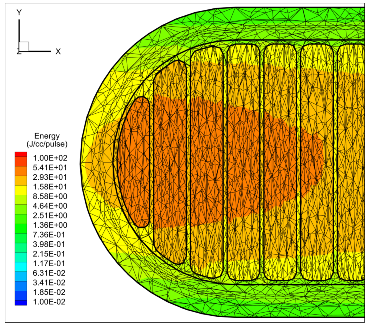
$$\text{Objective} = w_1 \times \frac{\text{PEAK}}{\text{PEAK}_{\text{ref}}} + w_2 \times \frac{\text{TINT}}{\text{TINT}_{\text{ref}}}$$

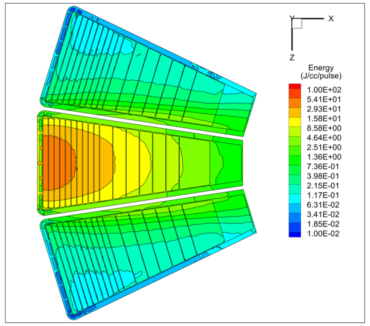
Set	w_1	w_2	T_{len} (mm)	R_{pm} (mm)	R_{Be} (mm)	X_{pos} (mm)	PEAK ($10^{-4}\text{cm}^{-2}\text{s}^{-1}$)	TINT (10^{-8}cm^{-2})
1	0	1	214	27.4	*220*	8	0.656 (88.7%)	1.944 (100%)
2	0.25	0.75	198	27.8	*220*	7	0.676 (91.5%)	1.931 (99.3%)
3	0.5	0.5	175	27.1	200	0	0.707 (95.7%)	1.874 (96.4%)
4	0.7	0.3	161	25.2	184	2	0.723 (97.8%)	1.826 (93.9%)
5	0.85	0.15	136	*25*	*180*	3	0.739 (100%)	1.700 (87.5%)
6	1	0	136	*25*	*180*	3	0.739 (100%)	1.700 (87.5%)

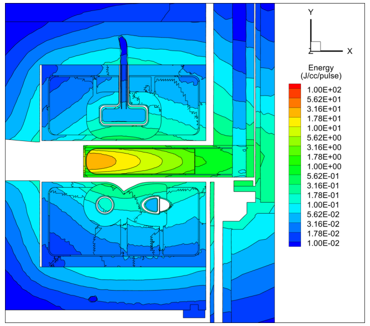
Coupled neutronics & structural optimization of the target

- **Detailed energy deposition distribution from MCNP as input to FEA**

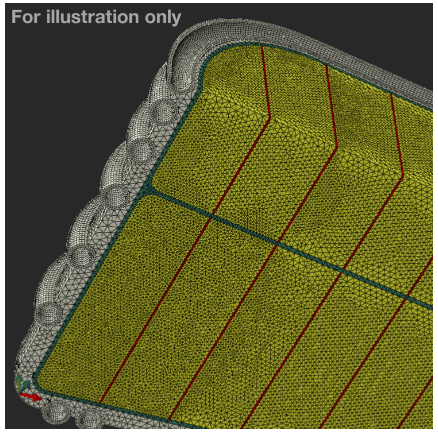


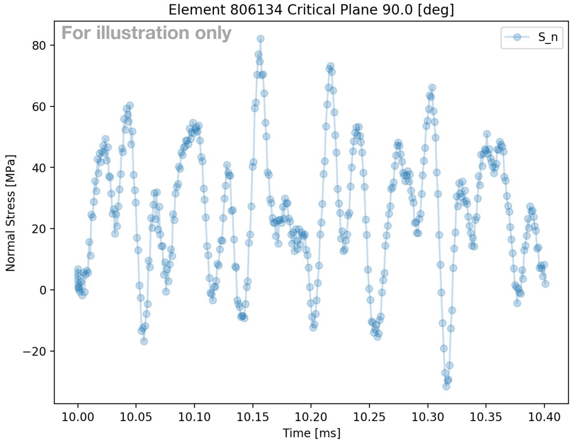


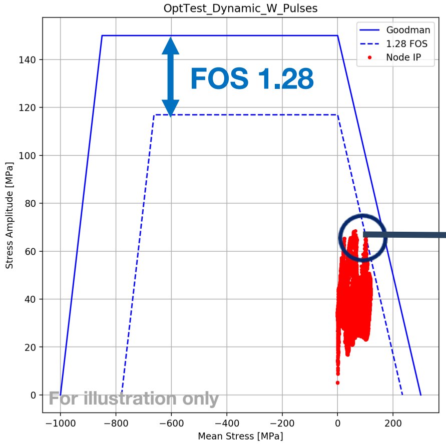


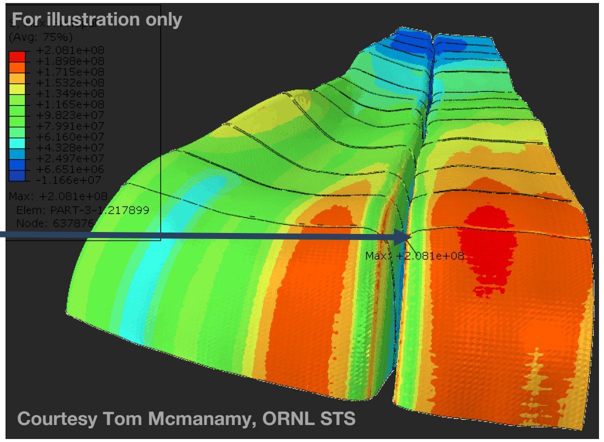


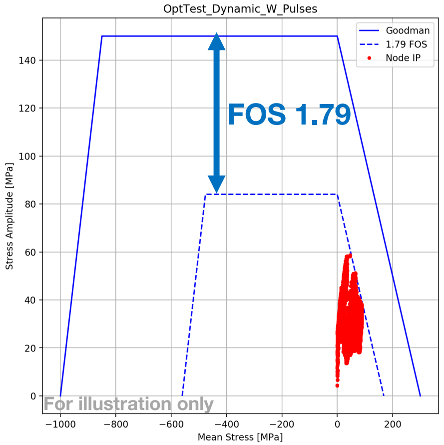
- **Factor of Safety (FOS)**
  – Measure for the mechanical performance of the target (irradiated after 10 years of operation)
  – Goodman diagram of a failure theory extracted from dynamic response





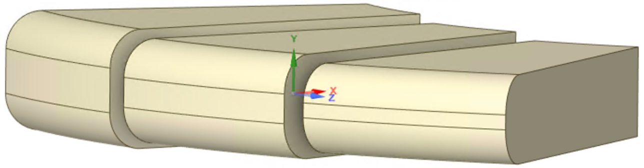


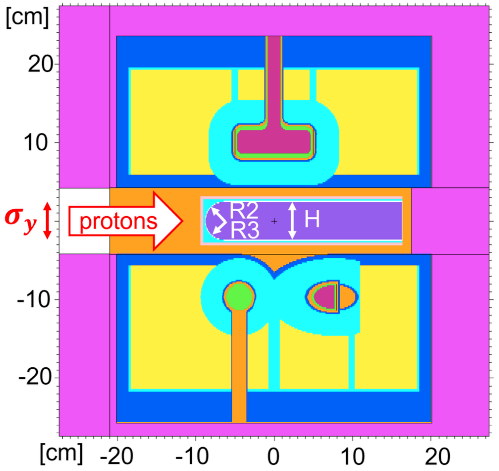


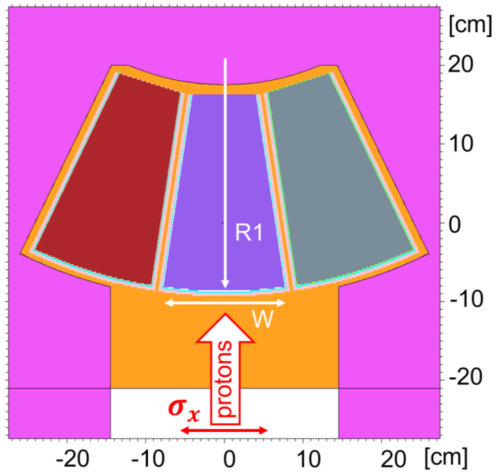


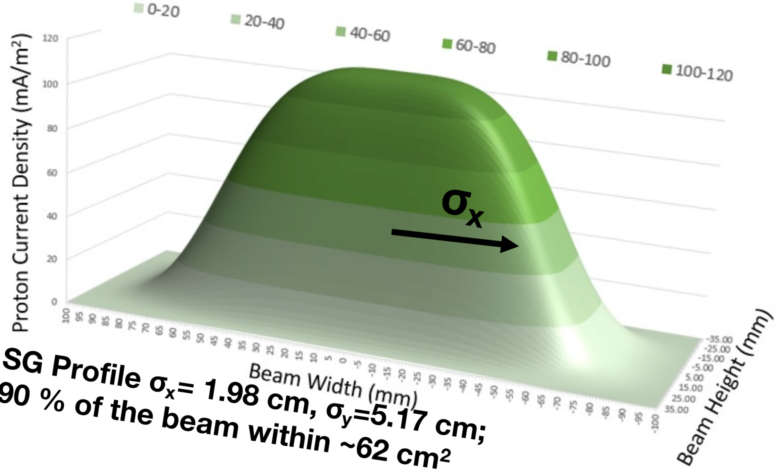
Coupled neutronics & structural optimization of the target

- **Simple target design**

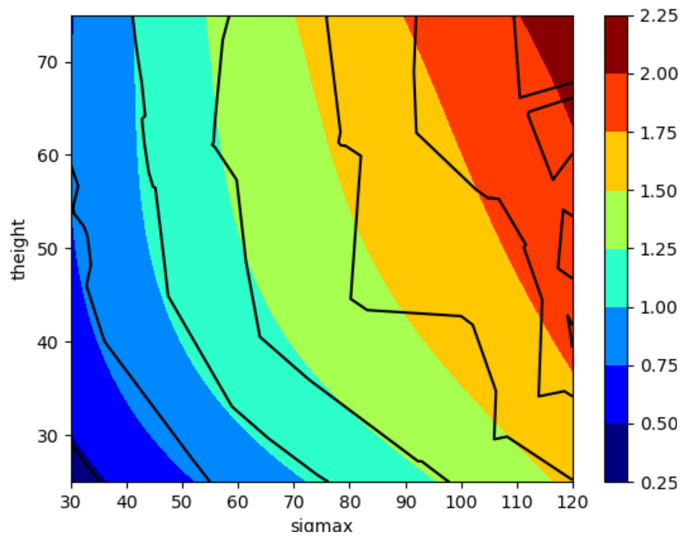


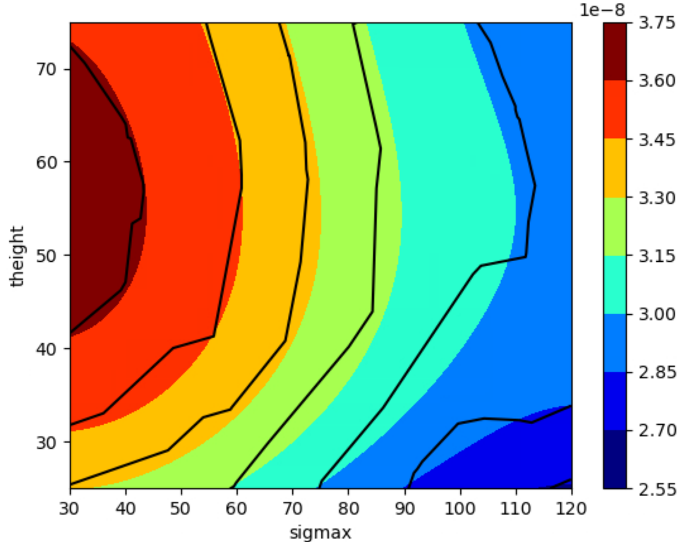


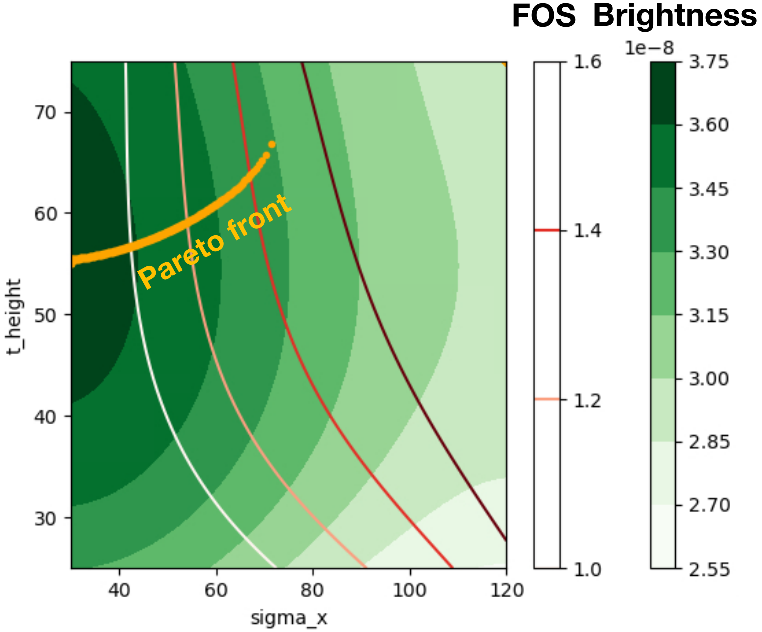




SG Profile σ_x= 1.98 cm, σ_y=5.17 cm; 90 % of the beam within ~62 cm²

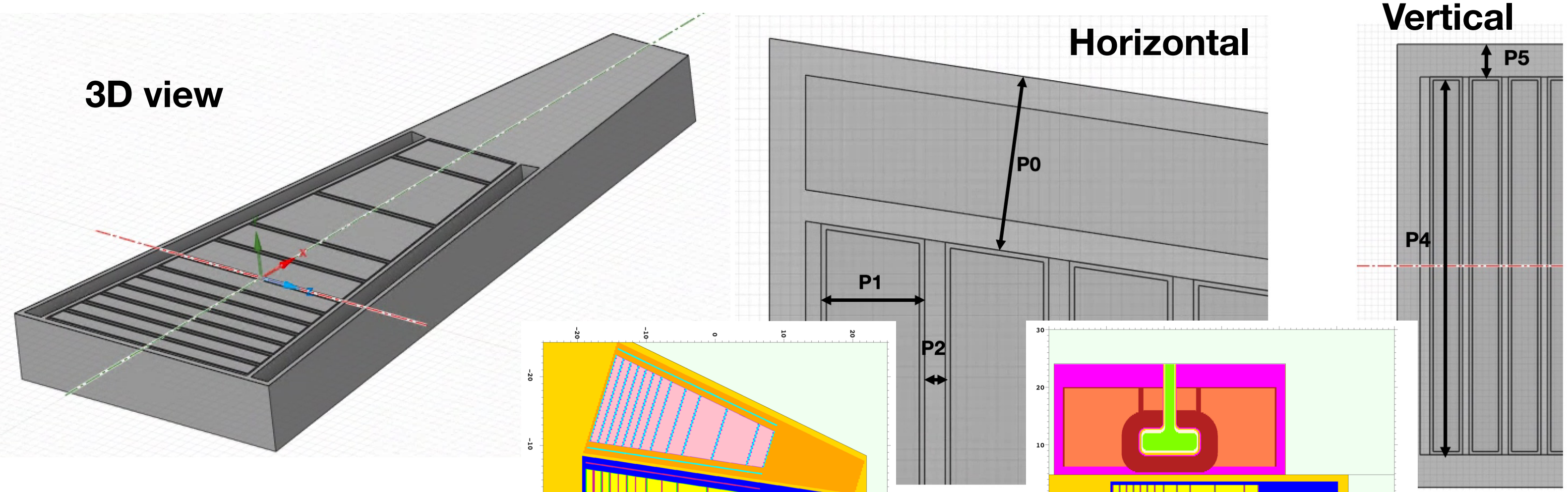


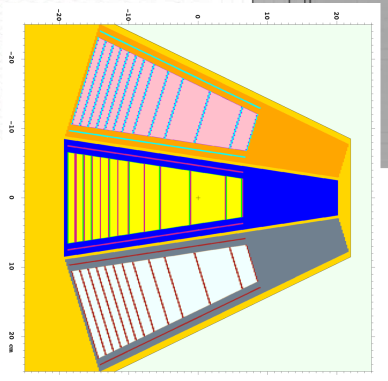


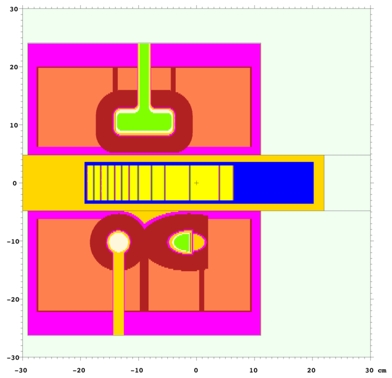


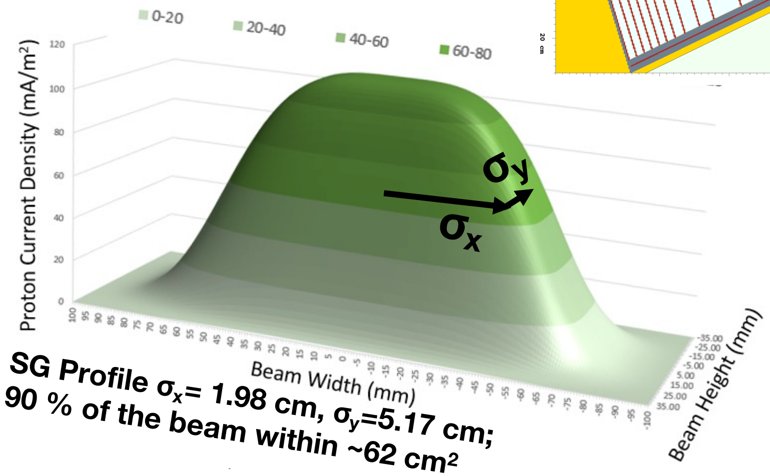
Coupled neutronics & structural optimization of the target

- **"Cheese wedge" target design**





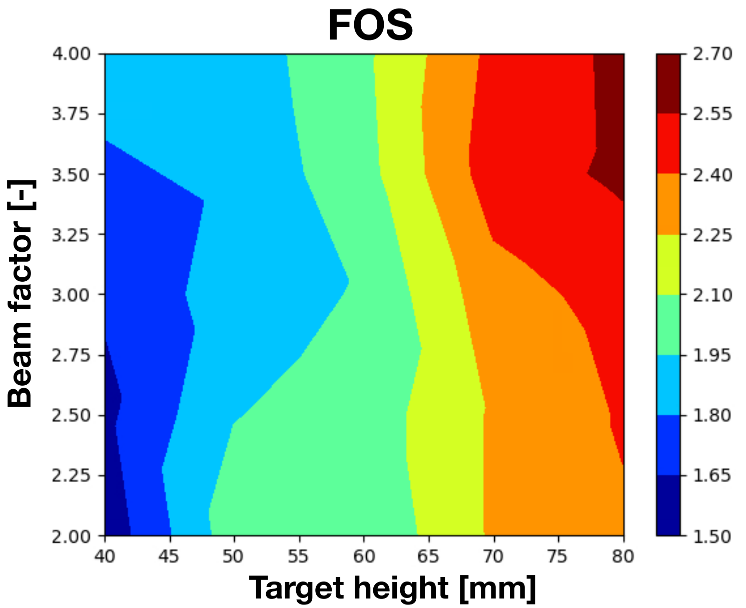


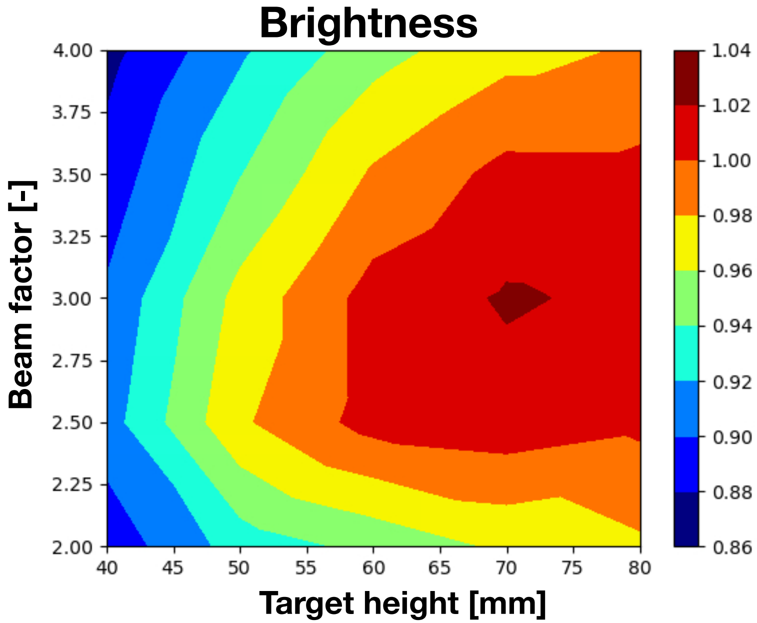


SG Profile σ_x= 1.98 cm, σ_y=5.17 cm;
90 % of the beam within ~62 cm²

Beam factor = $\frac{\text{Target height}}{\sigma_y}$

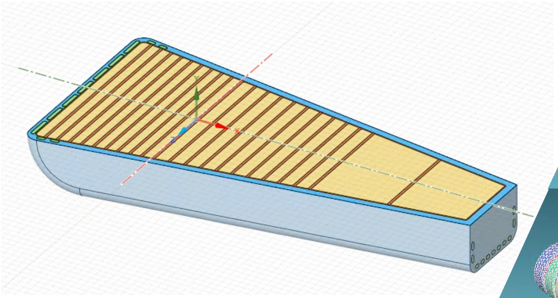
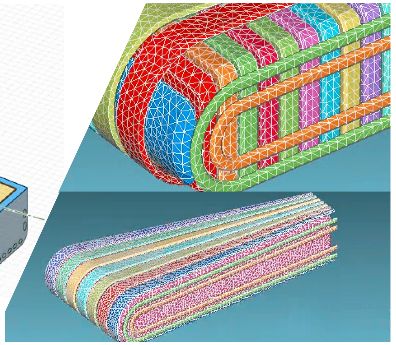
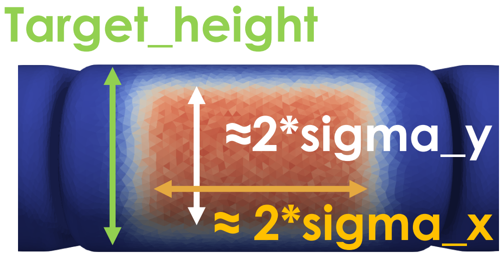
Large beam factor is small σ_y for a chosen target height

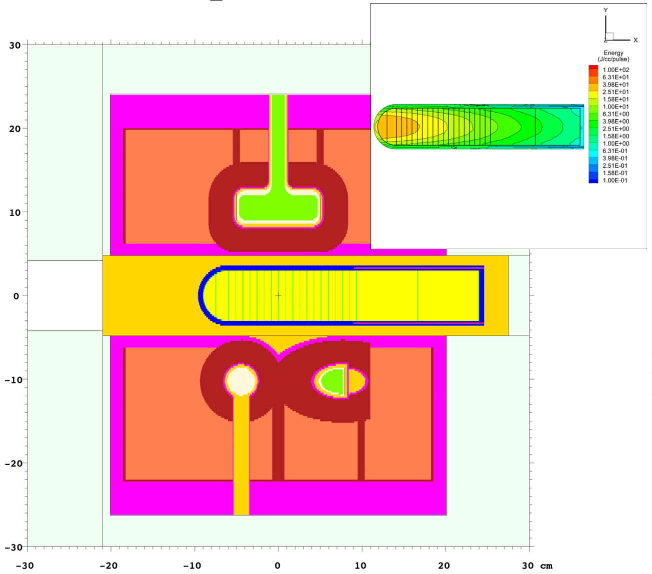


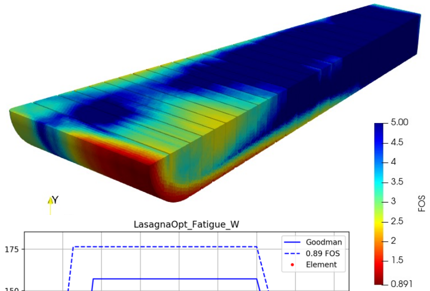
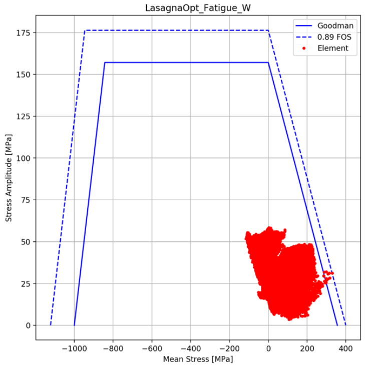


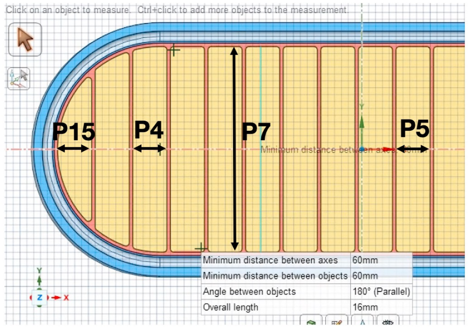
Coupled Target + Moderator + Beam optimization

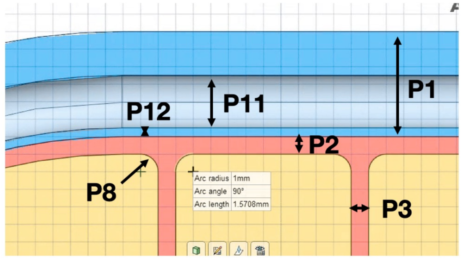
- **Latest target design**

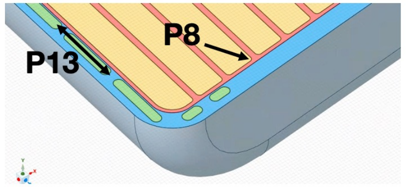




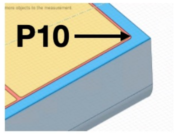


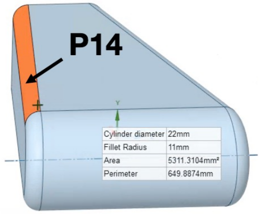



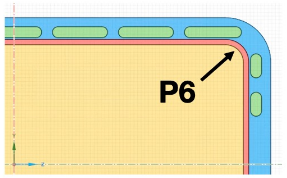


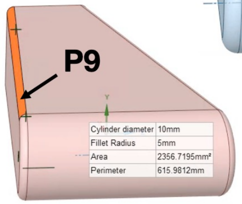


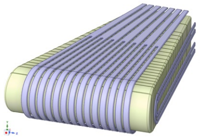
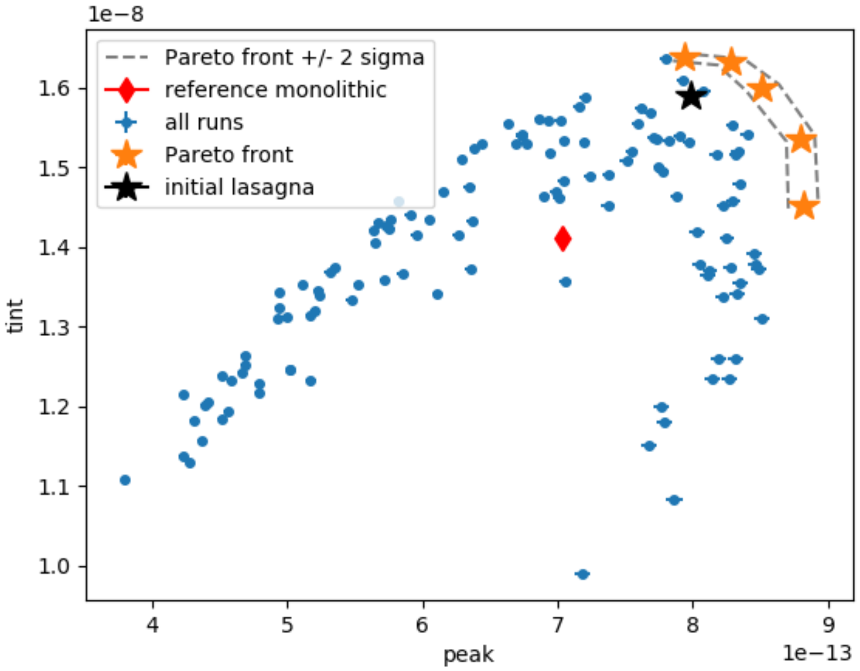


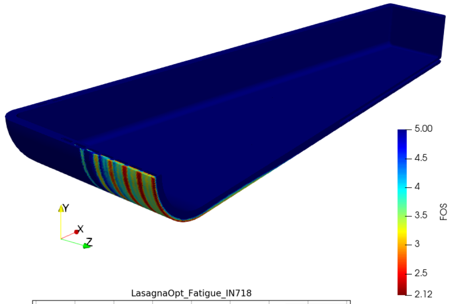
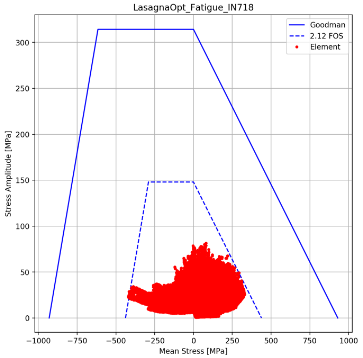








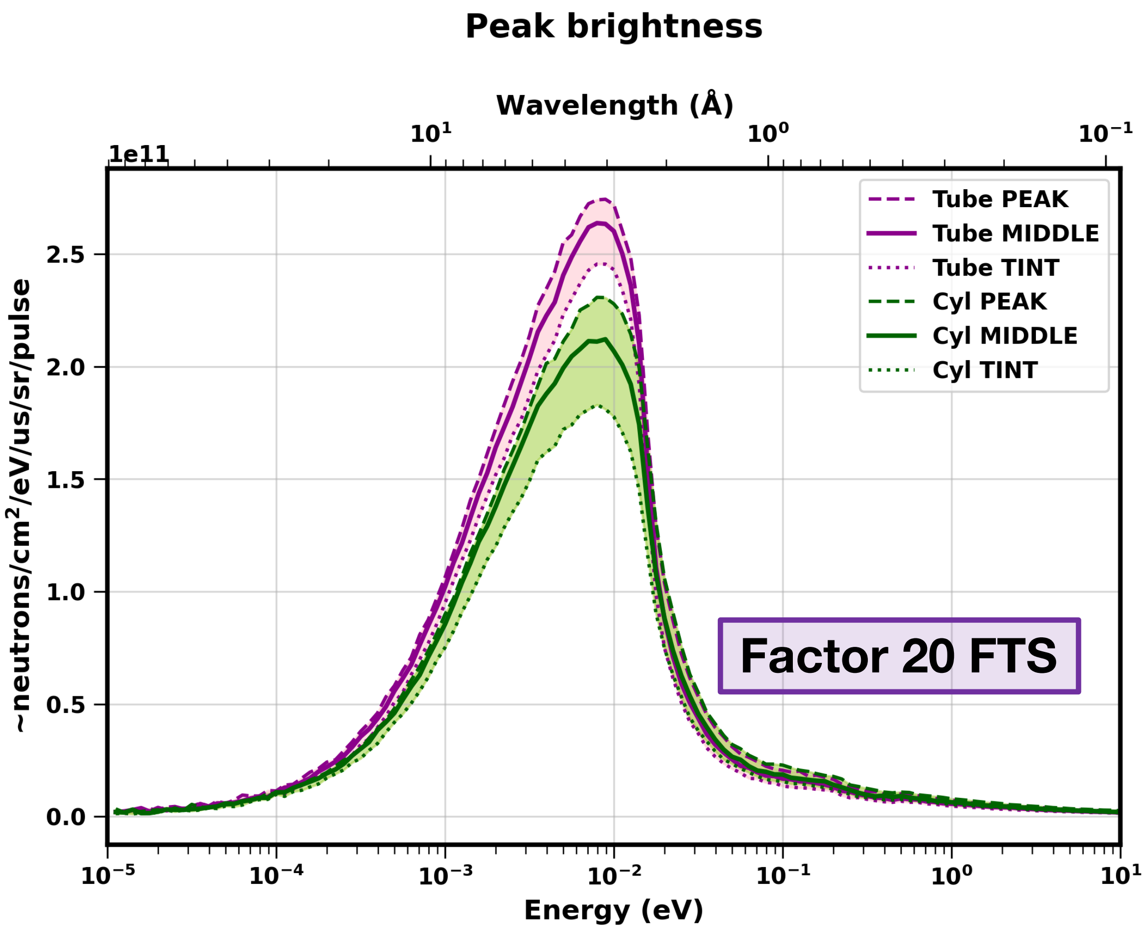
Conclusion

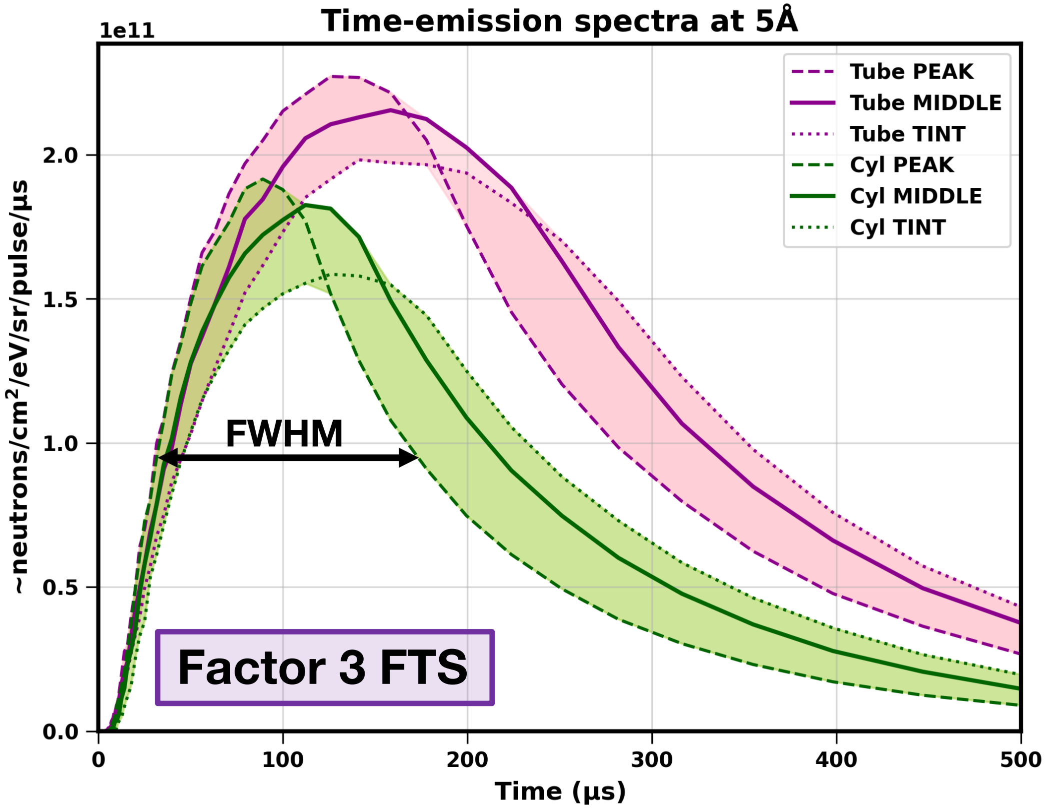
- **Developed an automated optimization workflow for coupled neutronics and structural stress analyses**
- **Reduced time per one iteration from weeks/months to hours**
- **Optimized moderators and several target designs**
- **Getting more efficient and moving towards more complicated problems**

- **Essential tool in the STS design process**
- **Can be applied at other research and accelerator facilities**

Thank you!

STS Moderator Performance





- **Tube moderator delivers superior brightness to eventually 6 instruments**
- **Cylindrical moderator has superior time resolution (event. 12 instruments)**