Direct Use of CAD Geometry in Monte Carlo Radiation Transport

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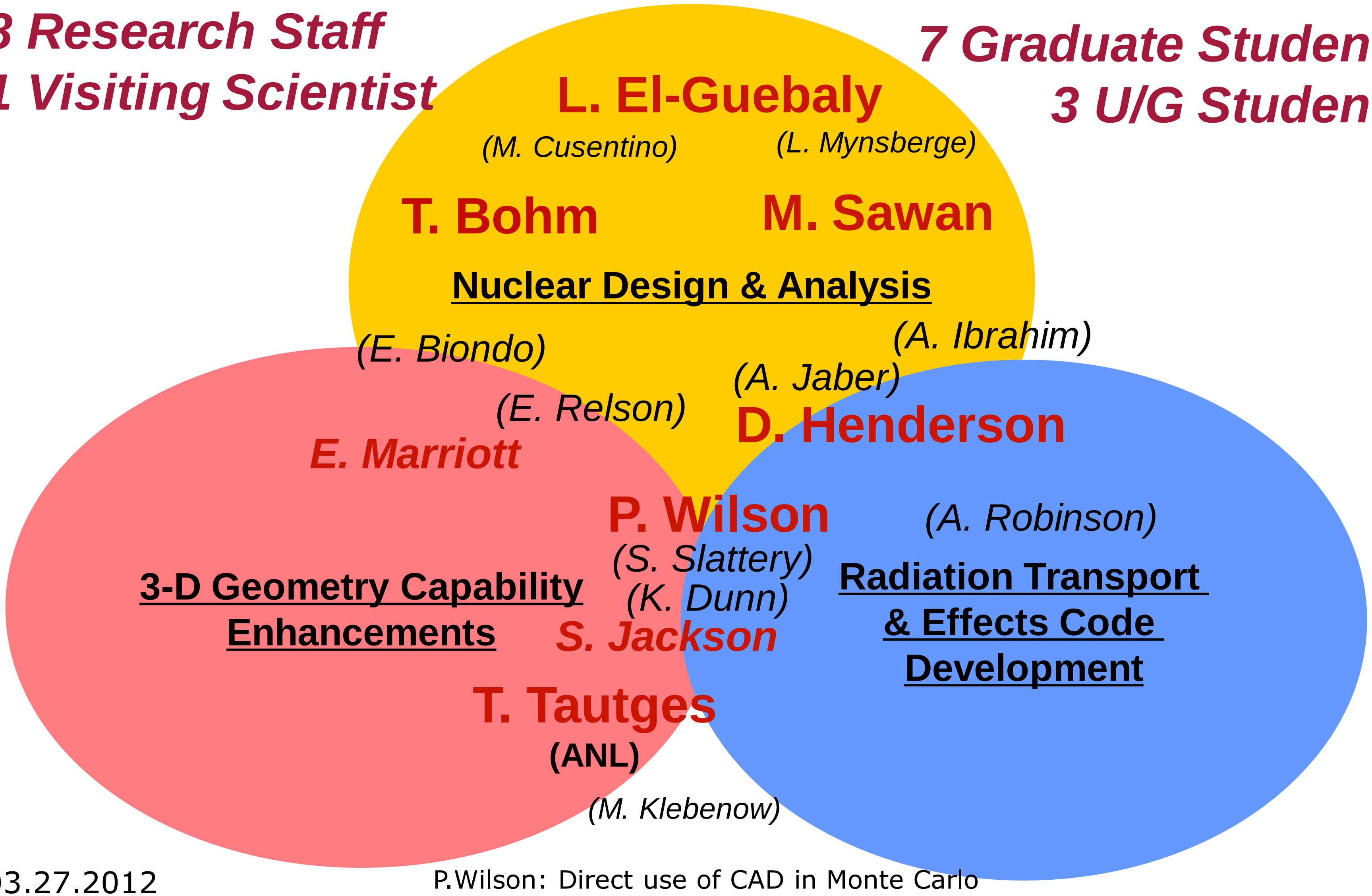


Overview

- Motivation
- Developer's Perspective
  - Core Software Infrastructure
  - Fundamental Geometry Operations
  - Methods & Accelerations
  - Performance
  - Robustness
- User's Perspective
  - Workflow
  - Examples
- Current Research

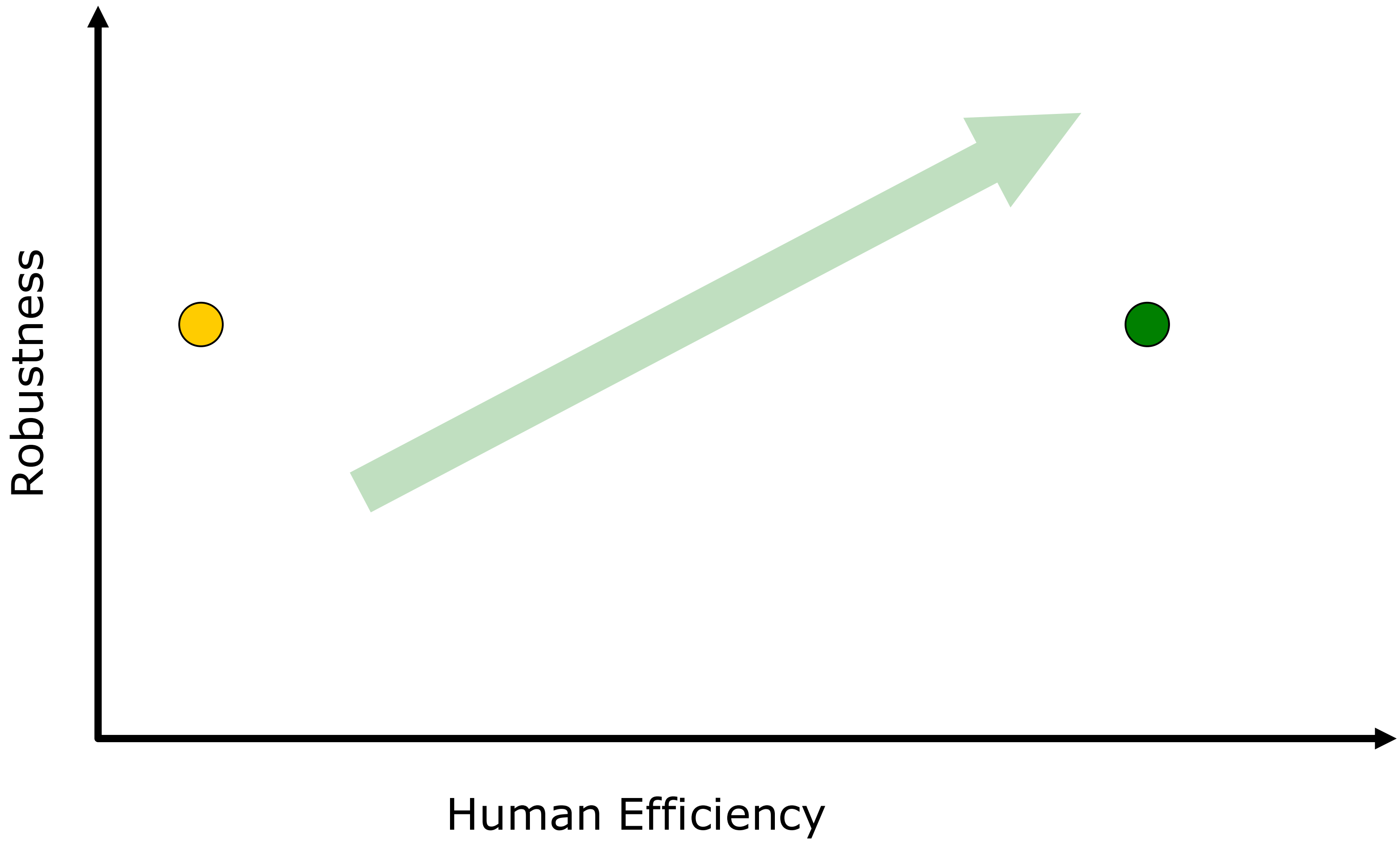
Monte Carlo Transport in Fusion Neutronics

- Complex shielding problems
  - Monte Carlo preferred
  - Intricate geometries created by hand
- Complex cell boundaries
  - Especially tori
- Small numerical gaps in geometry
- Lost particles accepted as necessary

Three Motivations for CAD-Based Monte Carlo Tools

- Faster
  - Reduce human effort – faster design iteration
  - **Provide common domain for coupling to other analyses**
- Cheaper
  - Reduce human effort
- Better
  - Avoid human error in conversion
  - **Include higher-order surface descriptions in analysis**

Promise of CAD-based Monte Carlo Transport

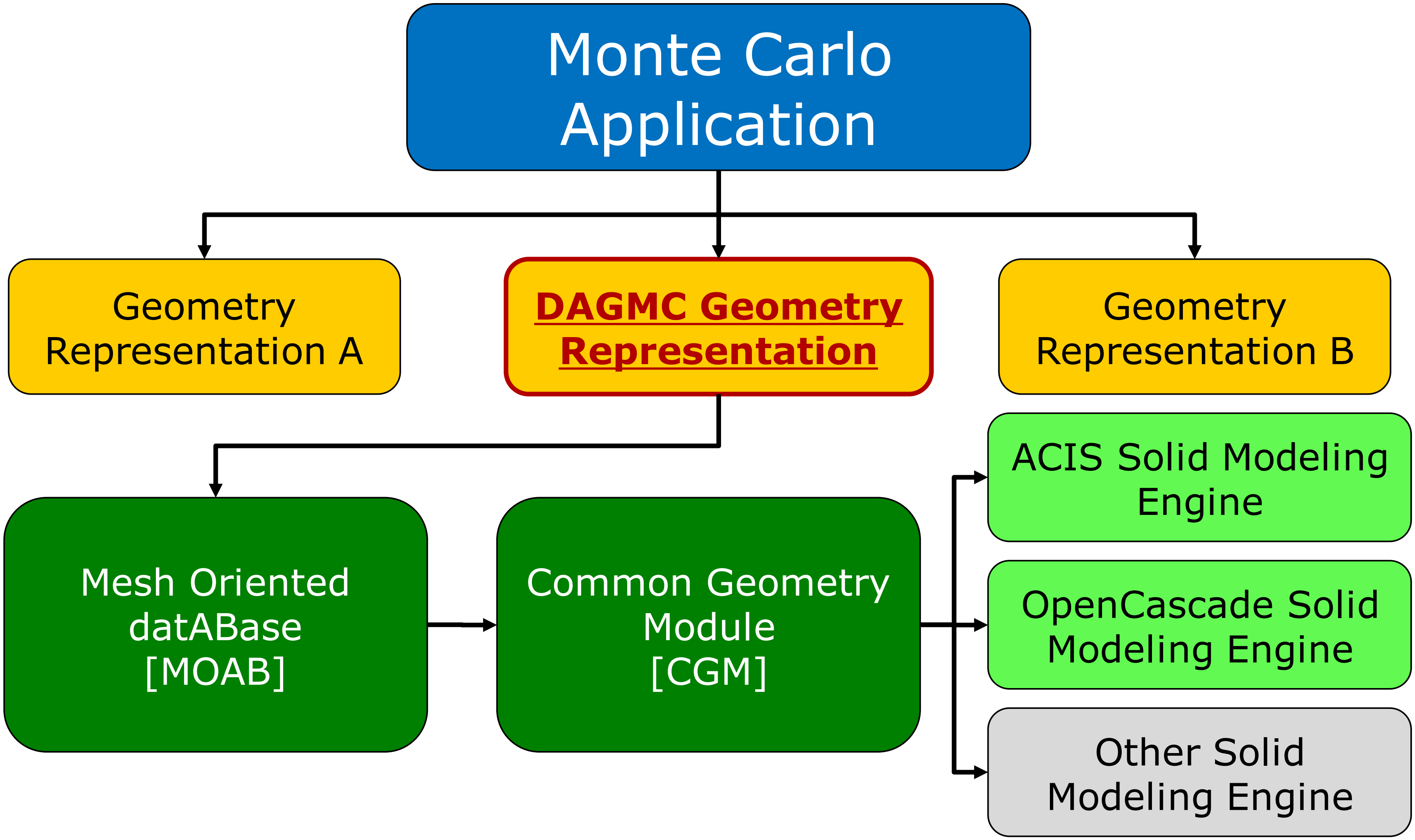


Developer's Perspective

THE UNIVERSITY of WISCONSIN MADISON

Developers Perspective: Software Infrastructure

Direct Accelerated Geometry Monte Carlo



Demonstrated Implementations

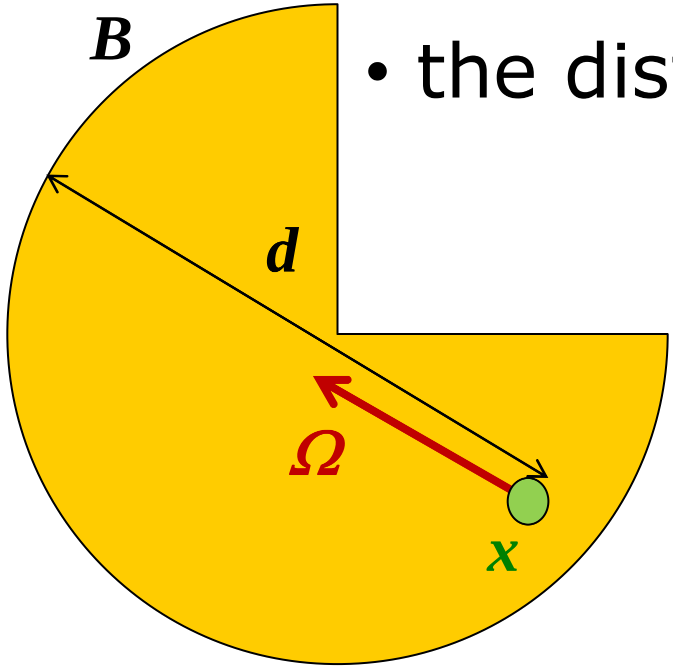
- MCNP5 (LANL)
  - Main development & testing platform
- Tripoli 4 (CEA/France)
  - UW implementation
- GEANT4
  - Implementation by S. Korean researchers
- FLUKA
  - Interest by NASA users and FLUKA developers
- MCNPX 2.x (LANL)
  - Initial development platform
  - Being merged with MCNP5 ⇨ MCNP6

Geometry & Mesh Infrastructure

- CGM
  - Common API to many solid modeling engines
  - Virtual geometry capabilities for merging and metadata
- MOAB
  - Robust & efficient mesh representation
  - Common API to many mesh formats
- Both are under independent with ongoing improvements
  - Access to other mesh operations/services
  - Other users benefit from developments

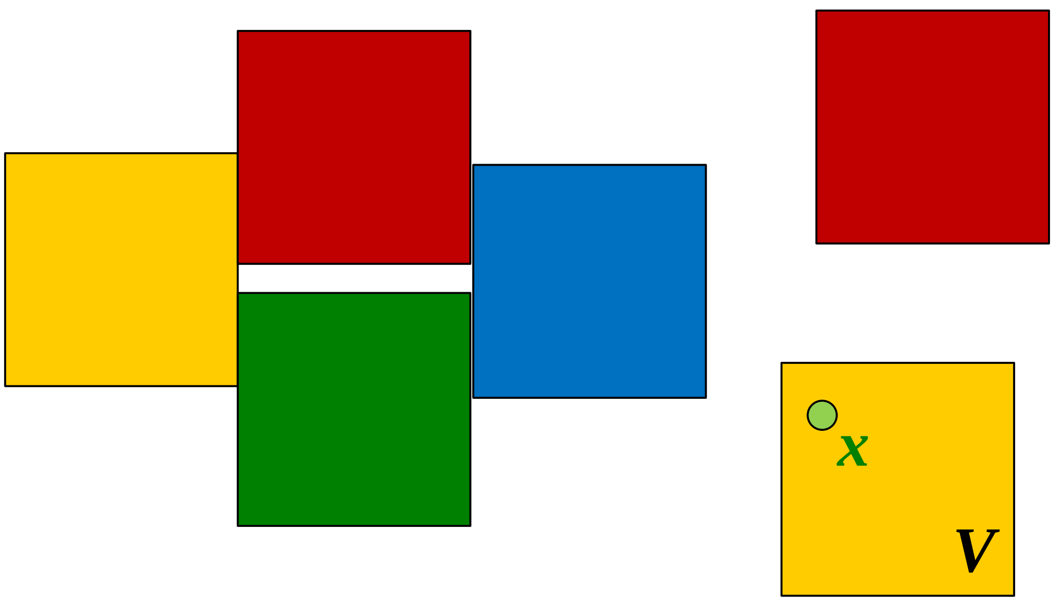
DISTANCE TO BOUNDARY

- For a given point, x, and direction, Ω, find
  - the nearest boundary, B, and
  - the distance, d, to that boundary



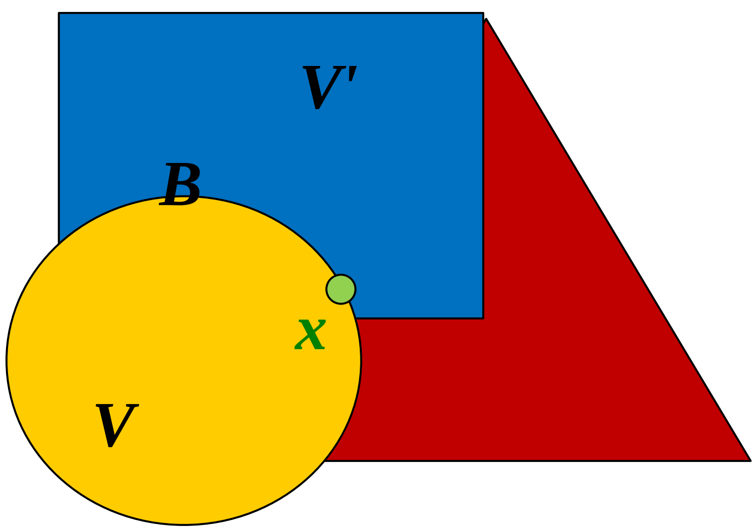
POINT LOCATION

- For a given point, *x*, find
  - the unique volume, *V*, containing that point



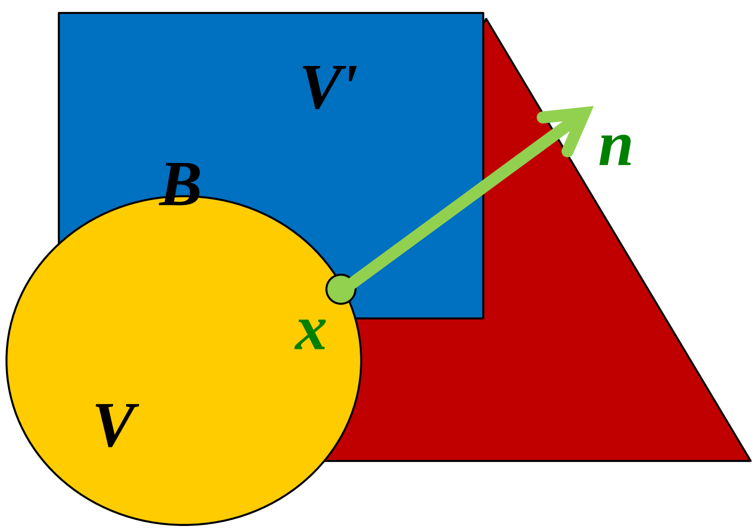
SURFACE CROSSING

- For a given point, x, on the boundary, B, of volume, V, find
  - which volume, V', will be entered next



SURFACE NORMAL

- For a given point, ***x***, on the boundary, ***B***, of volume, ***V***, find
  - the unit normal, ***n***, to that surface



METADATA QUERIES

- Metadata can be added to geometry to facilitate
  - Material assignment
  - Boundary conditions
  - Source definition
  - Tally/response definition
  - Variance reduction

The Need for Acceleration Techniques

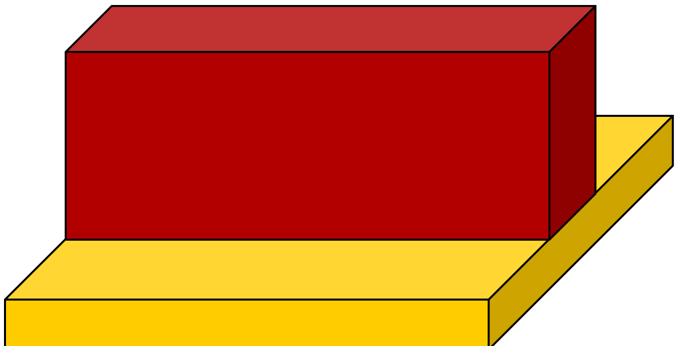
- Ray-tracing: fundamental operation of Monte Carlo transport
  - Ray-tracing on 2^{nd} order analytic surfaces is efficient
  - Ray-tracing on arbitrary high-order surfaces requires high-order root finding
  - Also need to detect curves where surfaces meet
    - More complexity with high-order surfaces

Accelerations

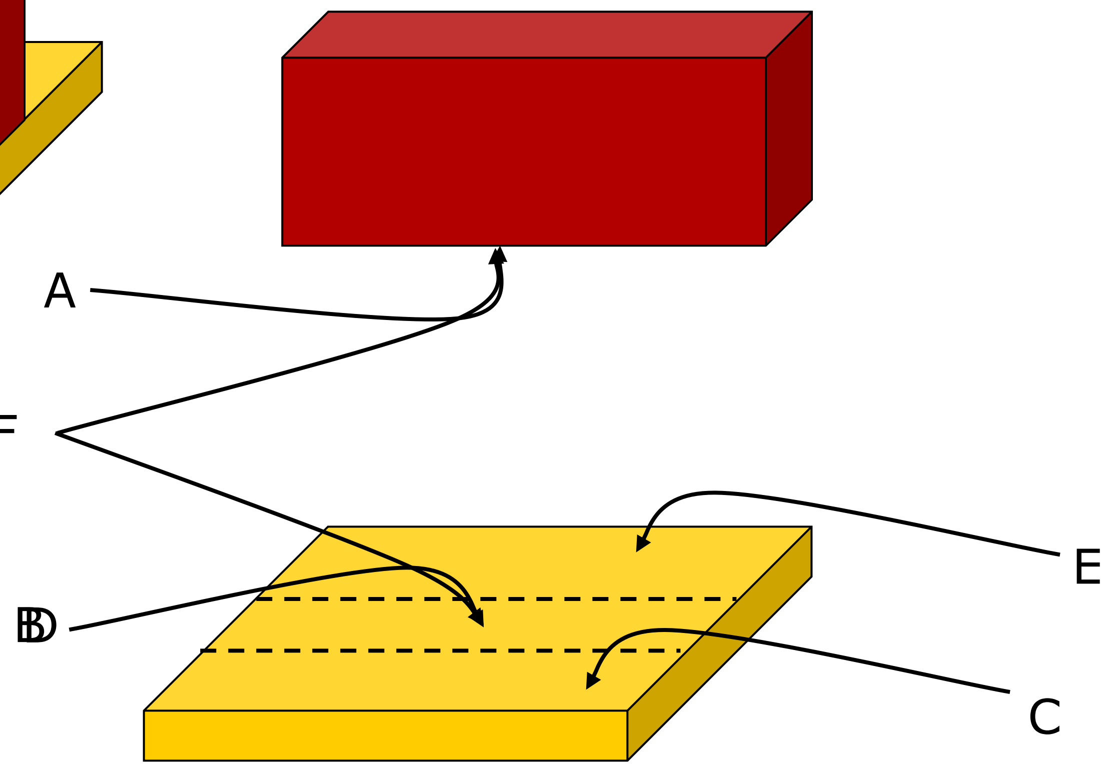
- Imprint & merge
  - Reduce complexity of determining neighboring regions in space
  - Reduce number of ray-firing operations
- Faceting
  - Reduce ray-tracing to always be on (planar) facets, but
    - introduce approximations
    - millions of individual facets
- Oriented Bounding Box Tree
  - Accelerate search of millions of surfaces
  - Reduce number of surface tests

Imprint & Merge

- Imprinting



- Merging
- Each surface in max. 2 cells

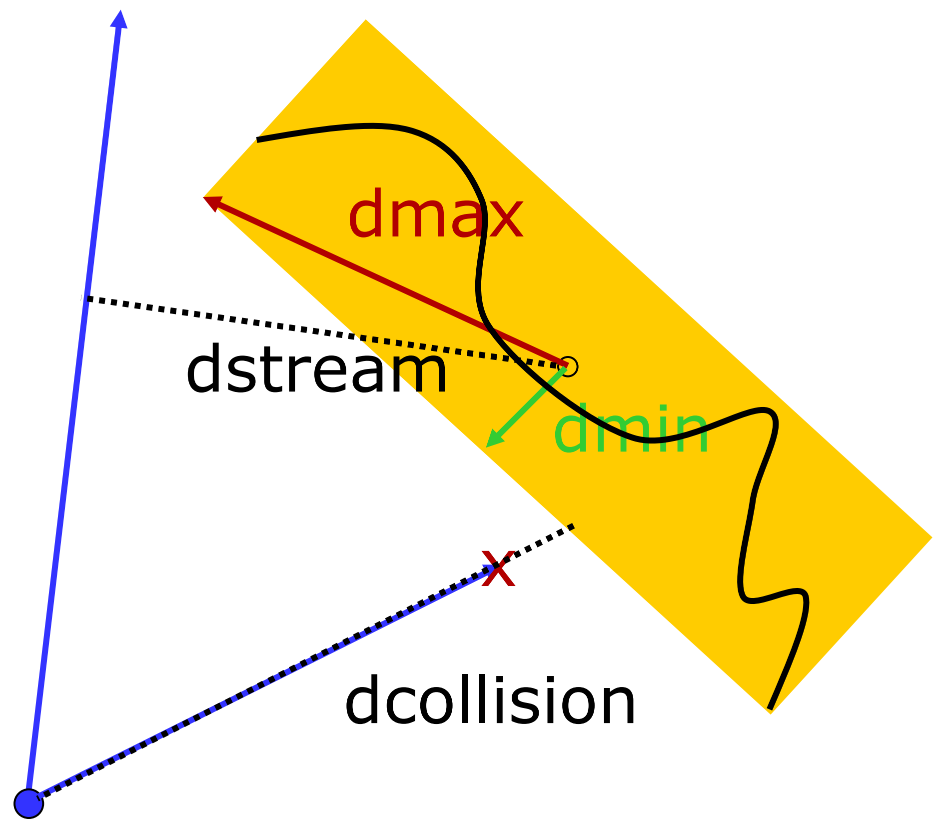


Avoiding the Explicit Calculation of the "Complement"

- CAD-based solid models do not typically represent non-solid regions
  - e.g. voids, coolants
- Explicit calculation
  - Boolean operations in CAD (or CUBIT)
  - Often computationally expensive
- Implicit determination
  - Volume bounded by surfaces with only 1 cell following imprint & merge

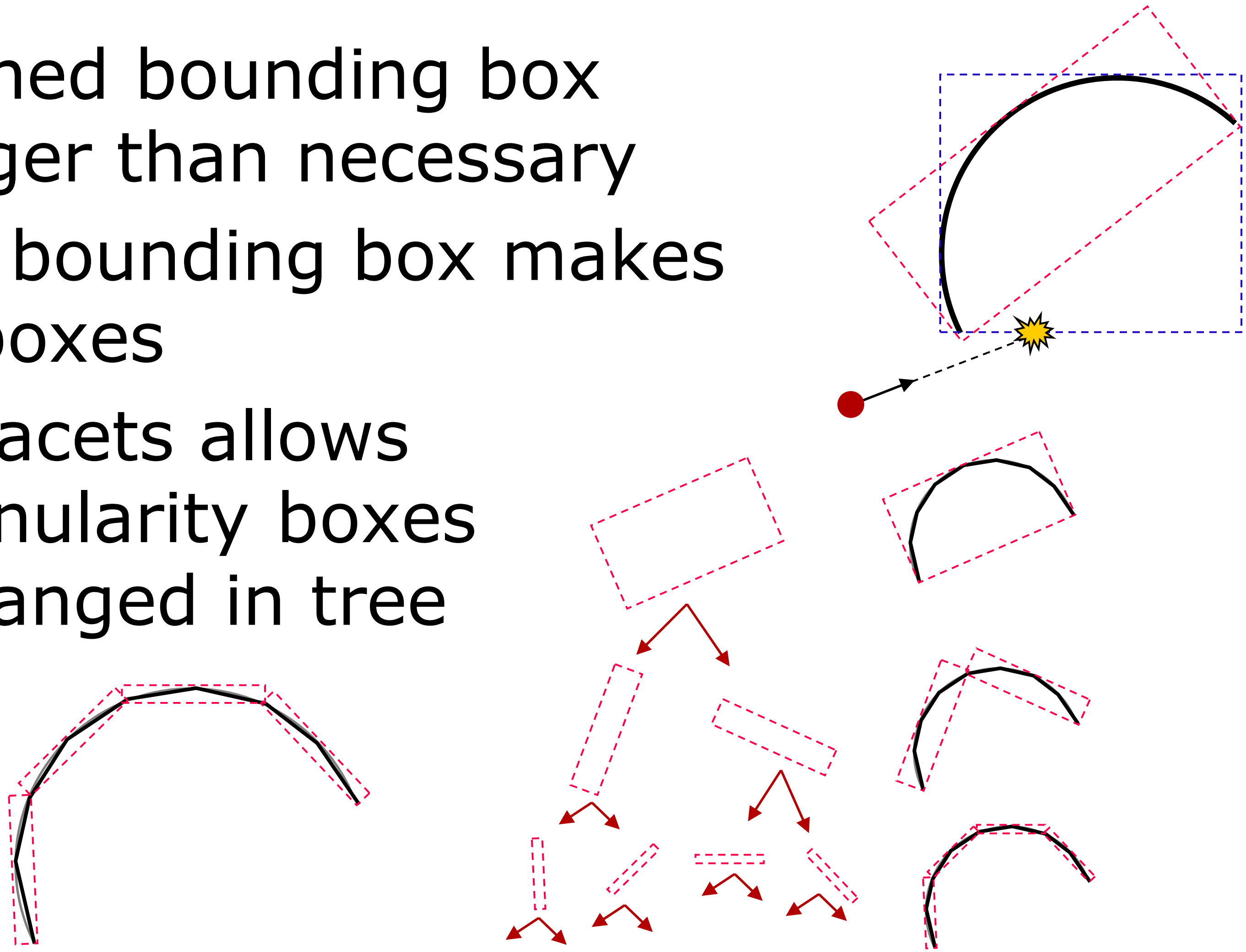
Accelerate Testing of Each Bounding Box

- Simple (inexpensive) bounding box test
  - Streaming distance to closest approach
  - Collision distance to closest approach

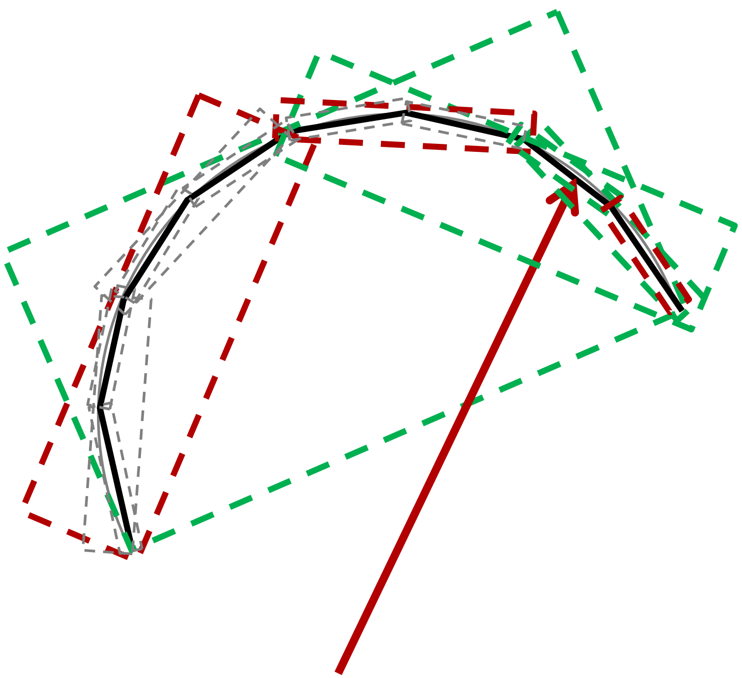


Oriented Bounding Box on Facets as Nodes in a Tree

- Axis-aligned bounding box often larger than necessary
- *Oriented* bounding box makes smaller boxes
- OBB on facets allows finer-granularity boxes to be arranged in tree



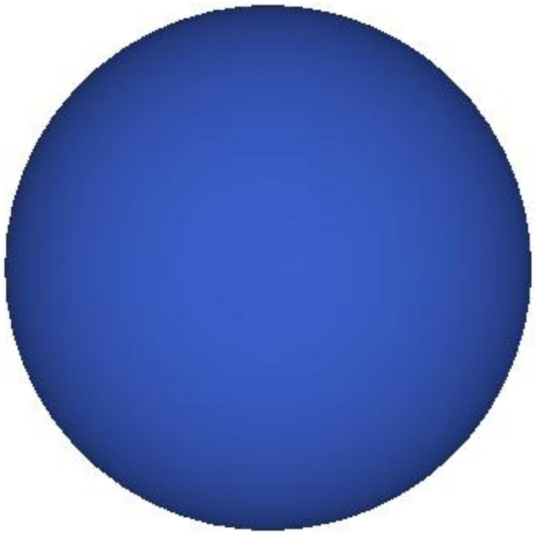
Tree Traversal Could Have $O(\log_2(n))$ Bounding Box Tests



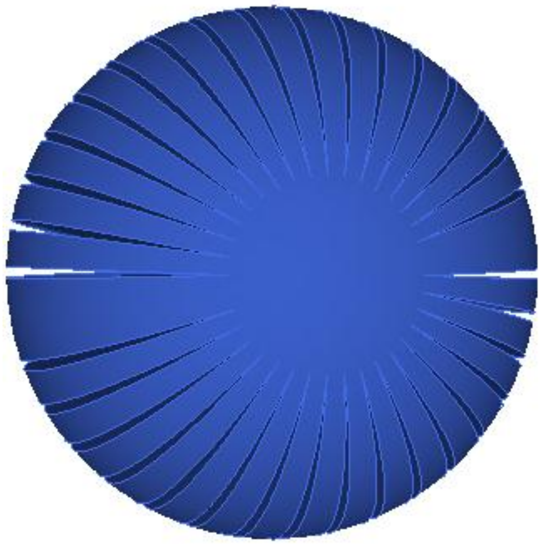
- Distance limit should guarantee improved performance
- Tree root for each cell/volume
  - Accelerate ray-tracing in implicit complement

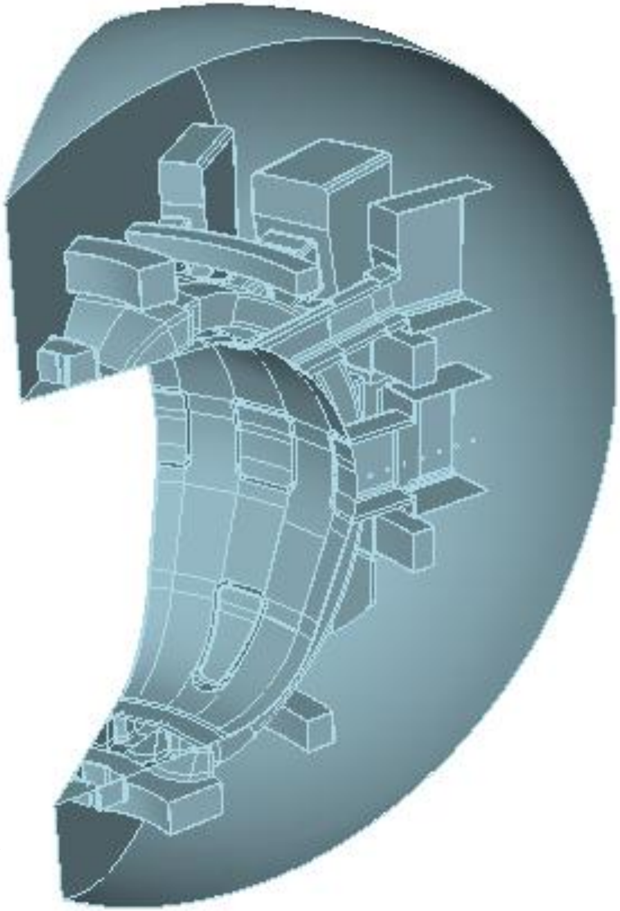
OBB-Tree Traversal Performance Tested on 3 Geometries

Sphere



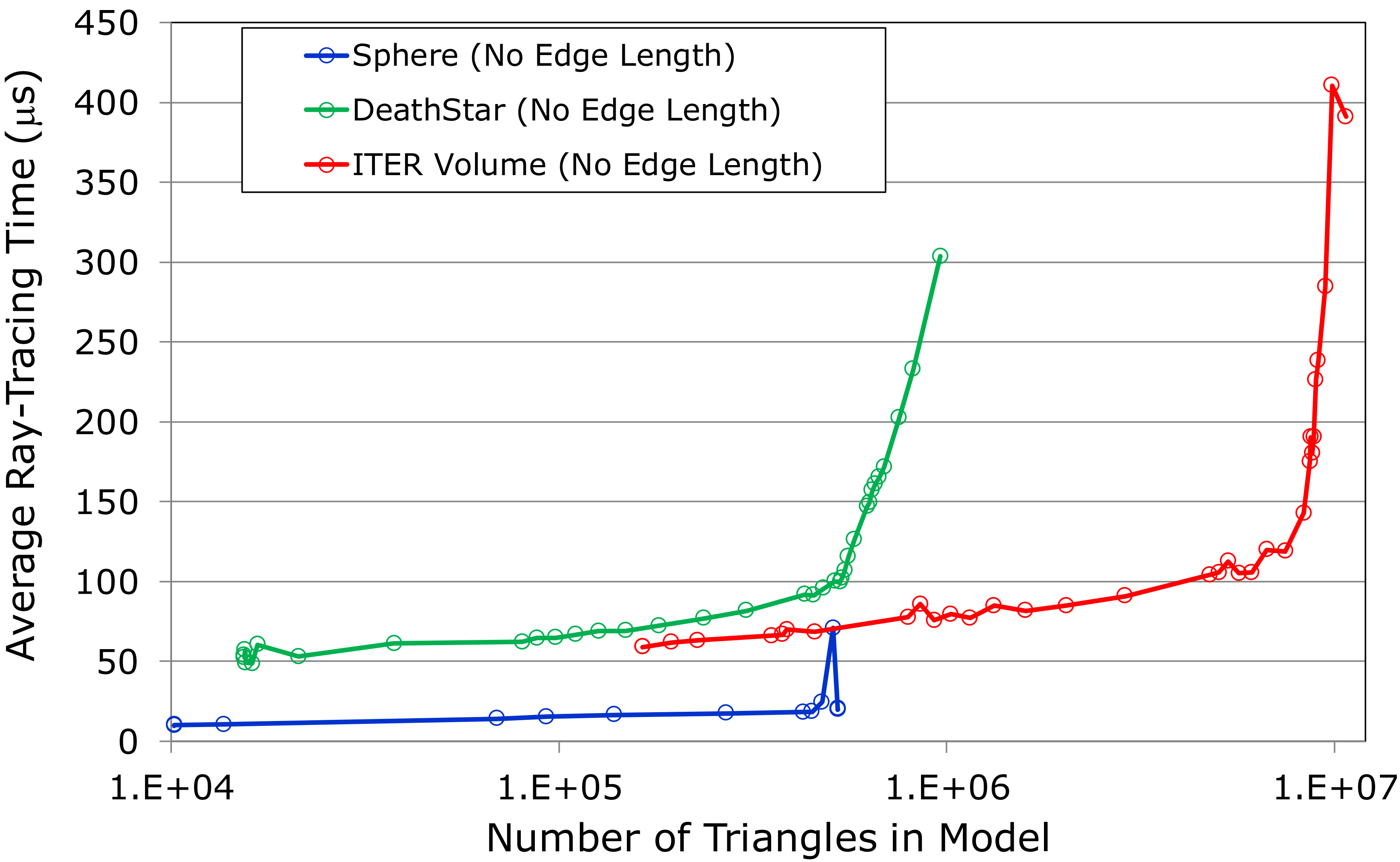
"Deathstar"



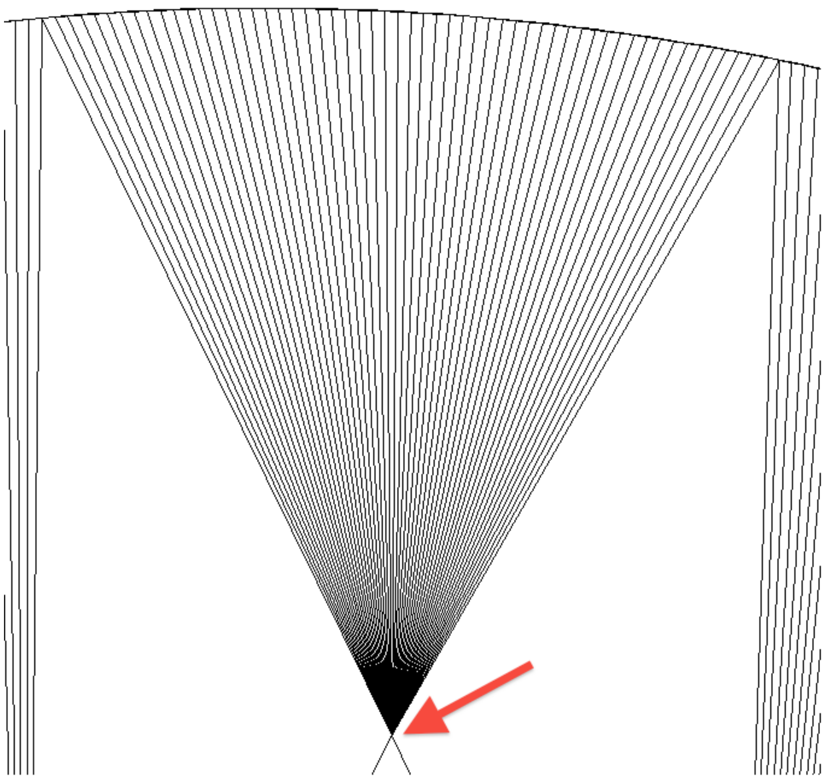


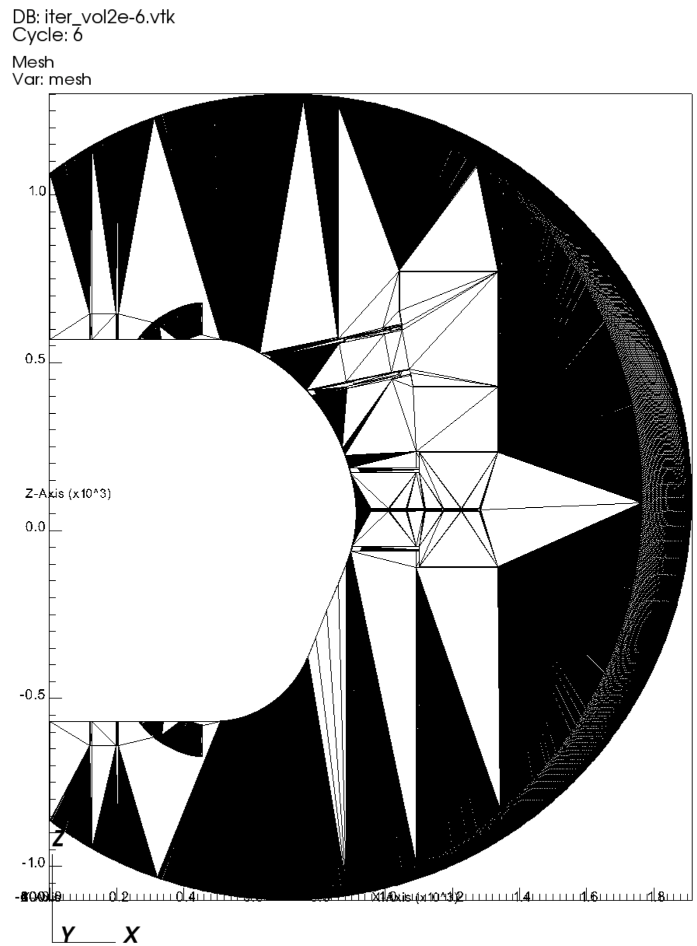
ITER Benchmark Complement

Performance does not meet expectations

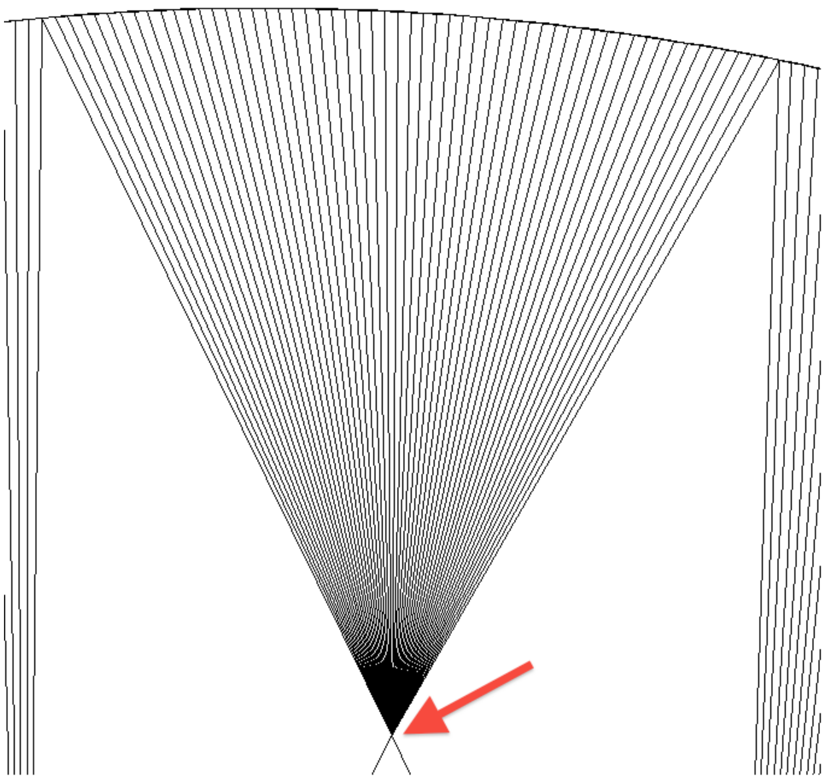


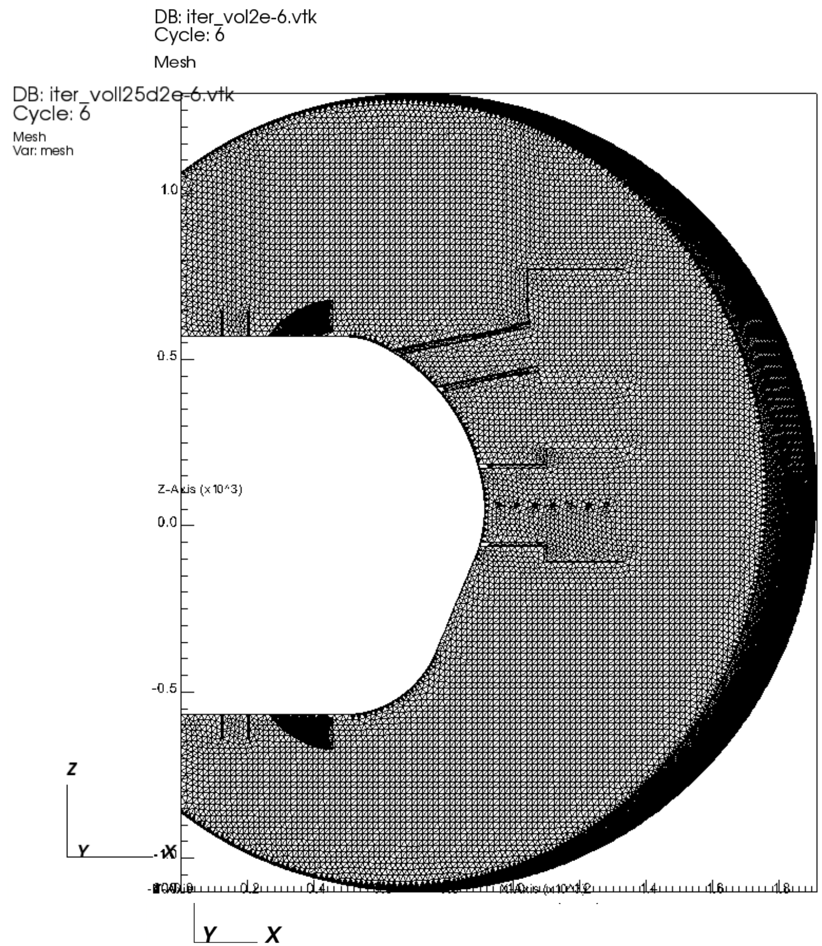
High Valence Vertices



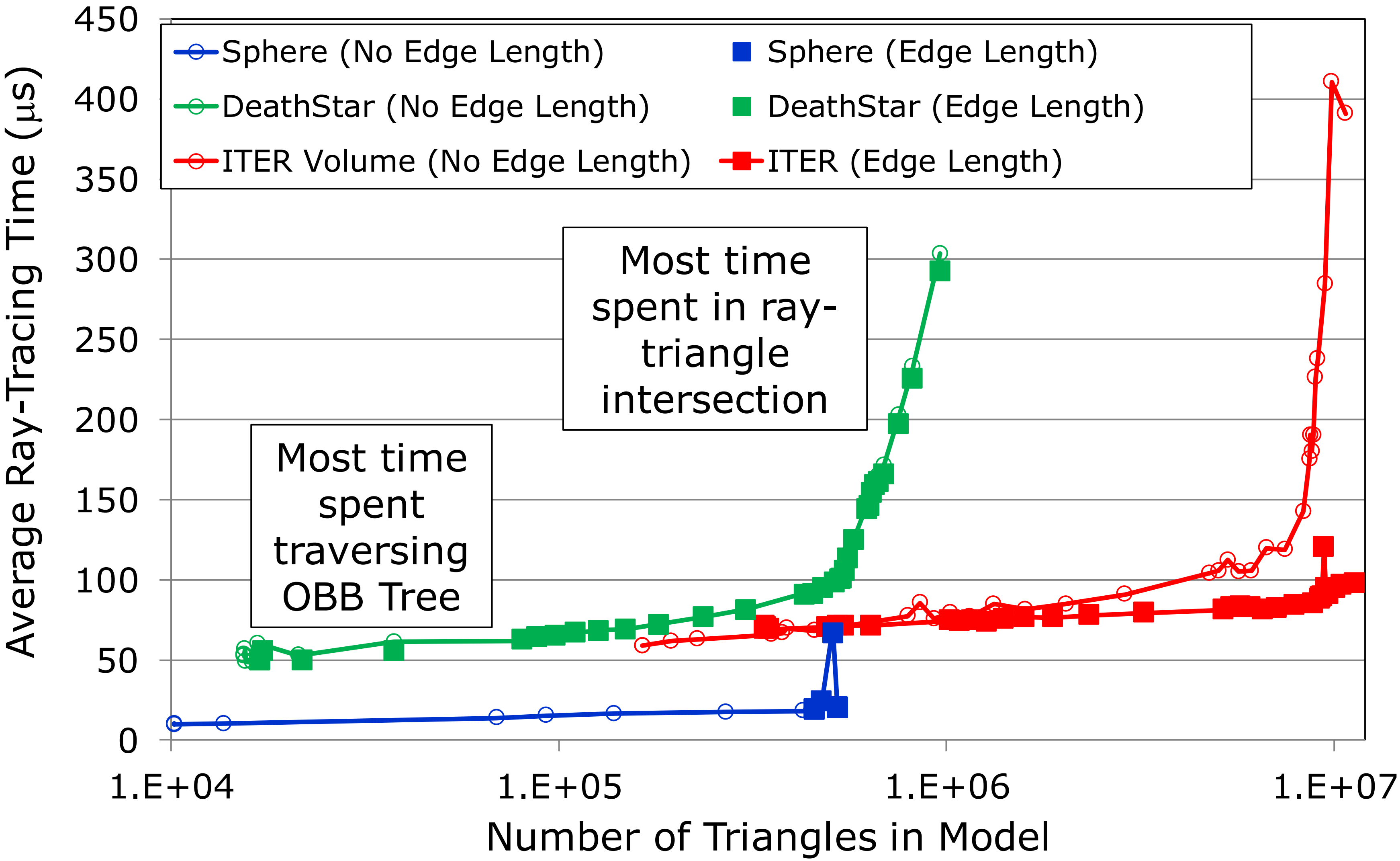


Edge Length Guidance





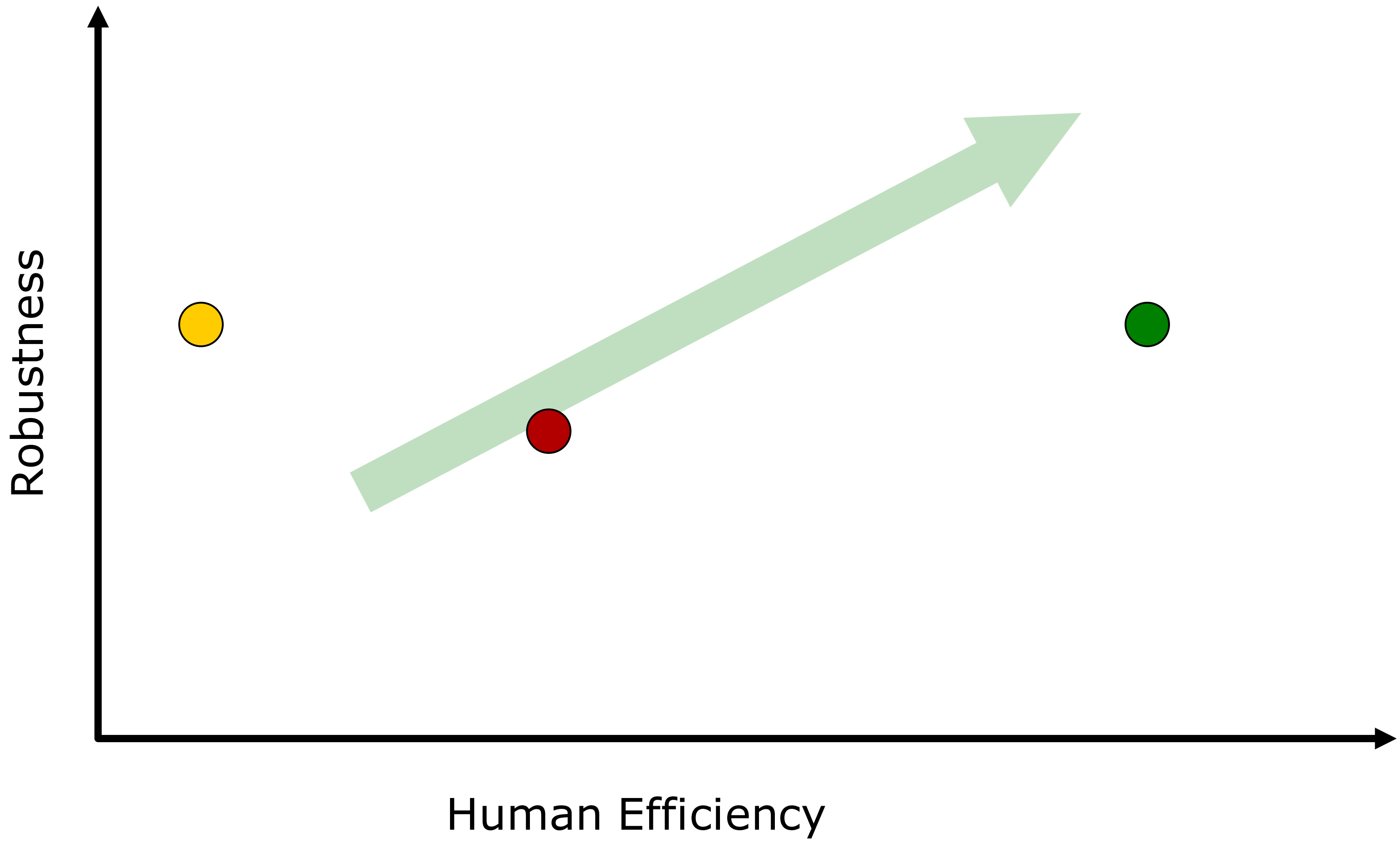
Improved Performance with Better Faceting



CAD-based Monte Carlo Neutronics

- Facilitates even more complex geometry
- More opportunity for
  - Small features and geometrical gaps
  - Automated precision to close gaps
- Impact on lost particles unclear
- Lost particle rate used as one performance metric ($< 10^{-5} – 10^{-6}$)

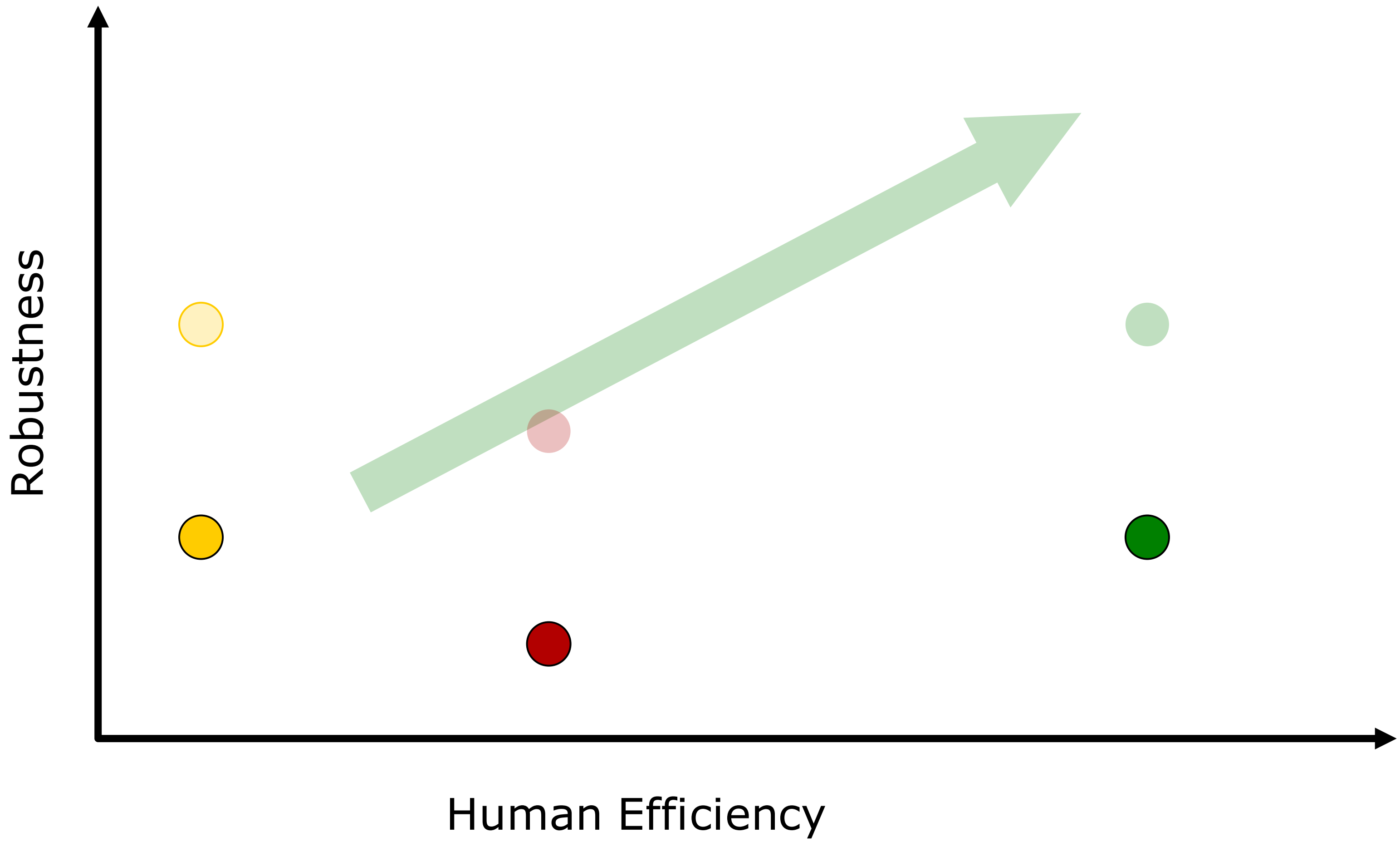
Initial Impact of DAGMC



New Problems with CAD-based Monte Carlo

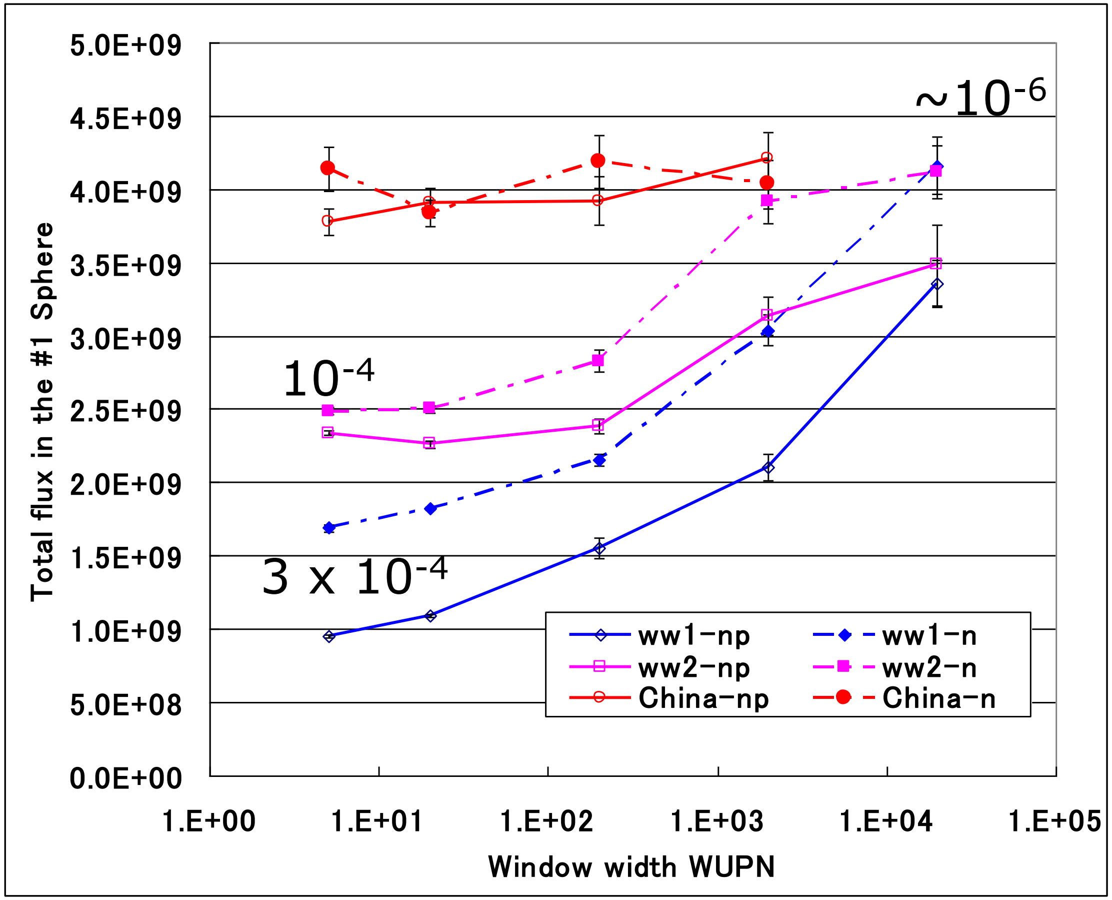
- Quality of CAD geometry
  - Small gaps & overlaps
  - Previous applications of CAD less sensitive
- Human efficiency gains reduced
  - New skills required
- DAGMC-specific challenges/opportunities
  - Inconsistent faceting
  - Robustness of tracking algorithm

Lost Particle Risk



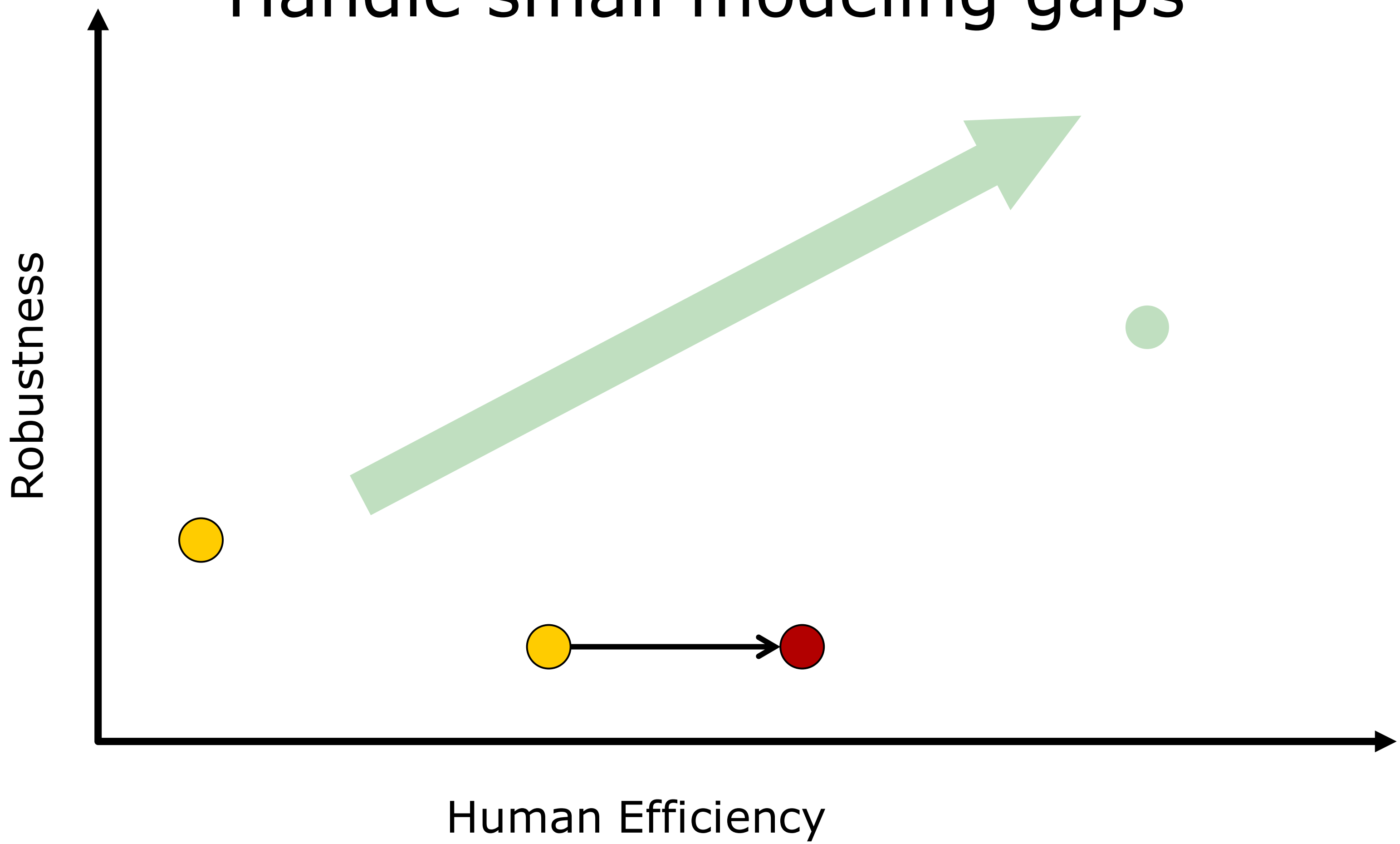
Lost Particle Risk

- H. Iida (2008)
- Intrinsically shielding/deep penetration
- Intense variance reduction necessary
- Some lost particles have high weight



Implicit Complement

Handle small modeling gaps

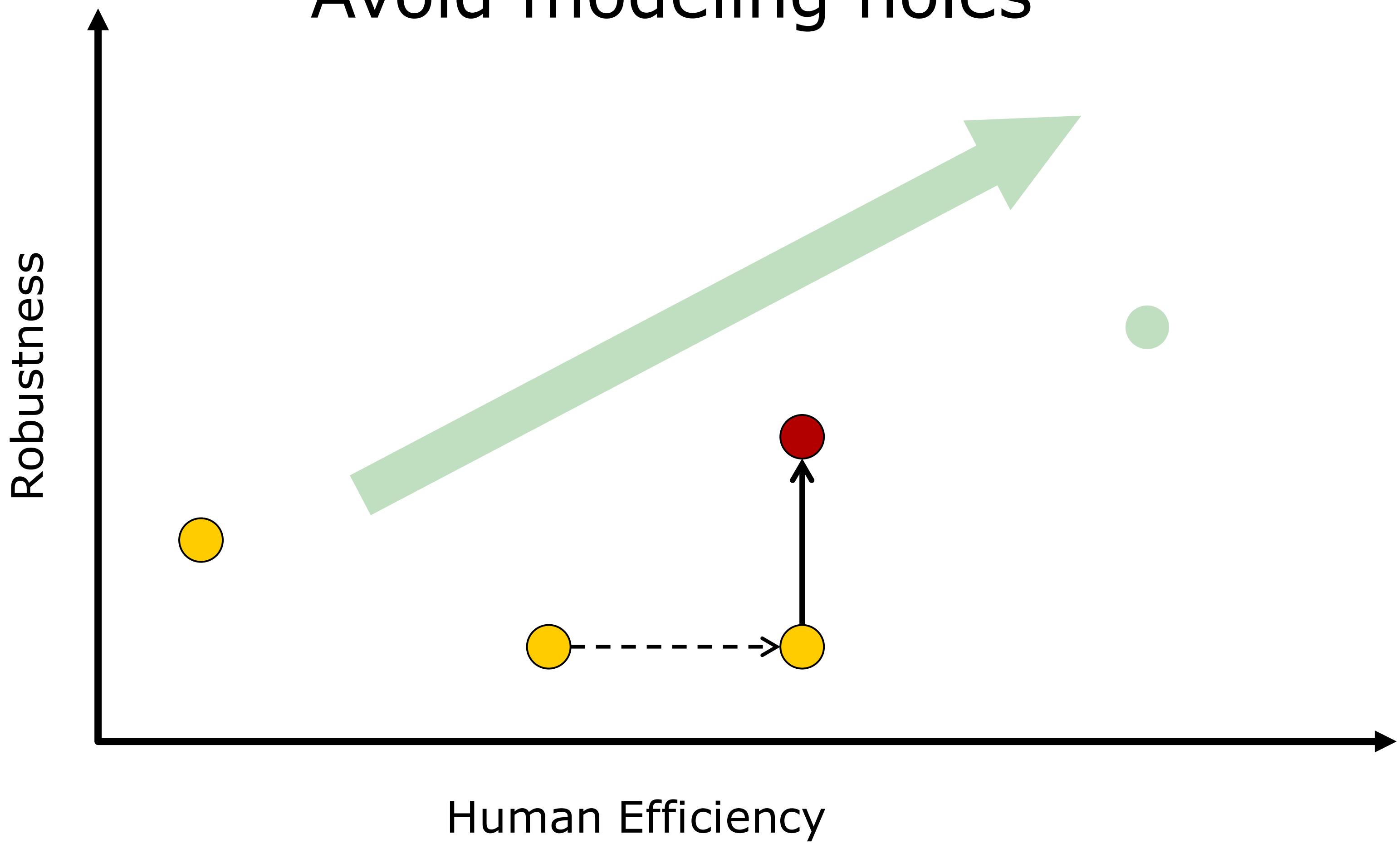


Implicit Complement

- Merging of adjacent surfaces accelerates ray-tracing
- Complex volume defined by all unmerged surfaces
  - Inefficient definition in native MCNP
  - OBB-tree preserves efficiency in DAGMC
- Small gaps between volumes are automatically captured in implicit complement

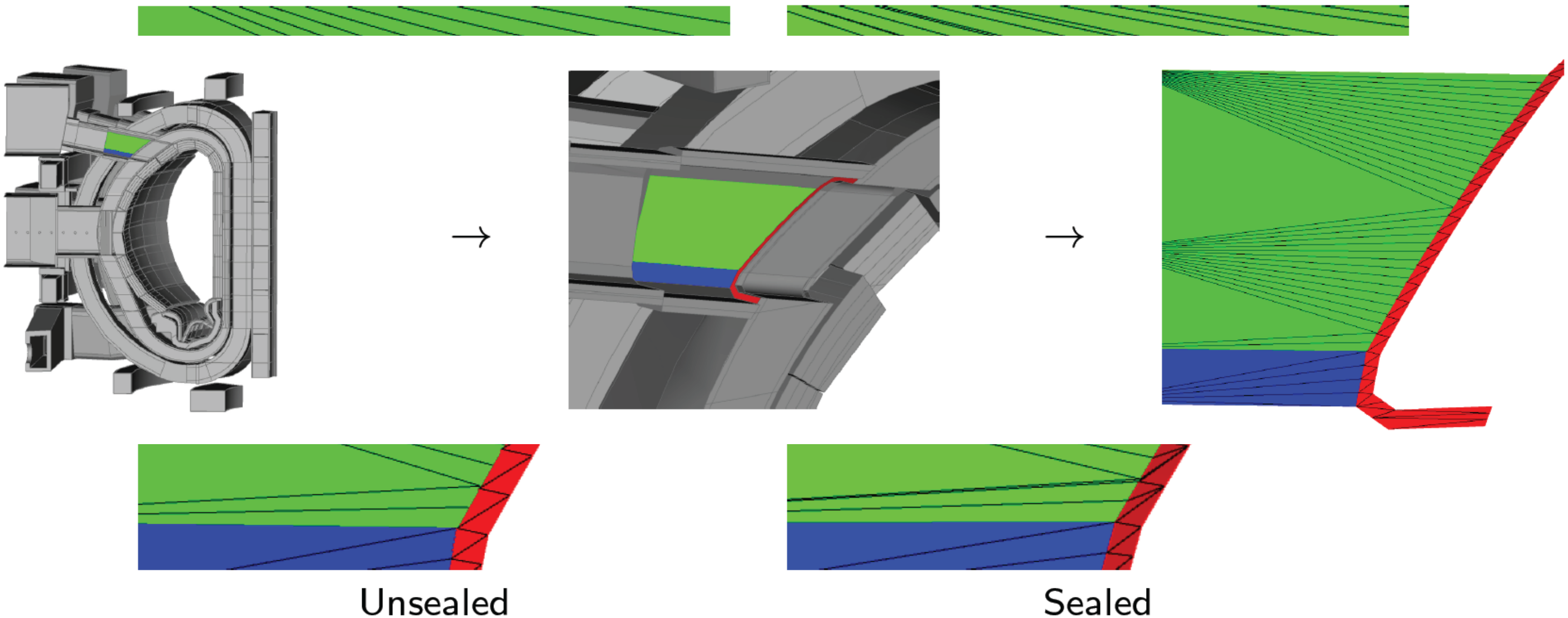
Watertight Faceting

Avoid modeling holes



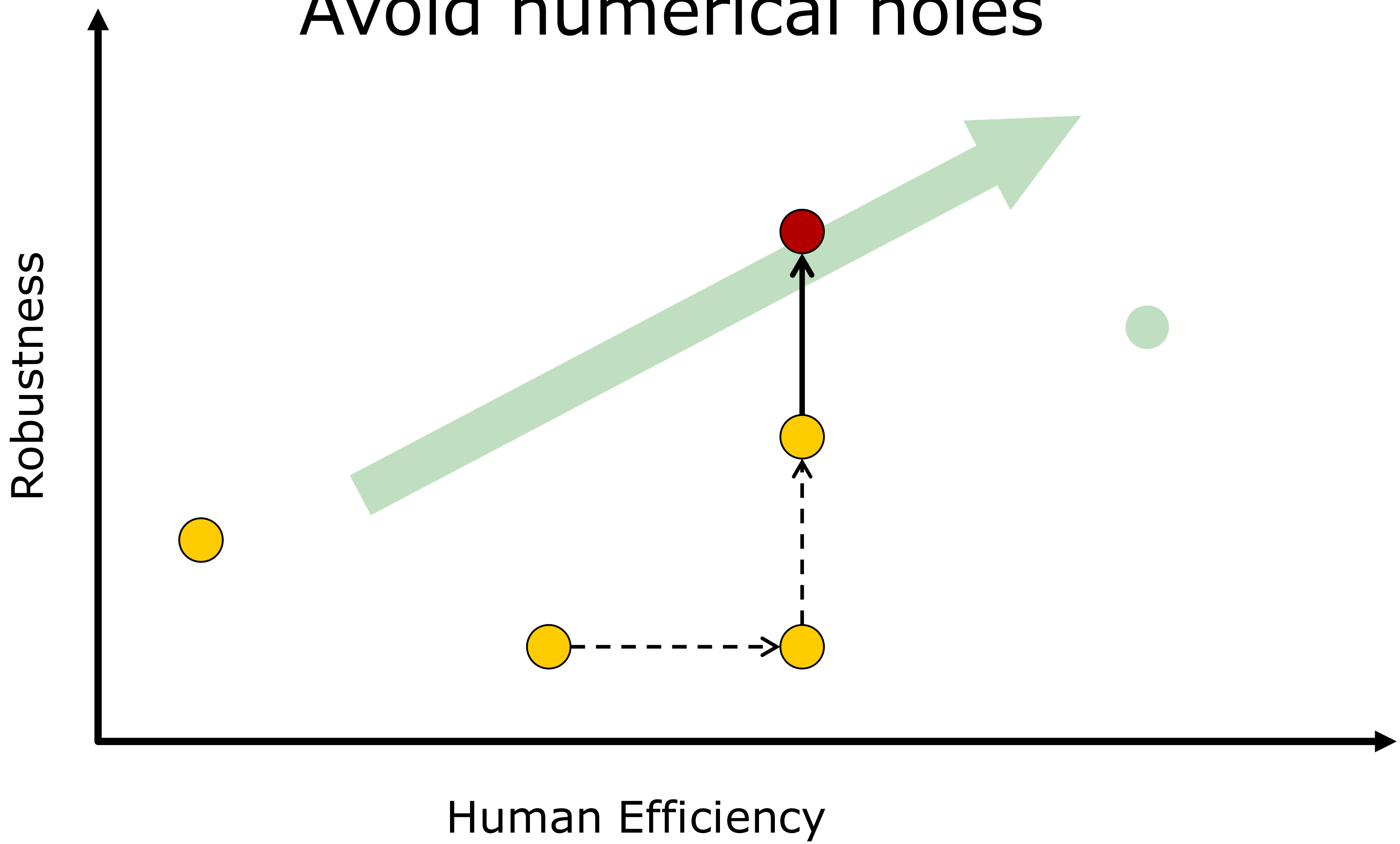
Watertight Geometry

- Watertight faceting not guaranteed in merged geometry



Robust Tracking

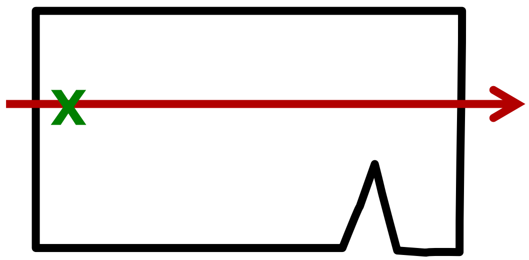
Avoid numerical holes



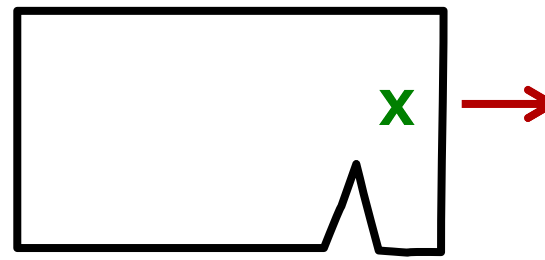
Robust Tracking

- Ray-tracing failure modes

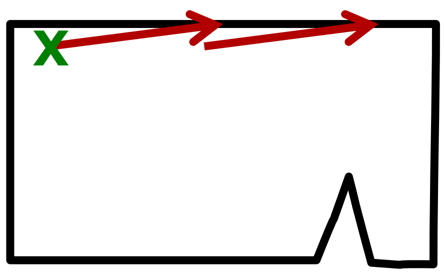
Behind previous surface (numerical)



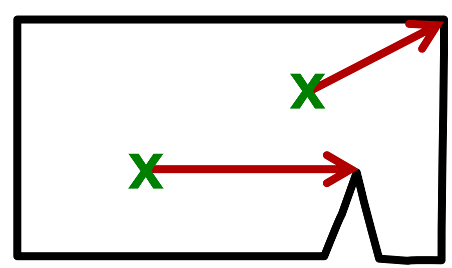
Ahead of next surface (numerical)



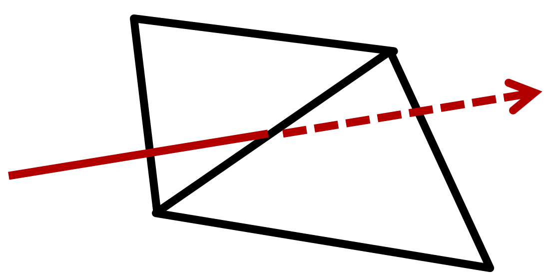
Tangent to Surface (numerical)



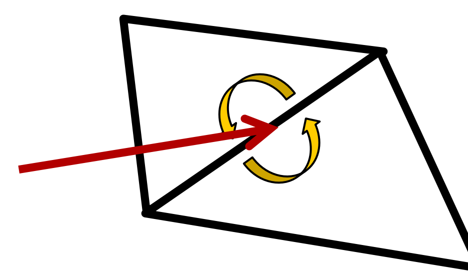
Edge/ Point Intersection (logical)



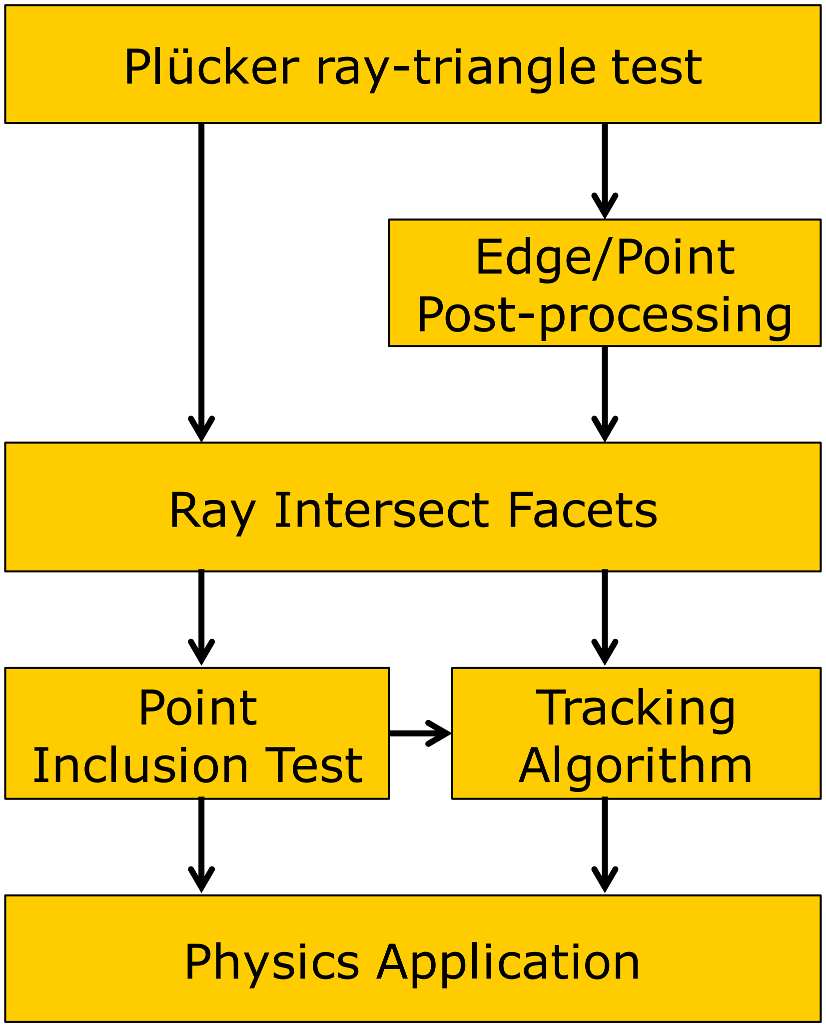
Leak Between Triangles (numerical)



Oscillate Between Triangles (logical)



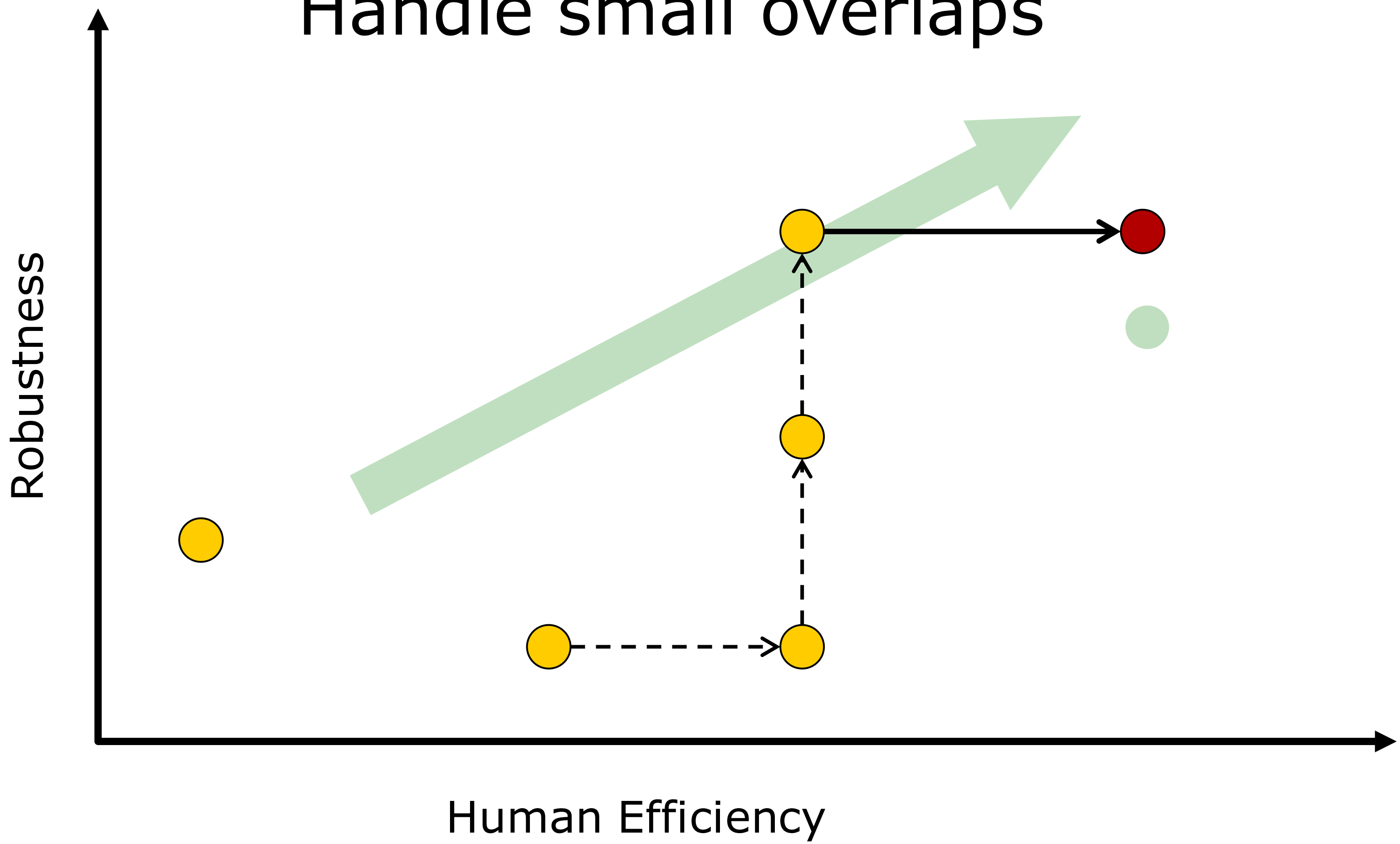
Robust Tracking



Model	Particles Simulated [millions]	Lost Particles	
		Original	Robust
UW Nuclear Reactor	41	5649 ± 178	0
Advanced Test Reactor	74	141 ± 32	0
40° ITER Benchmark	225	67 ± 39	0
ITER TBM	205	665 ± 184	0
ITER Module 4	59	59 ± 19	0
ITER Module 13	79	450 ± 60	0
FNG Benchmark	1310	31273 ± 989	0
ARIES First Wall	4070	25 ± 18	0
HAPL IFE	286	65 ± 19	0
Z-Pinch Fusion	409	2454 ± 317	0

Overlap Tolerance

Handle small overlaps



Overlap Tolerant Tracking

- User specifies an overlap tolerance
  - Only numerical tolerance in DAGMC ray tracing
- Search behind current point for intersection within tolerance
- Update logical location if in overlap
- Does NOT preserve exact physics in overlap region

Produced by University Communications

User’s Perspective

Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

Standard CAD software tools are used to define the solid model.

Models are exported to a standard geometric-model file format supported by Common Geometry Module (CGM).

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

Allocate materials and densities

Define boundary conditions

Define tally locations

Imprint & Merge

(Currently use CUBIT mesh generation tool for this step)

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

Skip cell definitions

Skip surface definitions

Provide data cards
- Material definitions
- Tally modifiers
- Source definition
- etc…

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

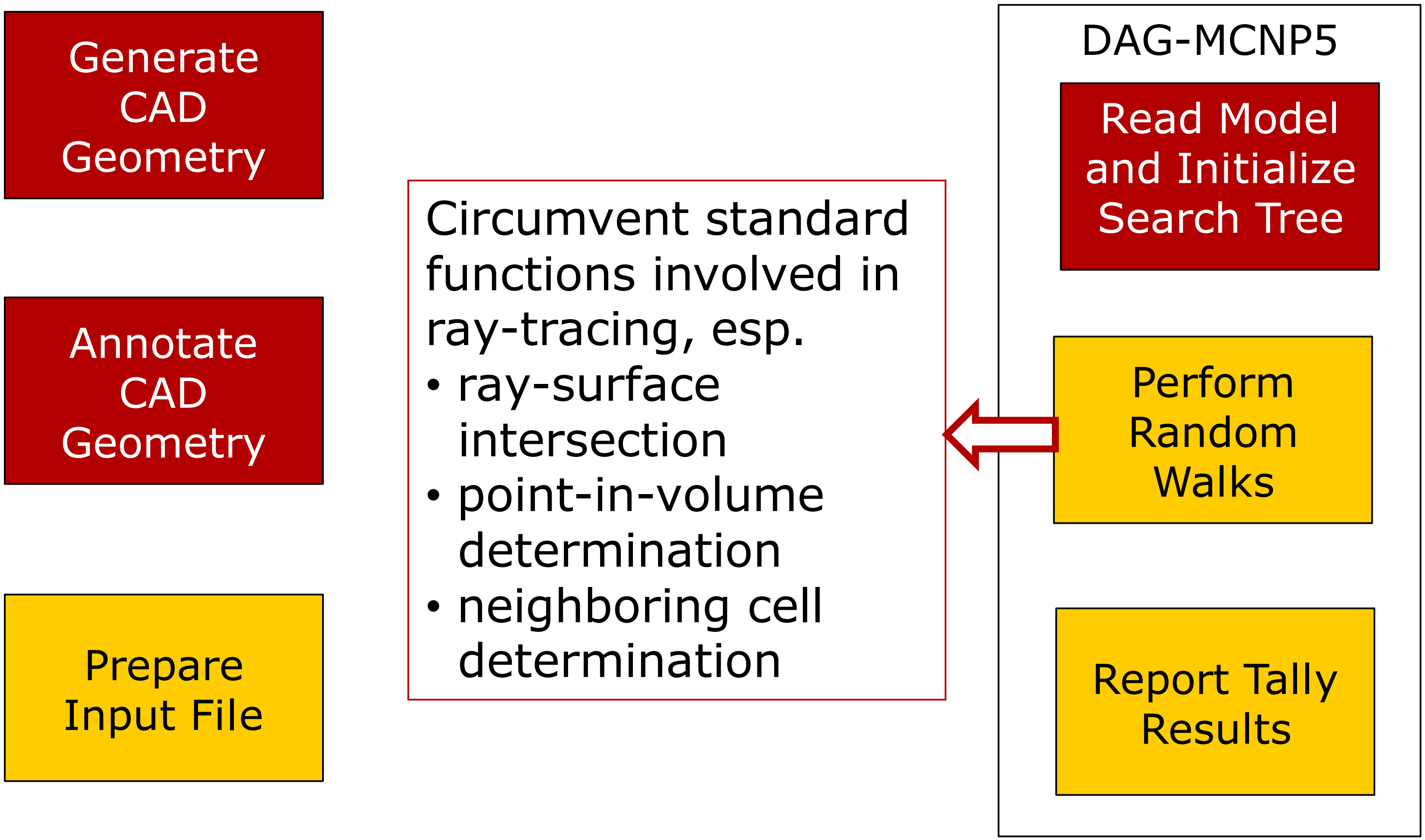
Prepare Input File

Generate *tree-based decomposition* of facets on model surfaces

DAG-MCNP5

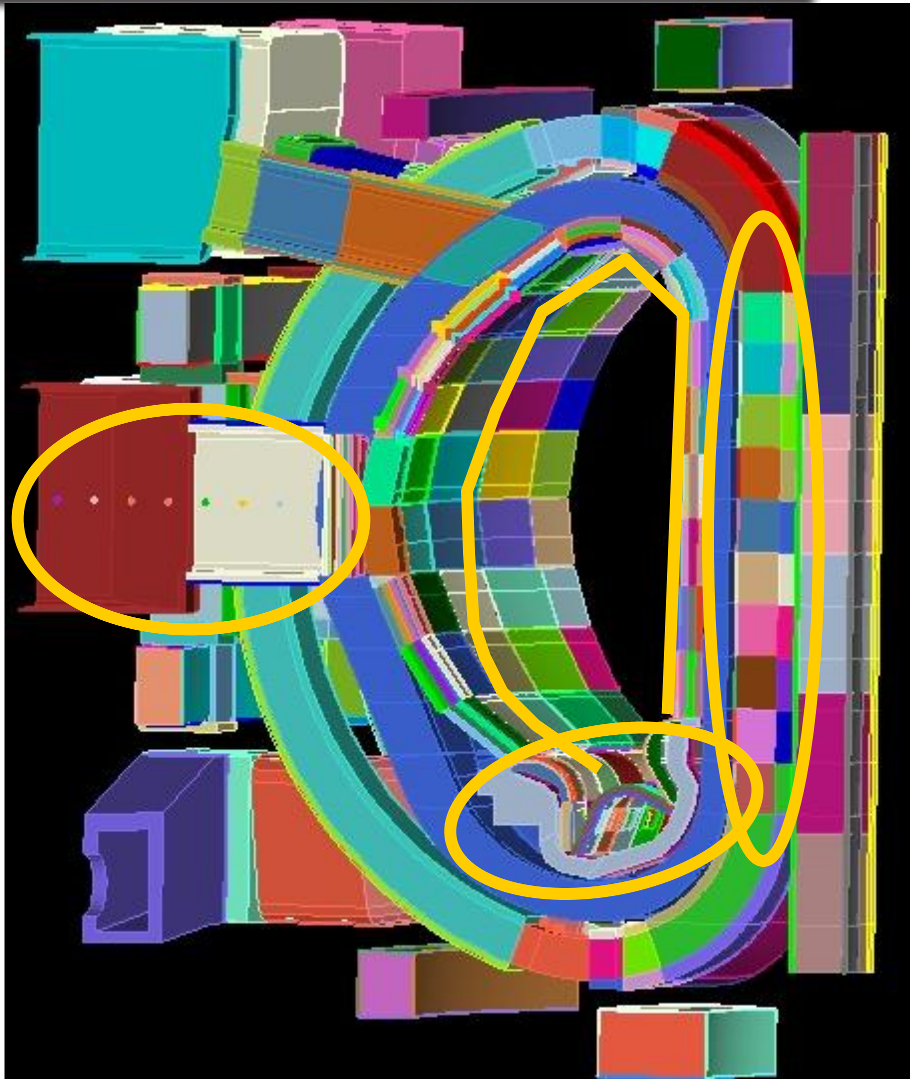
- Read Model and Initialize Search Tree
- Perform Random Walks
- Report Tally Results

Workflow Includes a Variety of New Tools and Skills

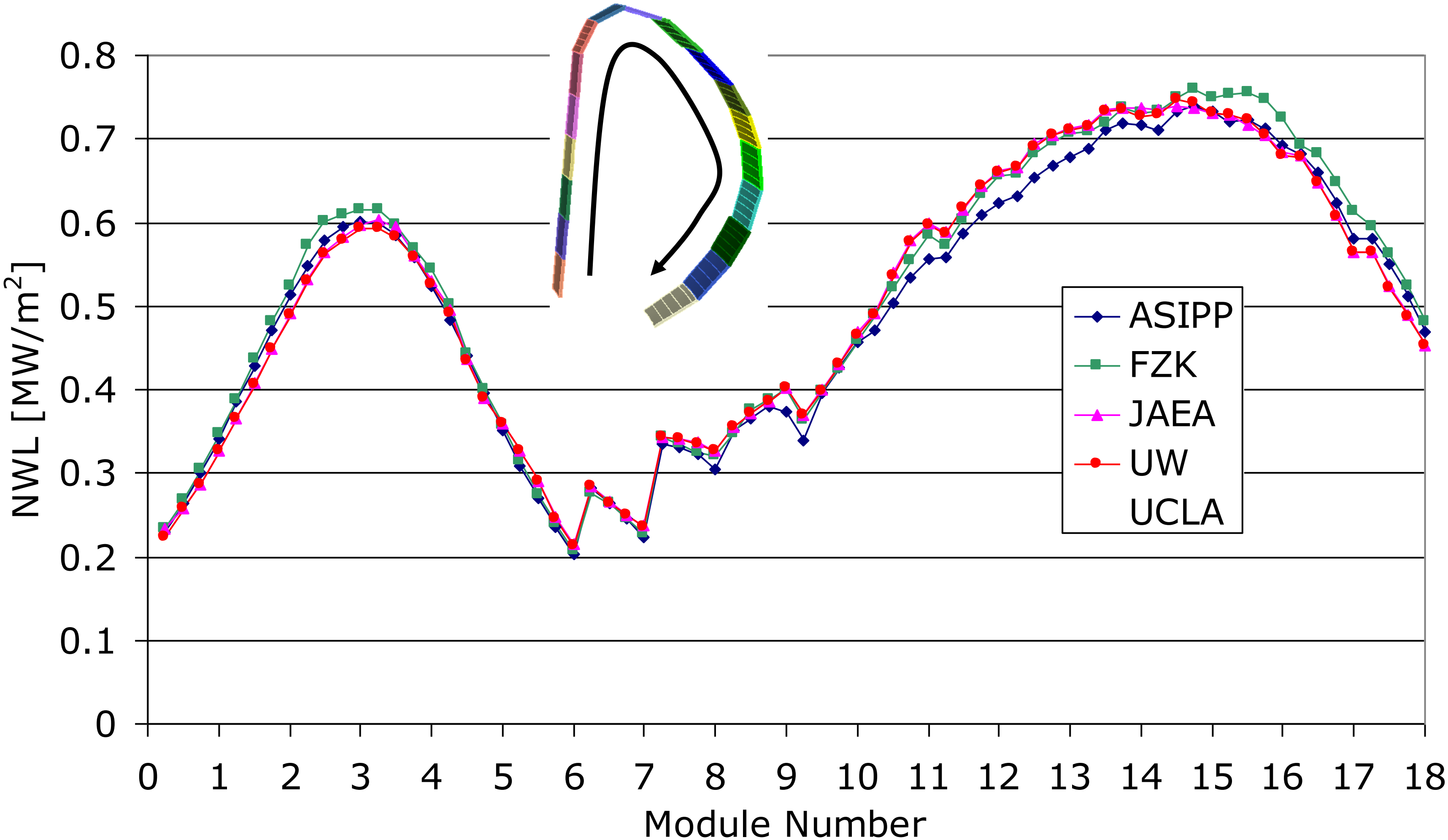


ITER Benchmark

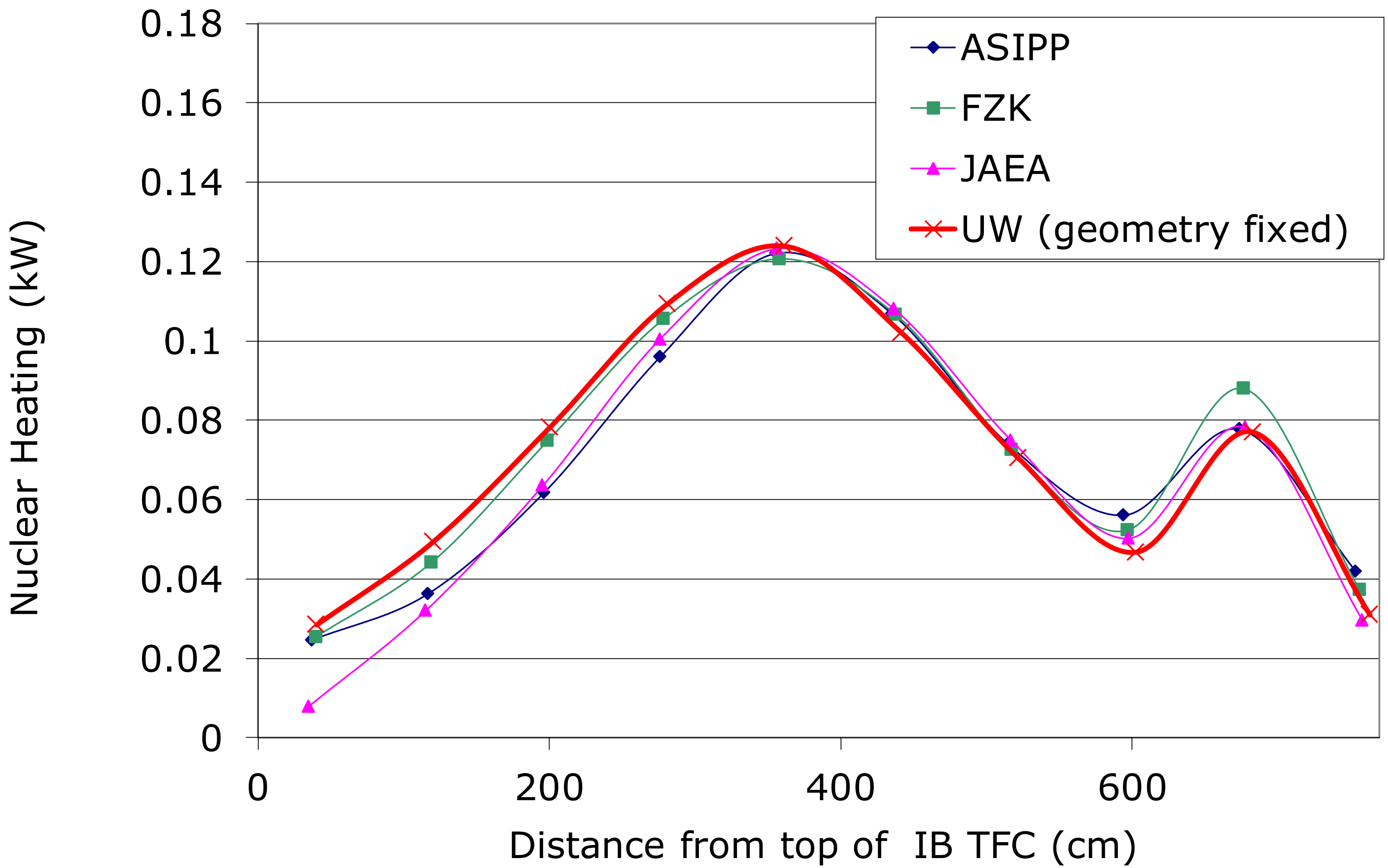
- Comparing 4 problems
  - Neutron wall loading
  - Divertor fluxes and heating
  - Magnet heating
  - Midplane port shielding/streaming
- Participants
  - UW, FZK, ASIPP, JAEA + ATTILA (UCLA/PPPL)



Neutron Wall Loading

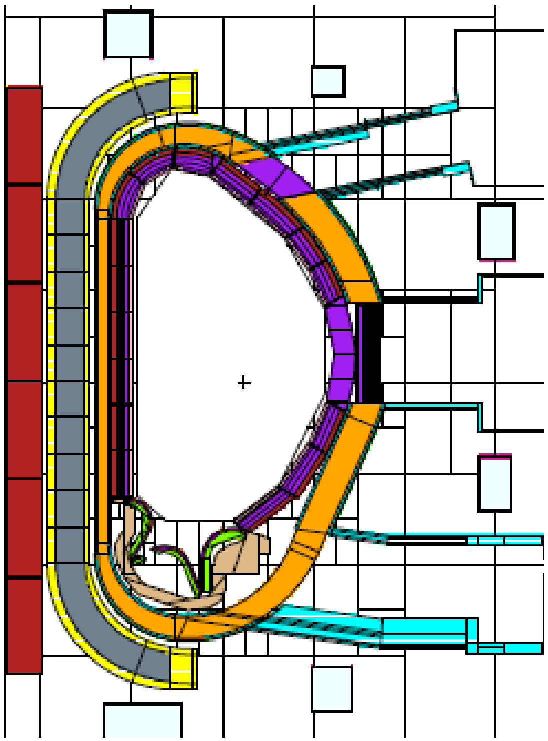


IB TFC heating

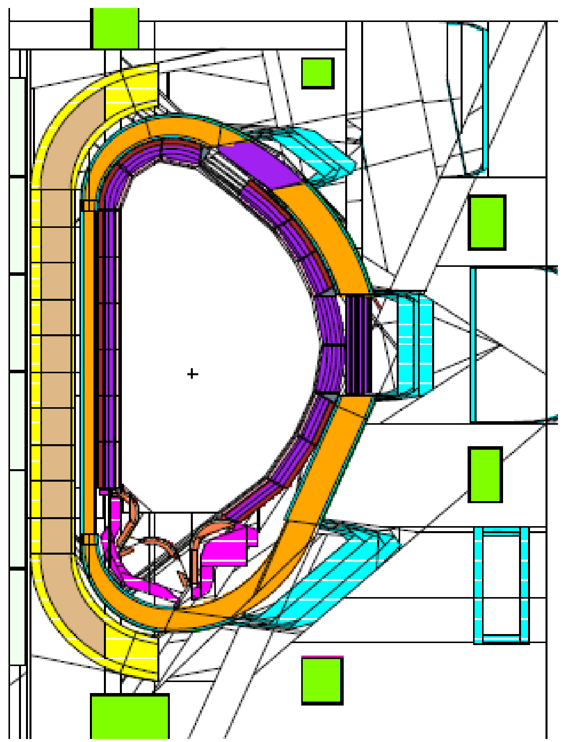


Performance Compared Using Translated Models

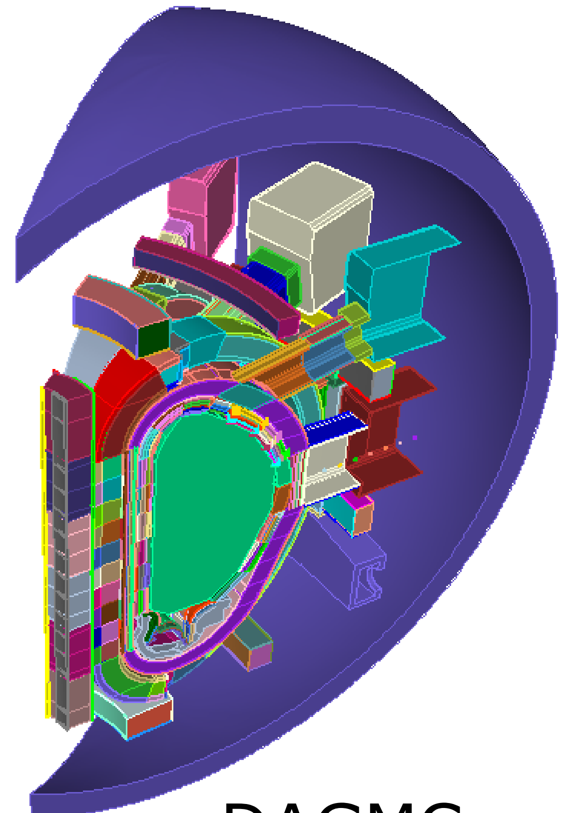
ITER Benchmark Model: >800 cells, ~10,000 surfaces



MCAM Translation



McCad Translation



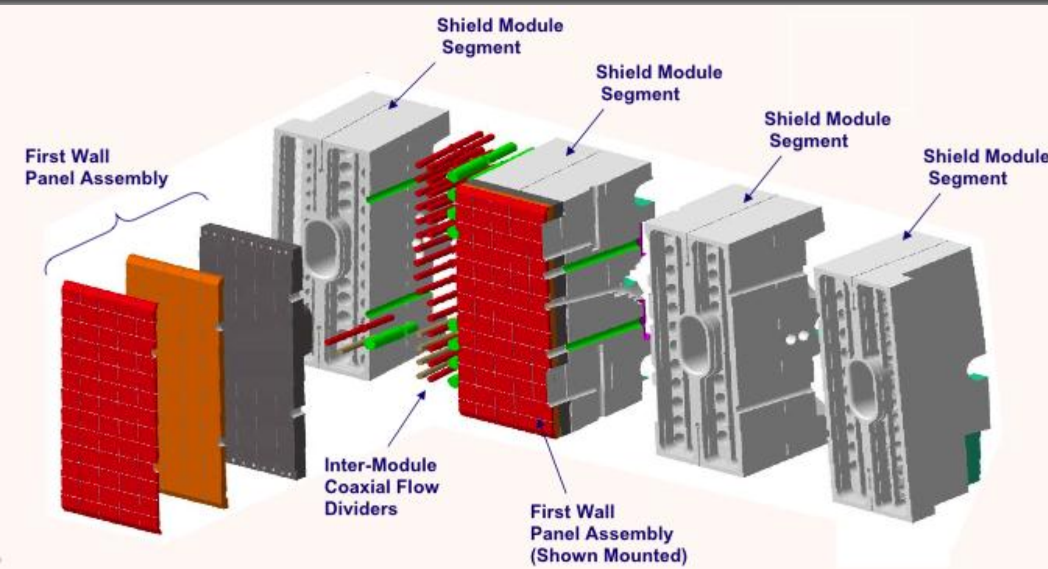
DAGMC Solid Model

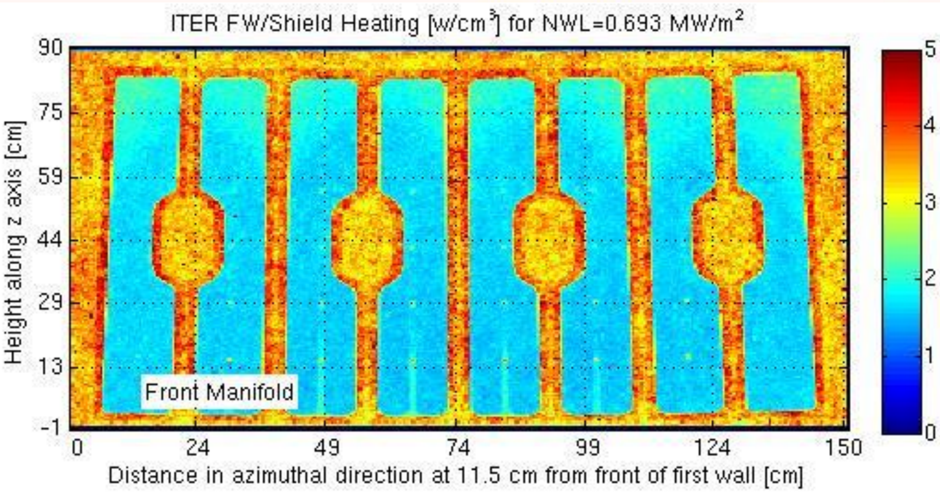
Overall Performance Less than 3x Slower than Native Geometry

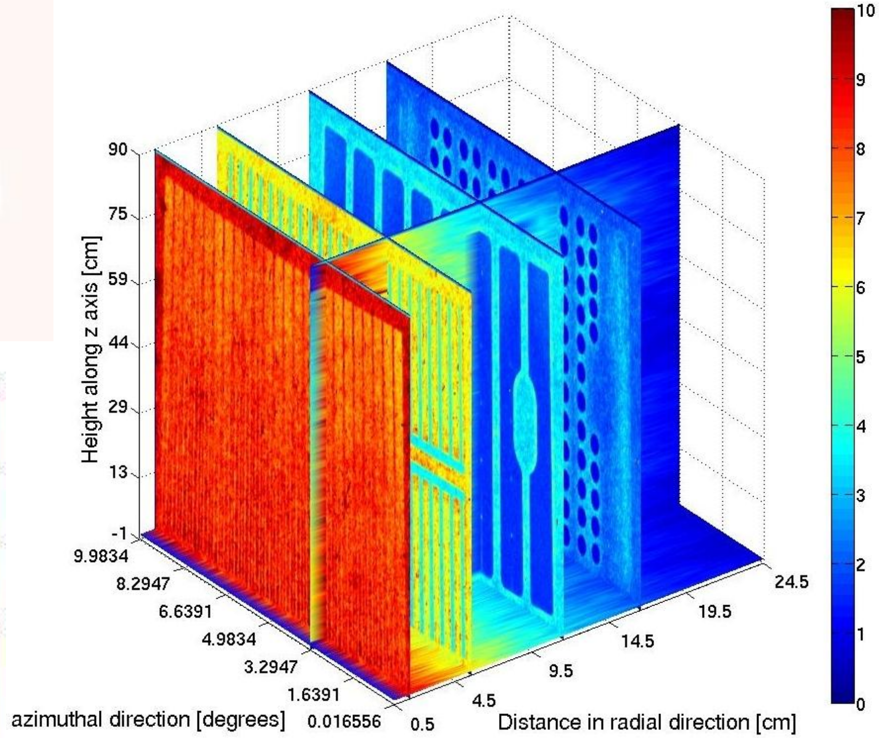
- Performance of translation approaches vary by 60%

Model	Number of Volumes	Number of Surfaces	**Relative CPU-Time**
MCAM translation	4148	3192	**1**
McCad translation	6031	3800	**1.63**
DAGMC	802	9834	**2.46**

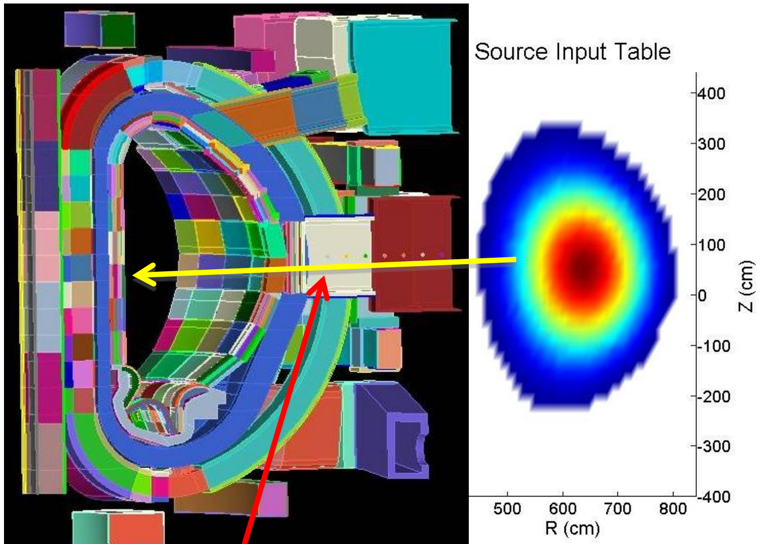
Analysis for an Initial Mod 13 Design

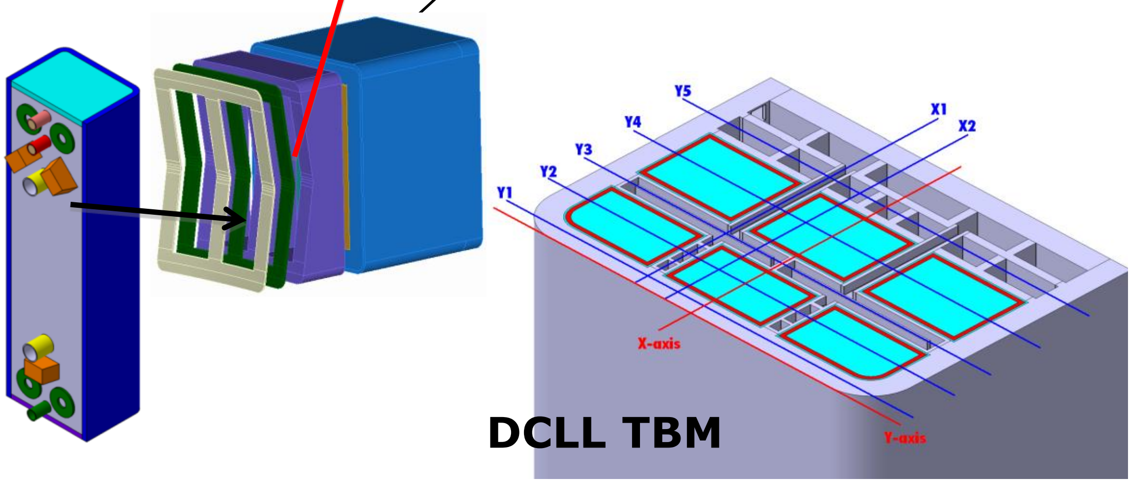




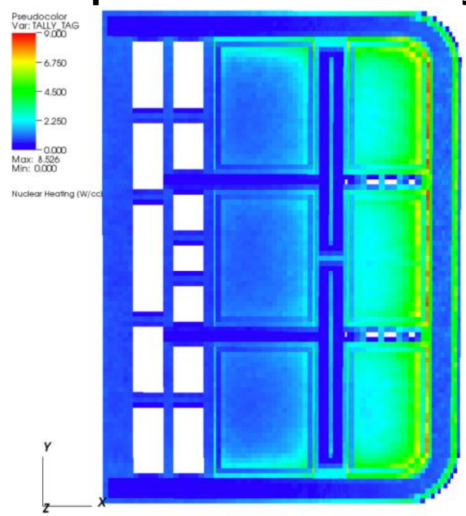


Detailed 3-D Neutronics for DCLL TBM

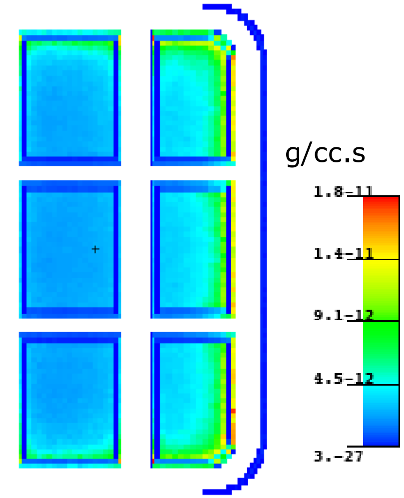




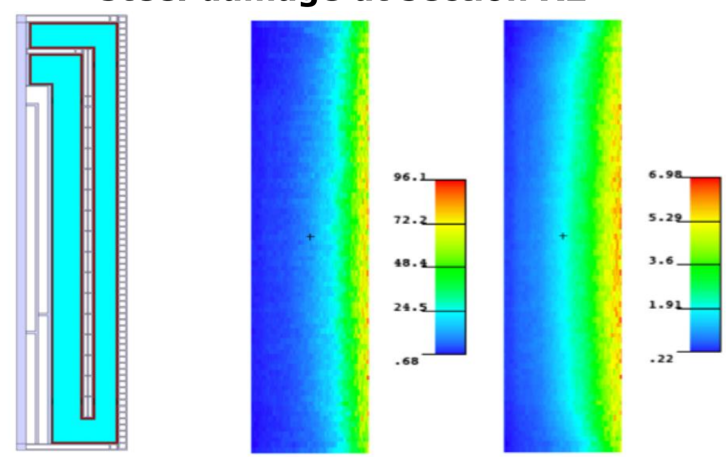
Mid-plane nuclear heating



Mid-plane T production

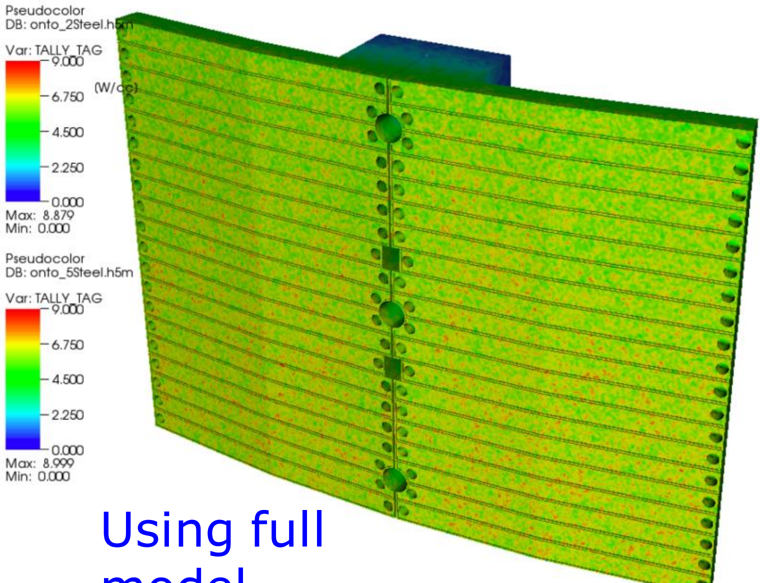


Steel damage at section X2



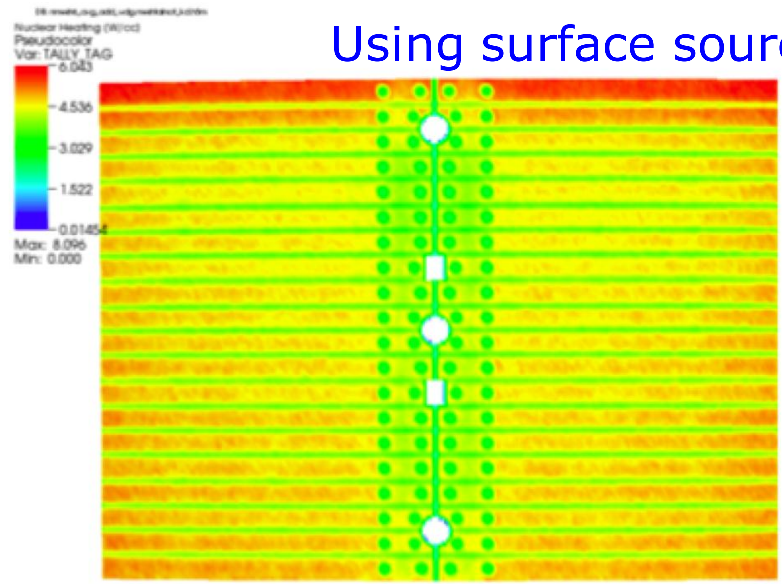
Cross section He appm/FPY dpa/FPY

Surface Source Approach Applied to ITER FWS Mod. 4



Using full model

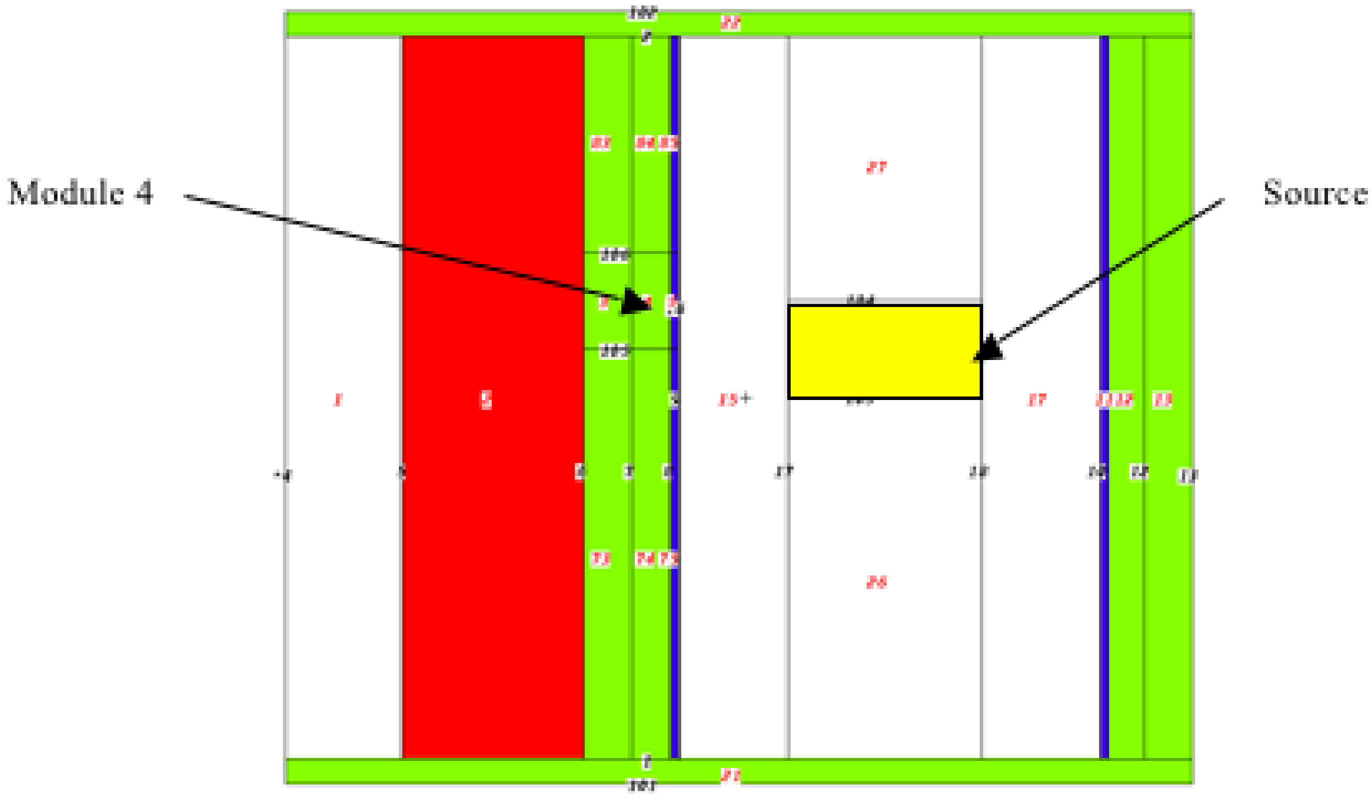
Using surface source



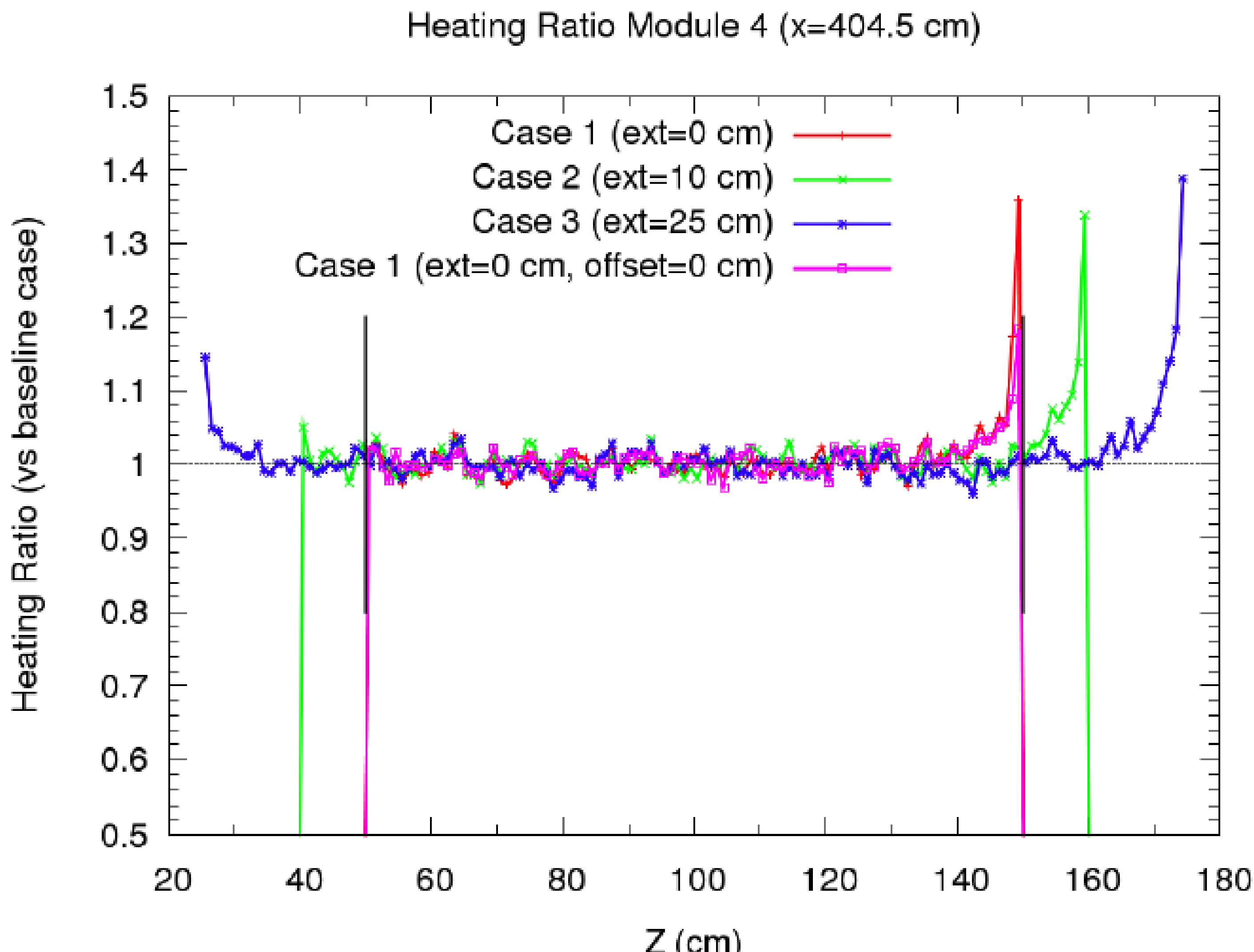
Overestimate in nuclear heating (MW) resulting from surface source.

	Full ITER Model	Surface Source Model	% Overestimate
Beryllium	0.0535	0.0543	1.50%
CuCrZr	0.0350	0.0356	1.71%
Steel	0.757	0.790	4.36%
Water	0.150	0.157	4.67%

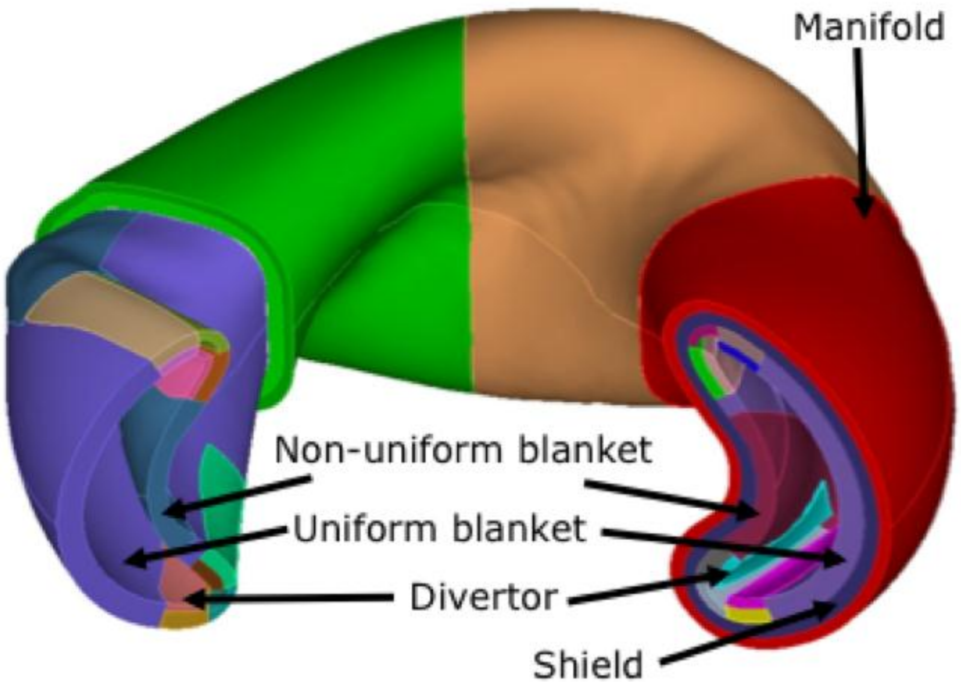
Assessment of Accuracy of Surface Source Approach



Assessment of Accuracy of Surface Source Approach



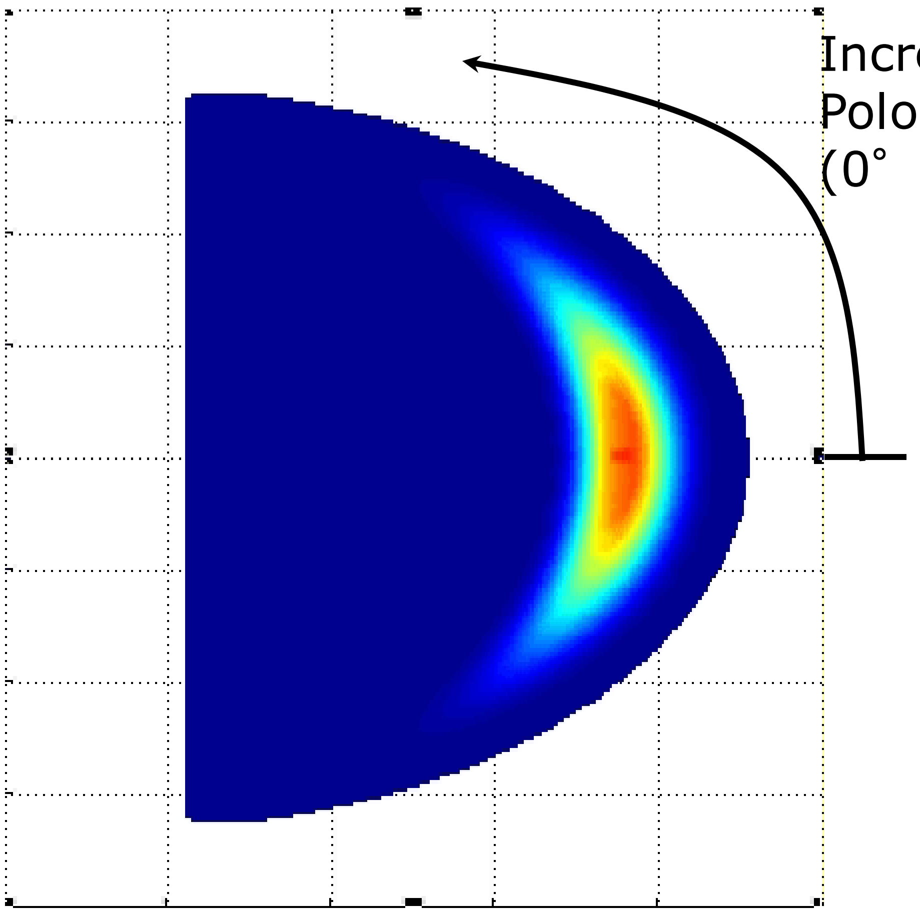
Application to ARIES-CS Compact Stellarator



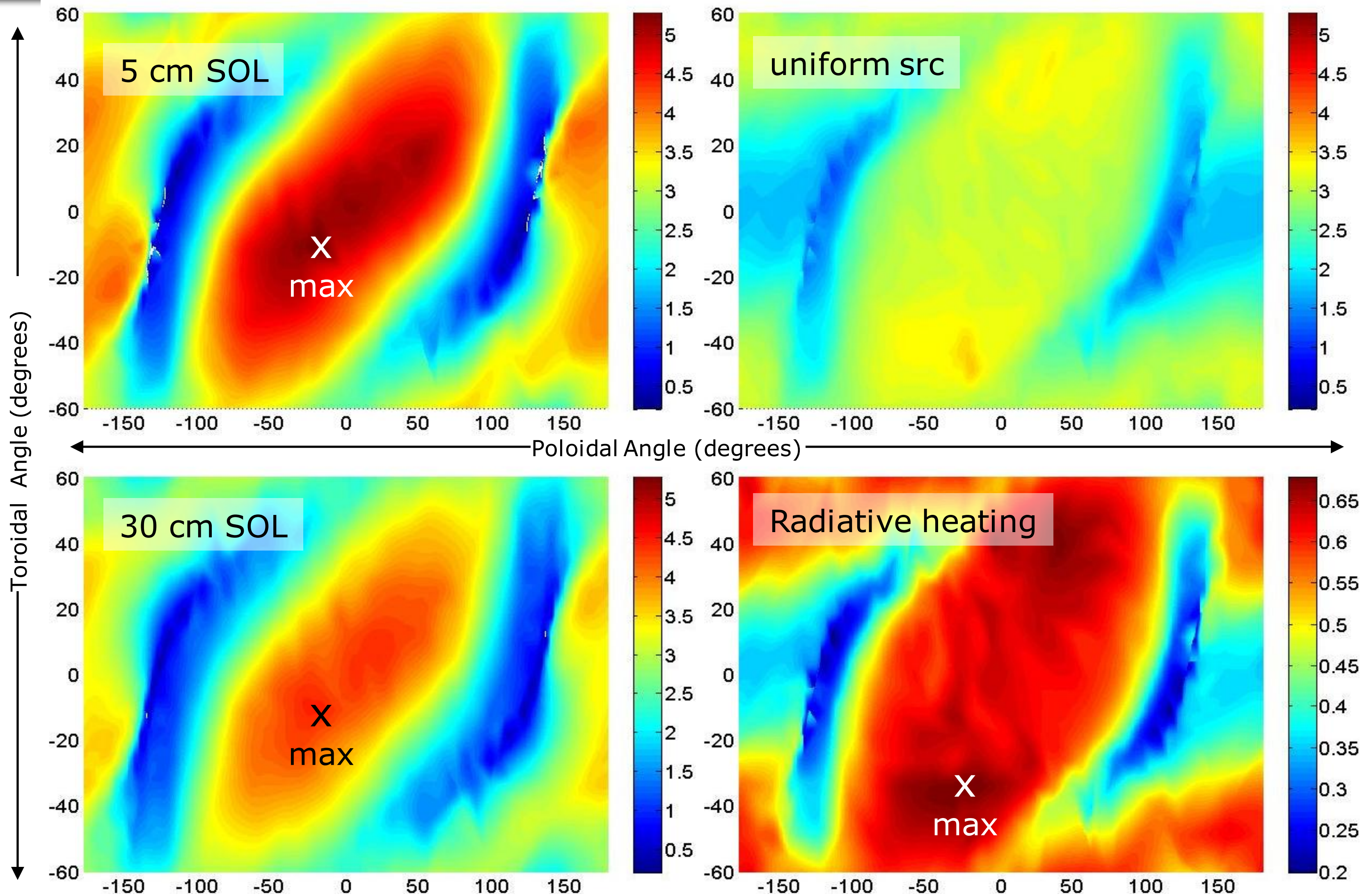
- Geometry complex
- FW shape and plasma profile vary toroidally within each field period
- Cannot be modeled by standard MCNP

Examined effect of helical geometry and non-uniform blanket and divertor on NWL distribution and total TBR and nuclear heating

Source Probability Map



NWL Maps (colormaps in MW/m^2)

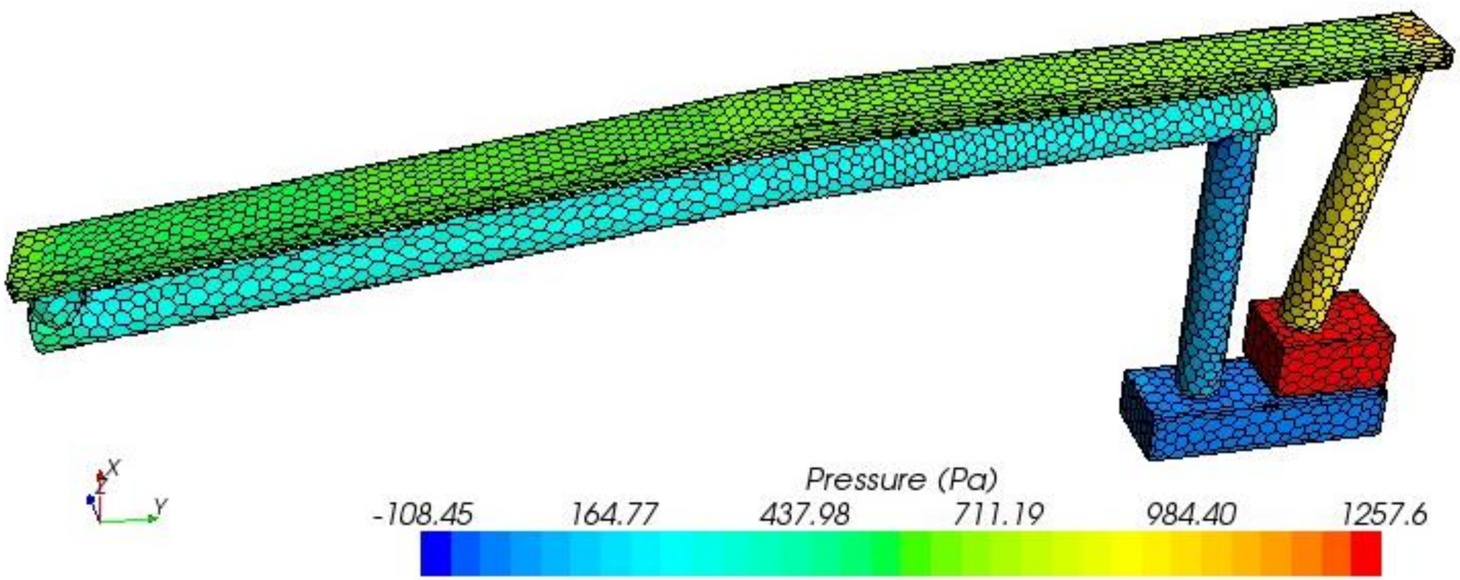


Multi-Physics: Coupling to CFD

- Fine mesh DAG-MCNP5 results
  - 1-3 mm Cartesian mesh overlay
  - Total nuclear heating
- Arbitrary mesh on CAD geometry
  - Tetrahedral
  - Polyhedral (Star-CCM+)
- Automated interpolation using MOAB

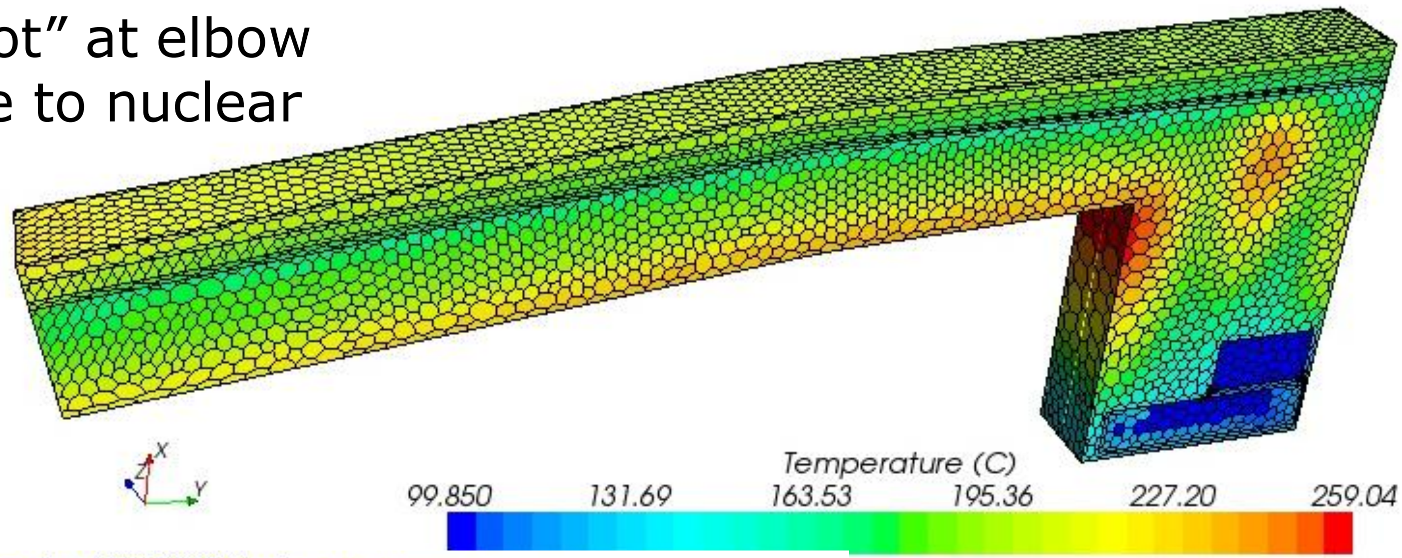
Multi-Physics: Coupling to CFD

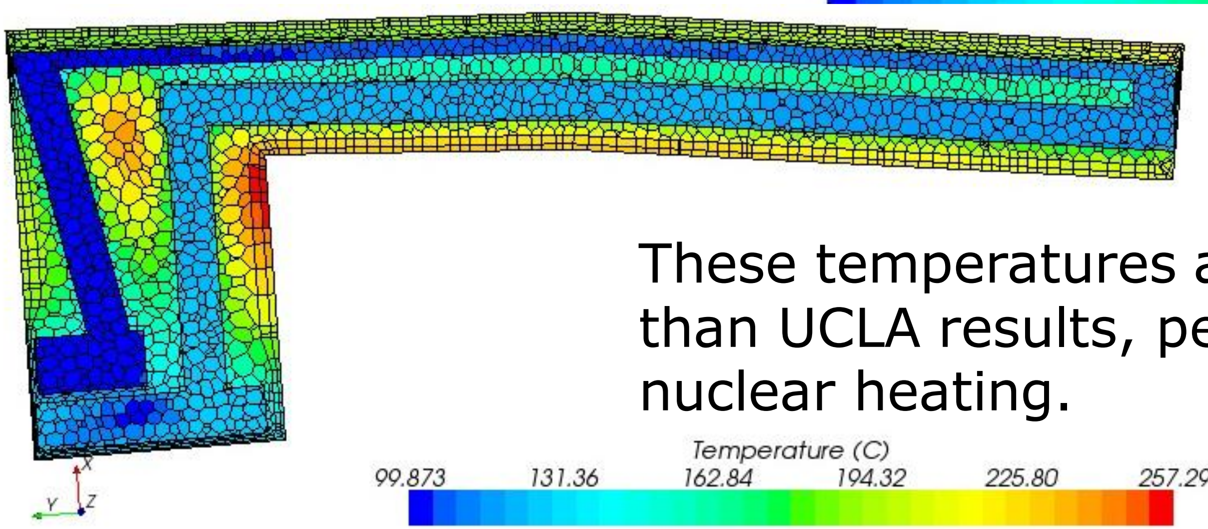
- 1 of 40 fingers in ITER First Wall concept
- Beryllium plasma facing component
- CuCrZr heat sink into pressurized water
- Steel backing for structural support
- 0.2 MW/m^2 heat flux onto Beryllium
- Inlet: 0.2 kg/s water, 373 K, 3 Mpa



Neutronics+CFD Coupling

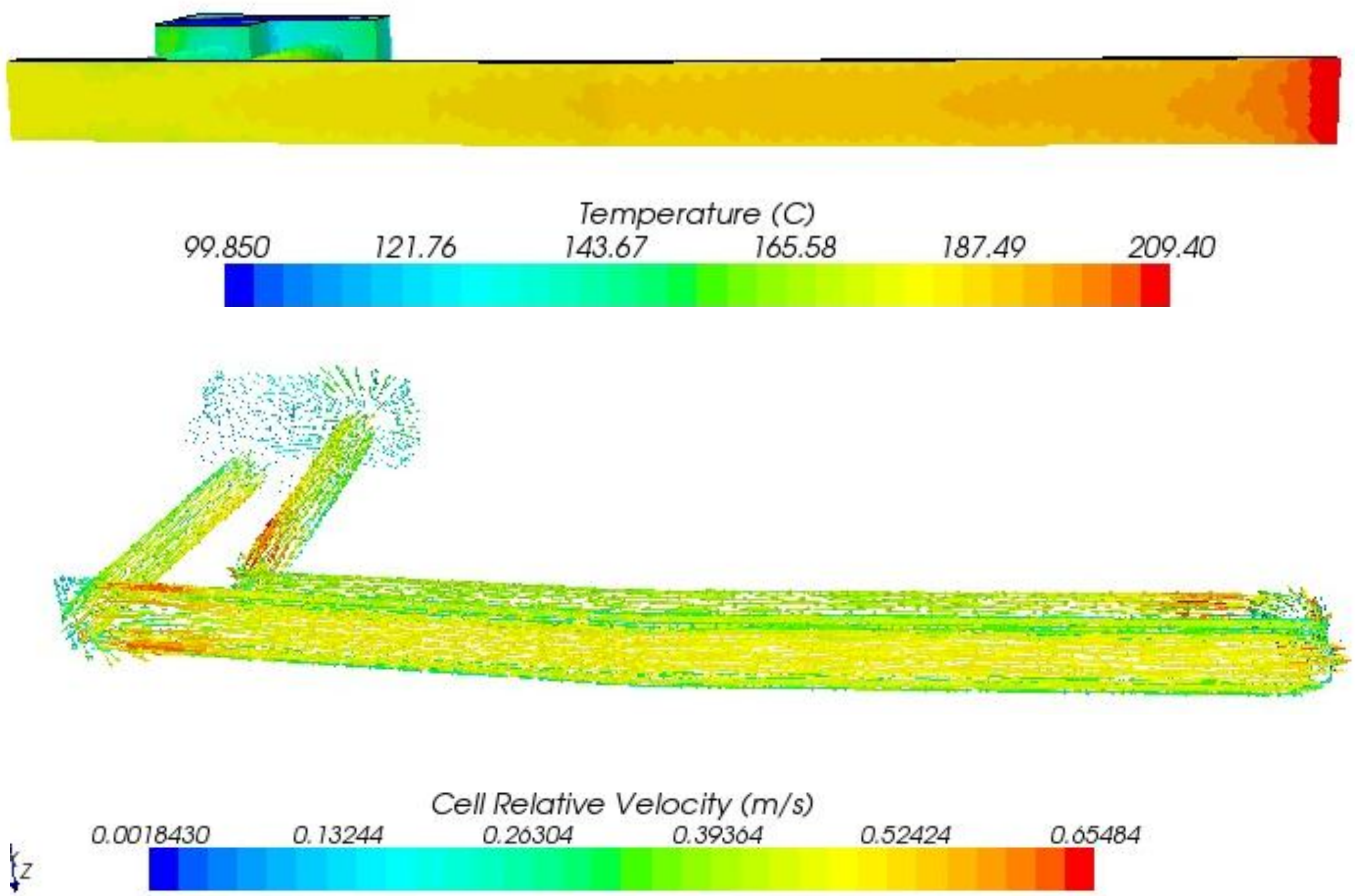
Notice “hot spot” at elbow and center due to nuclear heating.



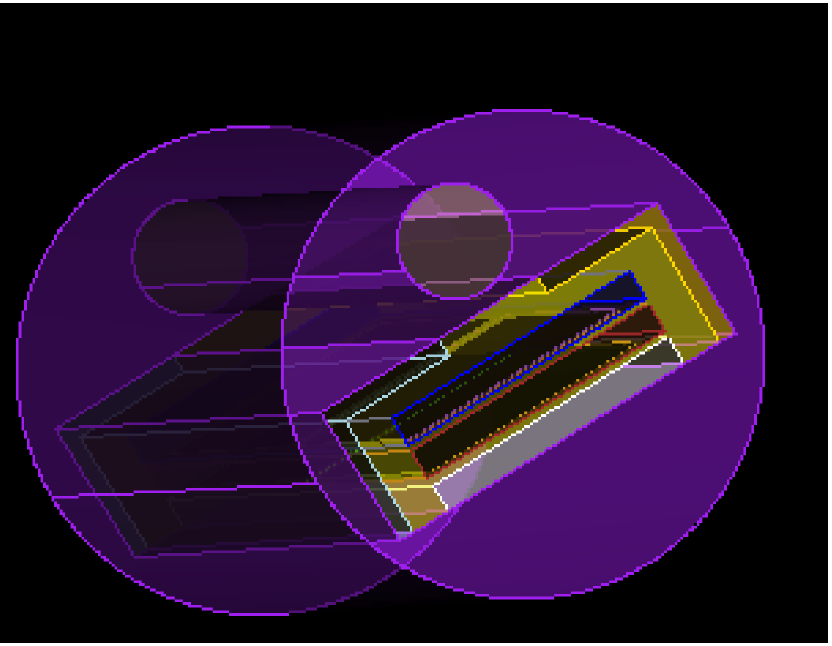


These temperatures are ~30C higher than UCLA results, perhaps due to nuclear heating.

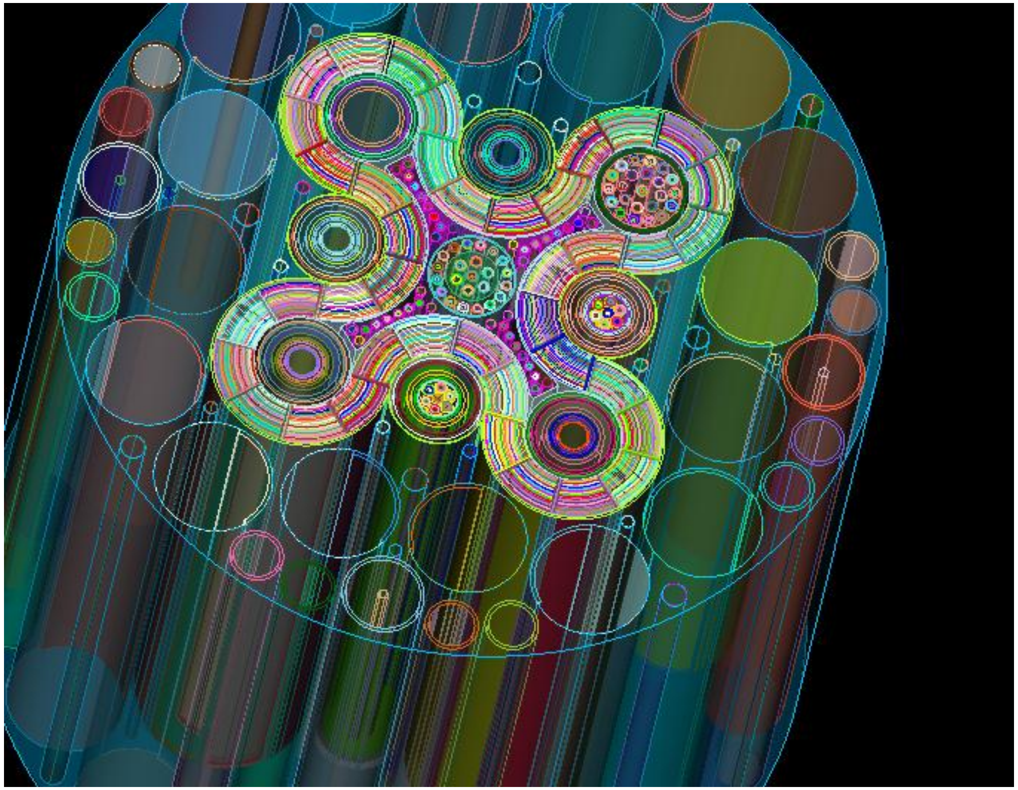
Fluid Temperature & Velocity



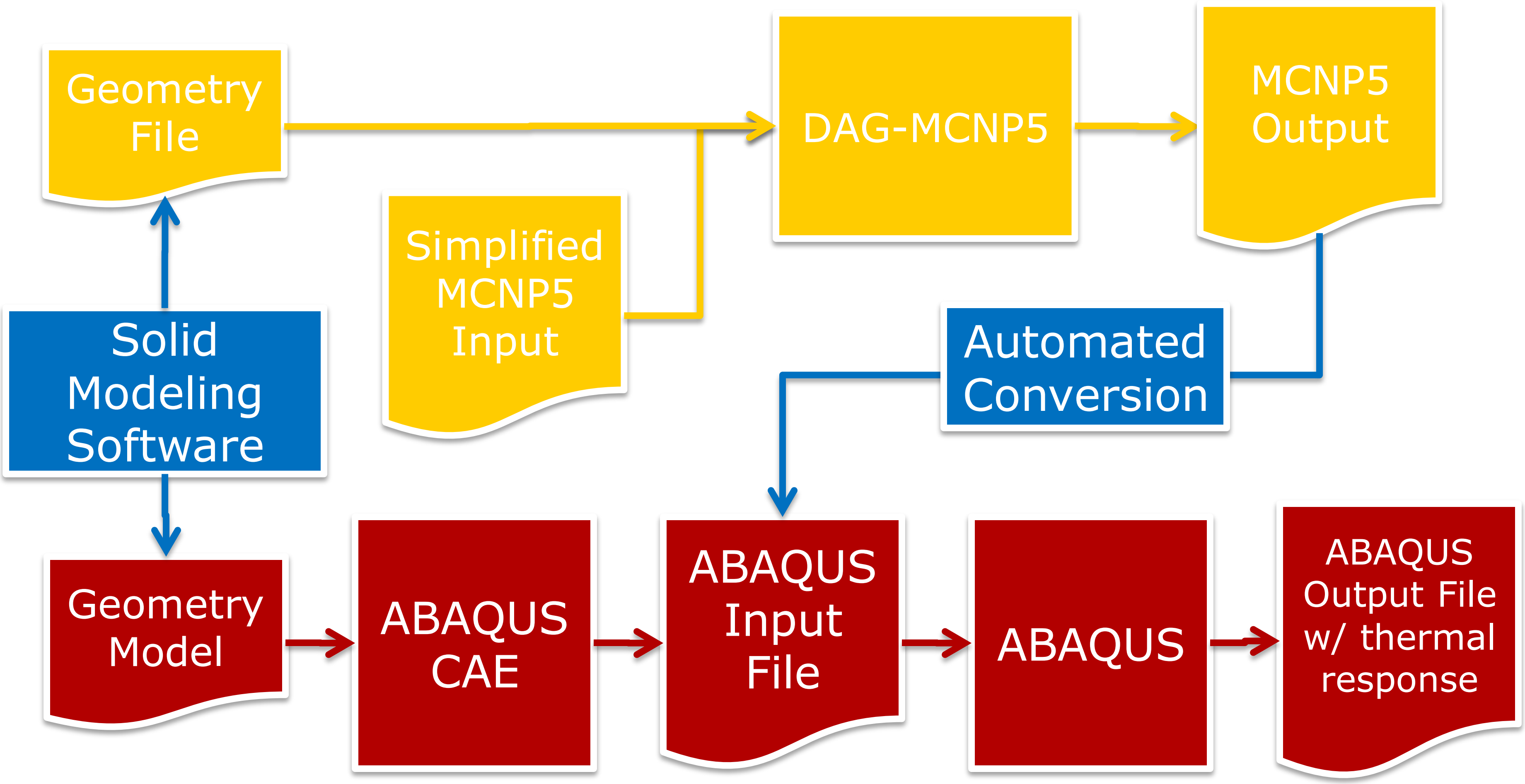
Fission Applications
ATR National Science User Facility



AFIP Experiment In CFT

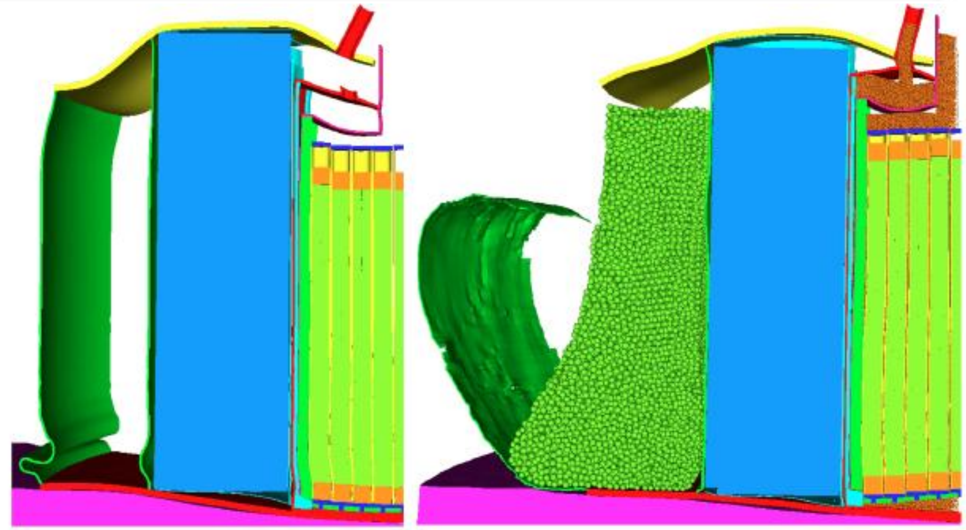
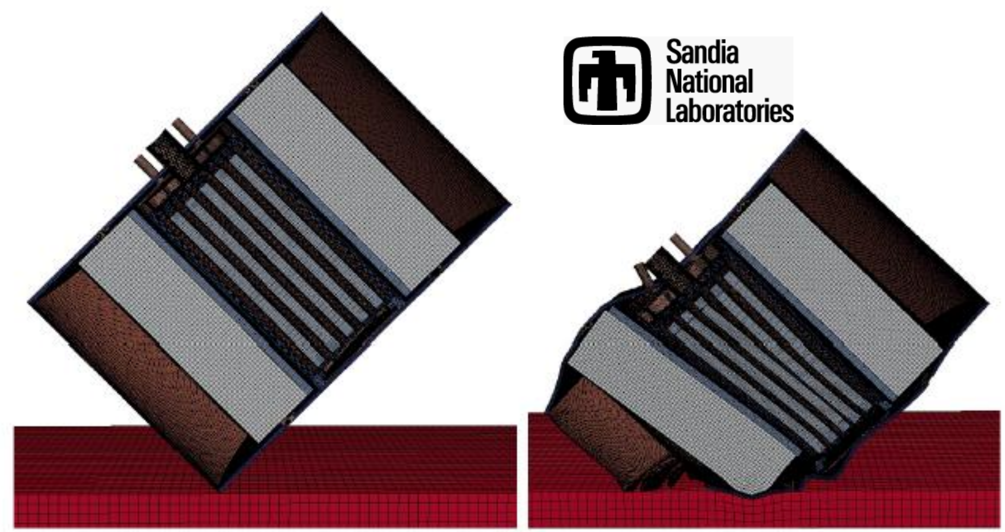


Fission Applications
Irradiation Experiment Design



Neutron Transport in Deformed Geometries

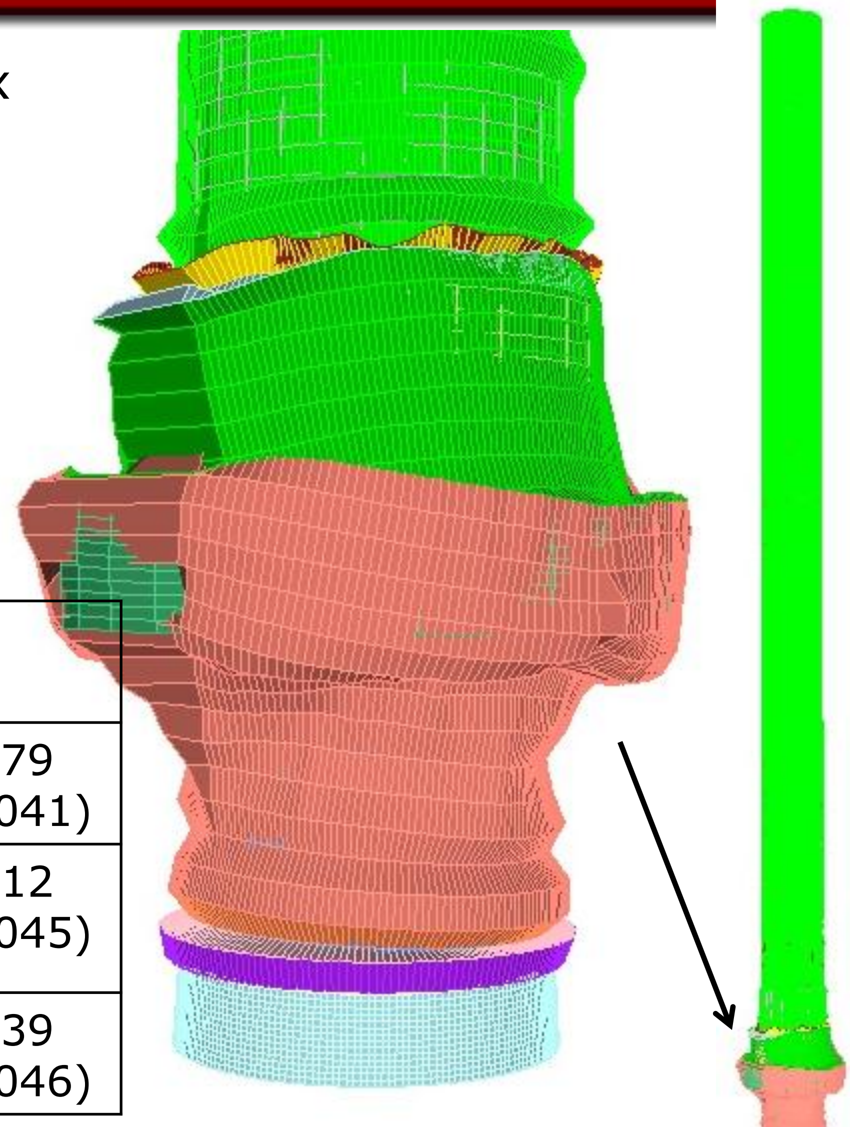
- Space reactor launch accidents may result in reactor return to earth
- Criticality of intact reactor well understood
- Impact likely to deform reactor
- Is criticality possible?

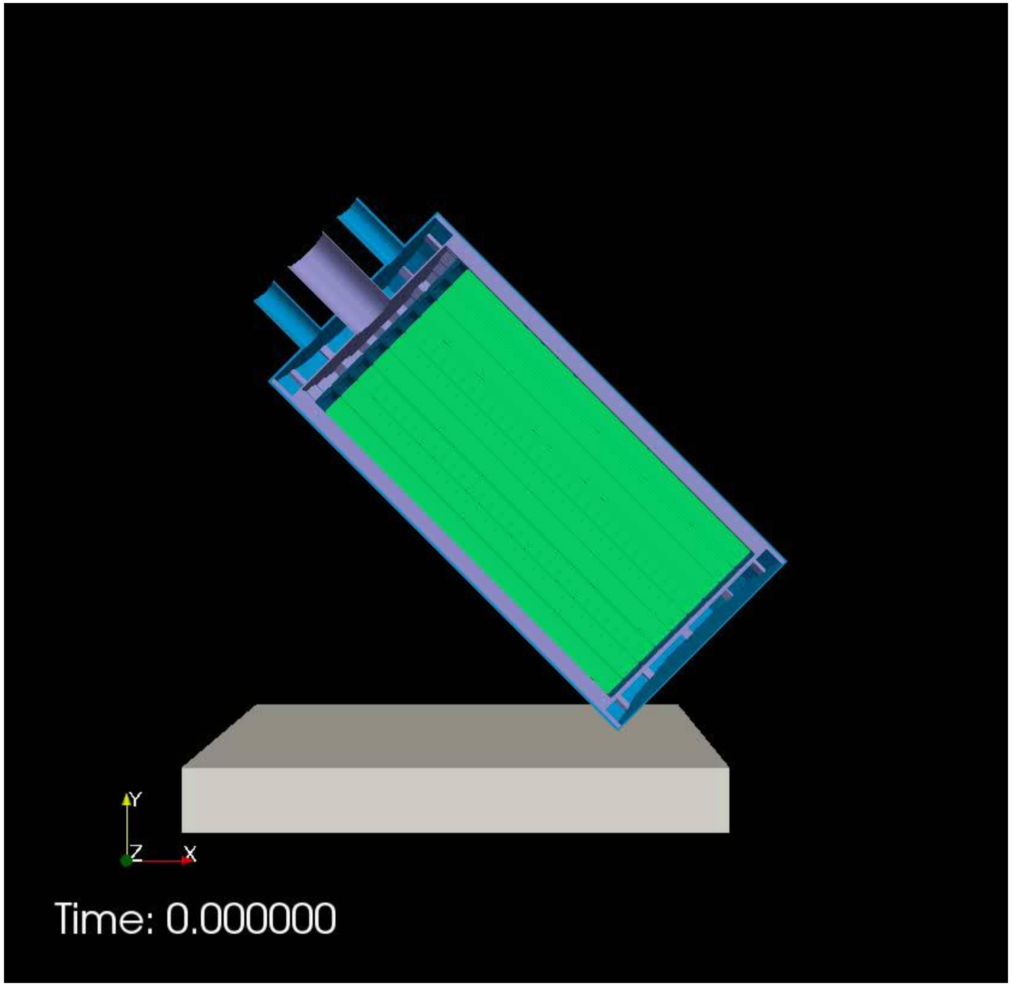
The single pin k_{eff} increases with deformation.

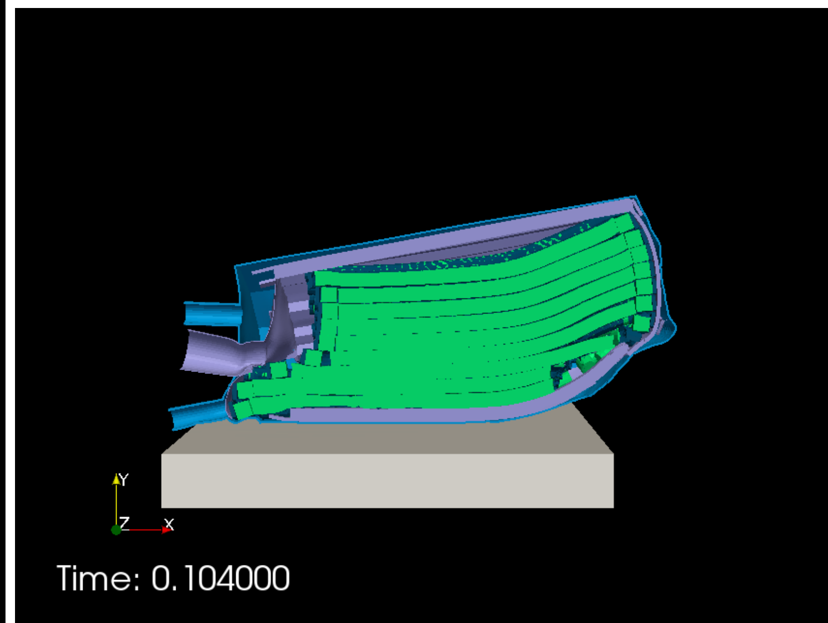
- 33 volumes, 113 surfaces, 103k hex elements
- Clad is not explicitly modeled
  - Clad is homogenized with fuel
- Fuel pin is surrounded by void
- Same MCNP material density was used pre/post deformation

Time Step	Stage	k_{eff}
1	Undeformed	0.84479 (0.00041)
29	Last deformed step w/out dead elements	0.92412 (0.00045)
50	Last deformed step	0.96939 (0.00046)



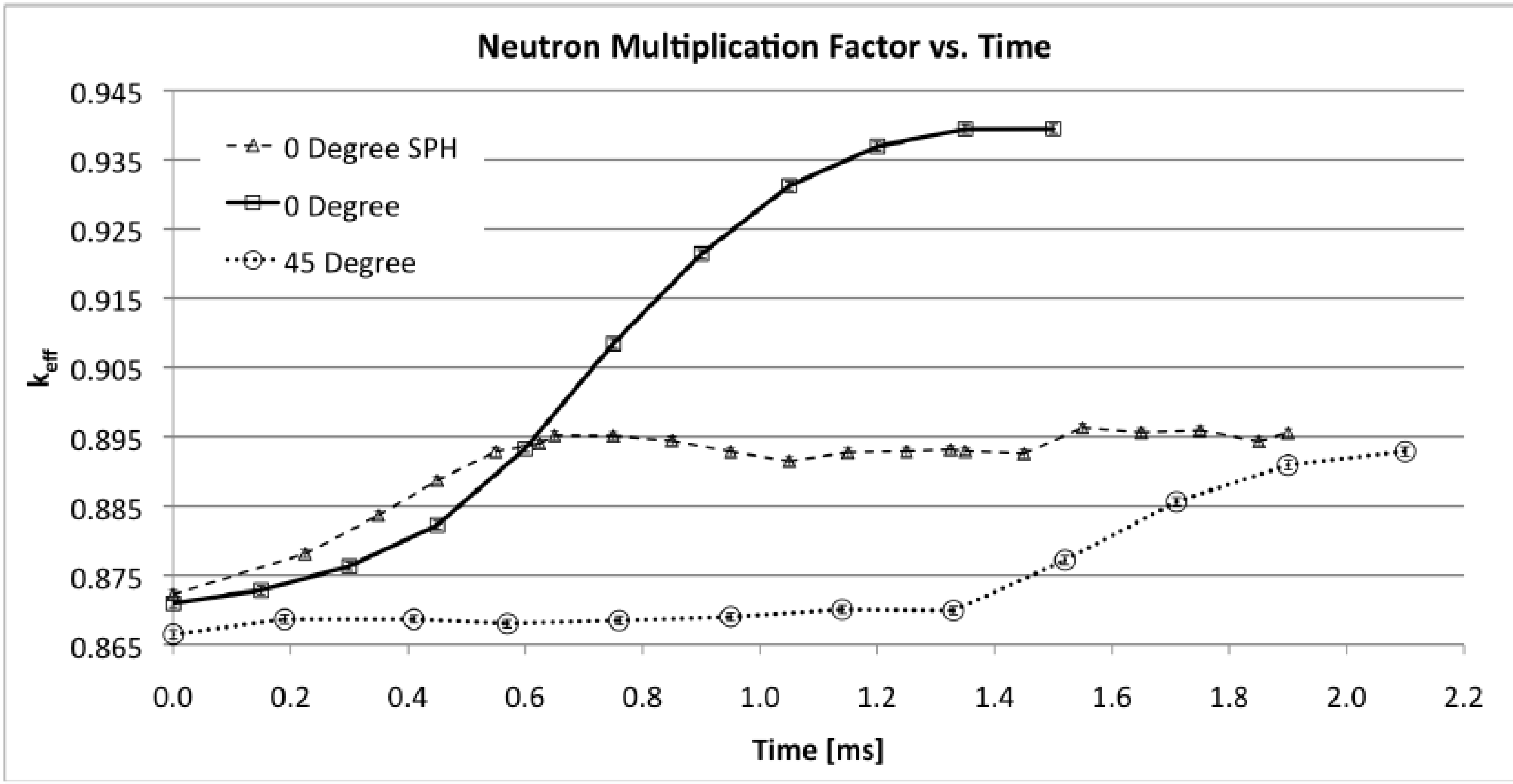
Fission Applications
85-Pin Full-Scale Space Reactor Impact





40 m/s on concrete

Neutron Transport:
85-Pin Full-Scale Space Reactor Impact

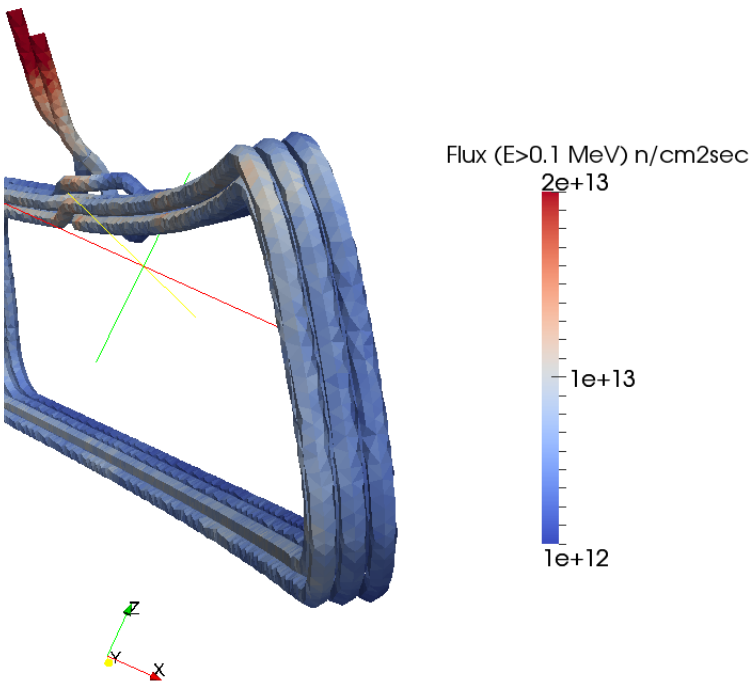


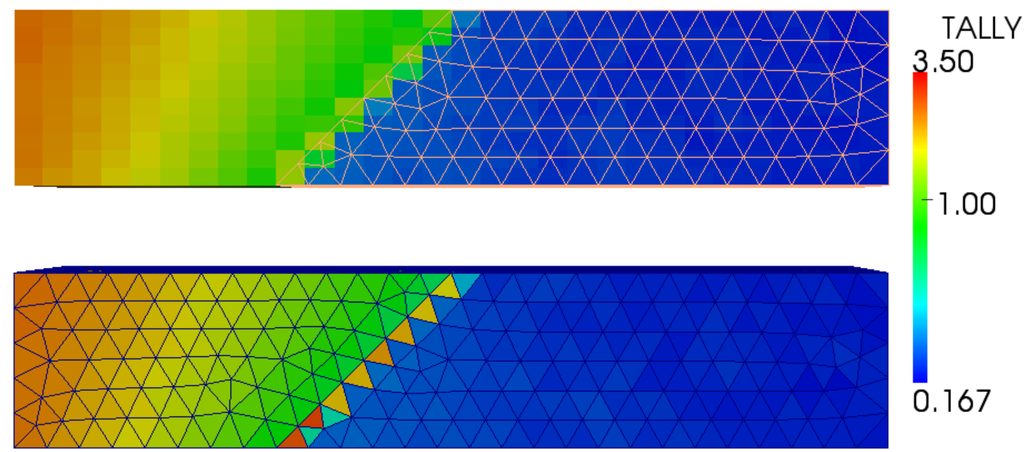
Advanced Mesh Tallies

- Perform track length tallies on arbitrary polyhedral mesh
  - Prototype exists for tetrahedral mesh
- Develop alternative tally estimators
  - Functional expansion tallies
  - Kernel density estimators
- Explore $hp\sigma$-adaptivity of advanced mesh tallies

Next Steps: Human Efficiency

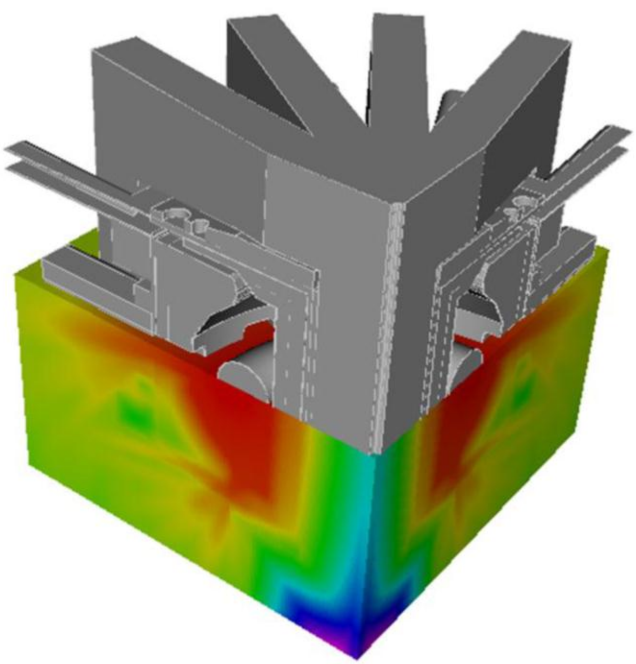
- Unstructured mesh tallies
  - Small volume fraction tallies
  - Multi-physics coupling

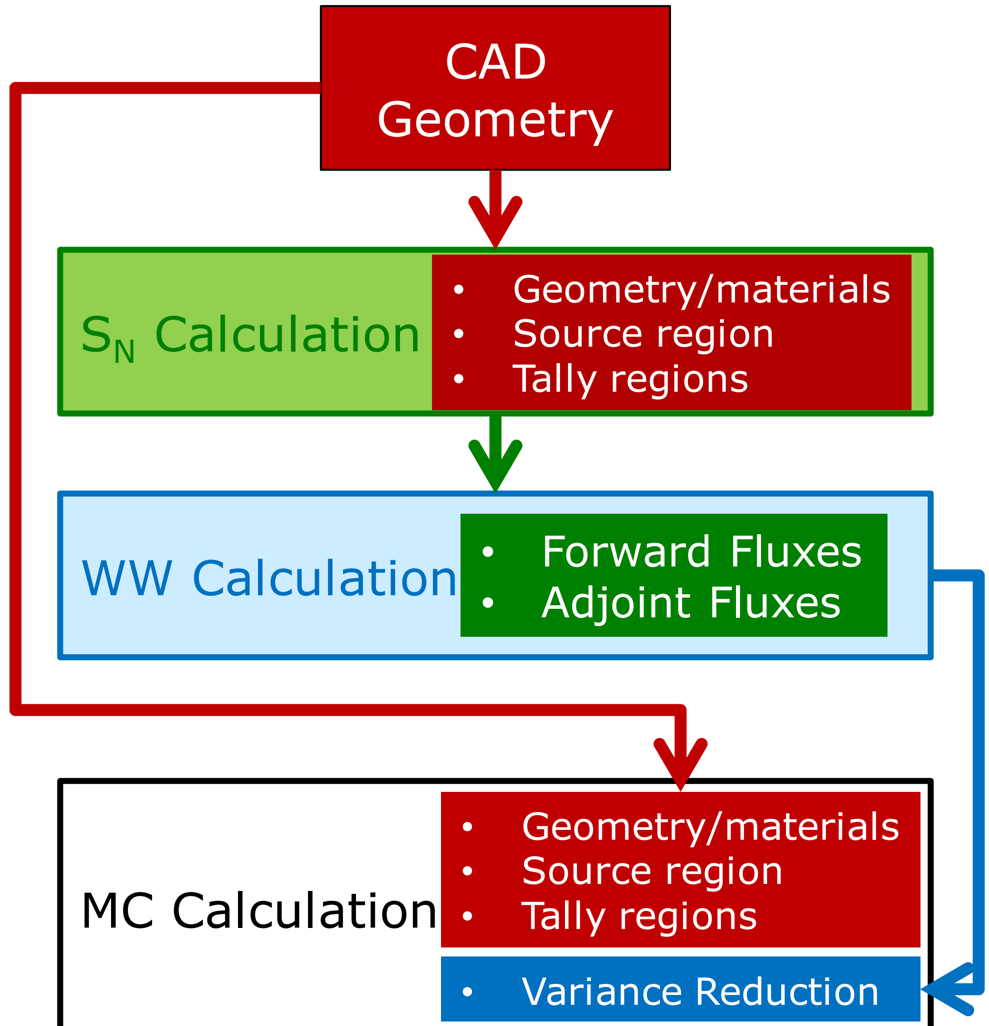




Next Steps: CPU Efficiency

- Hybrid Transport
  - Automated mesh generation based on CAD model





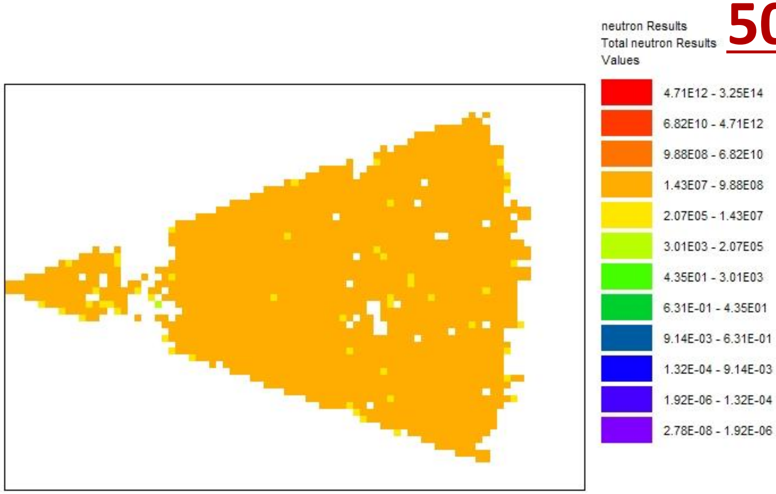
Research Directions
Hybrid Methods

- Monte Carlo not well-suited to deep penetration problems
- Deterministic methods not well suited to gap streaming problems
- Use deterministic methods to develop importance maps for Monte Carlo problems

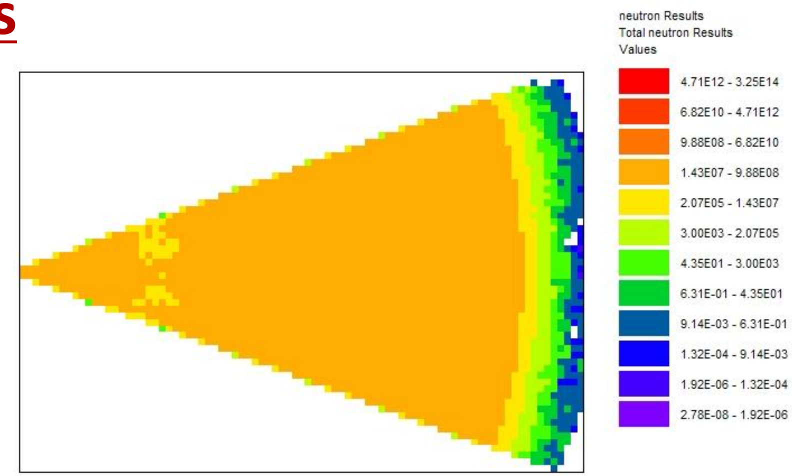
Research Directions

Hybrid Methods

50 CPU-days

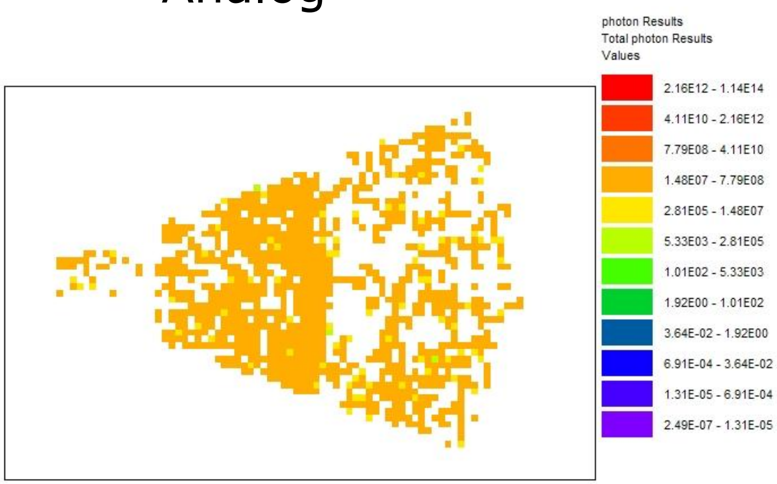


Neutrons

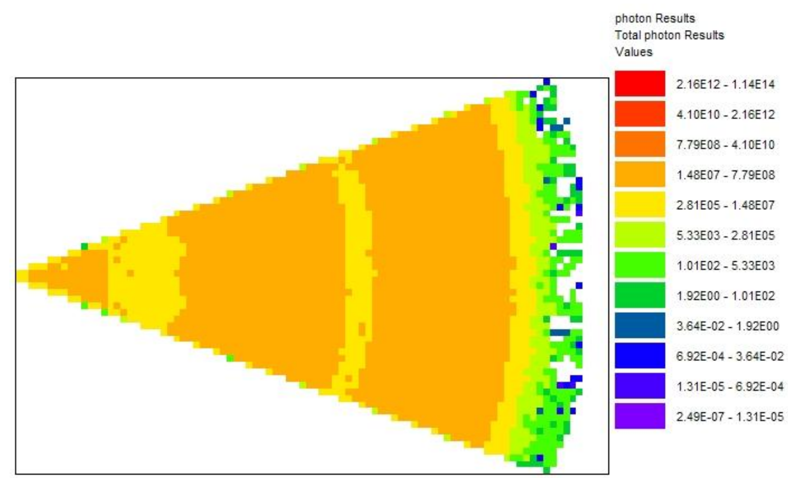


Analog

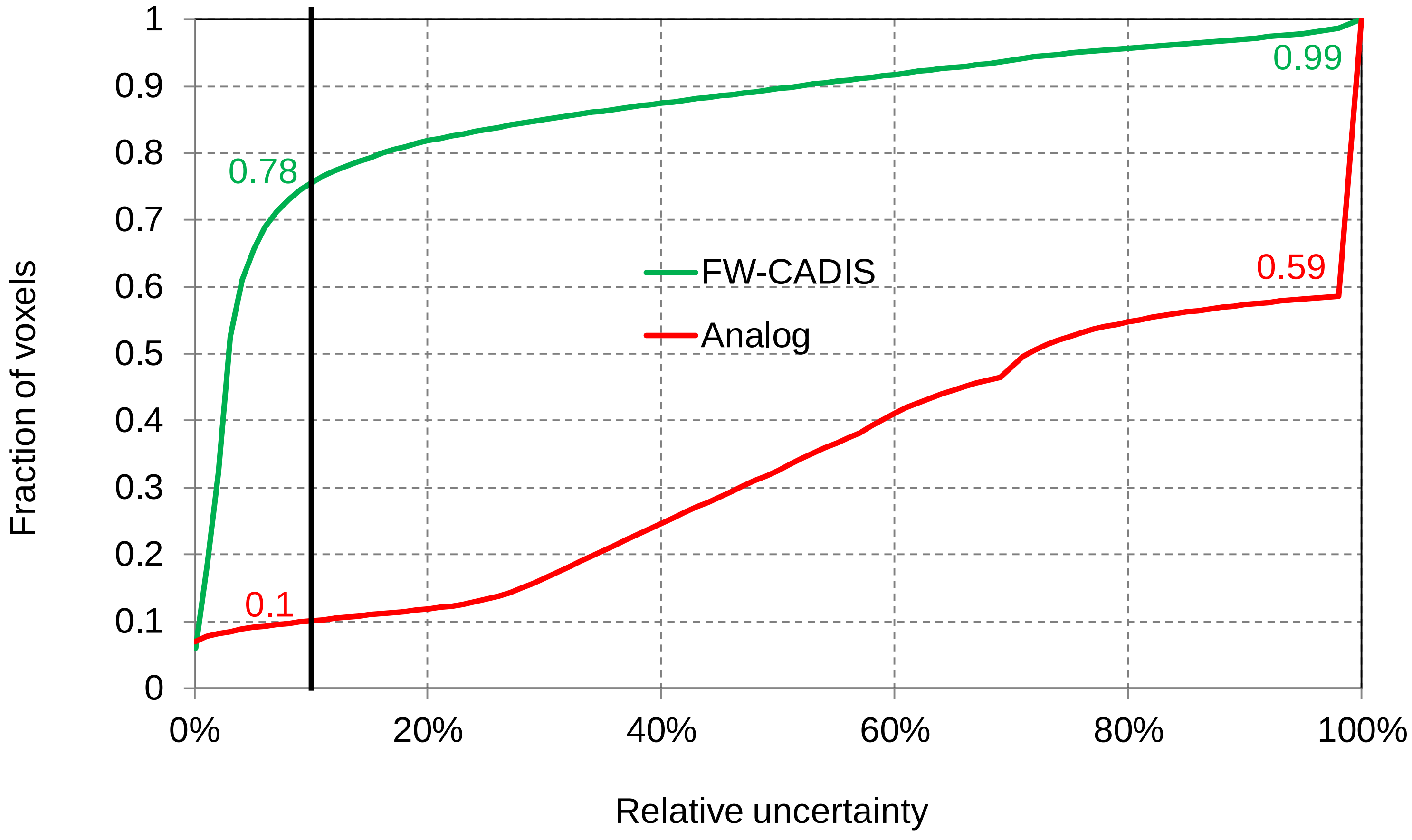
FW-CADIS (ORNL)



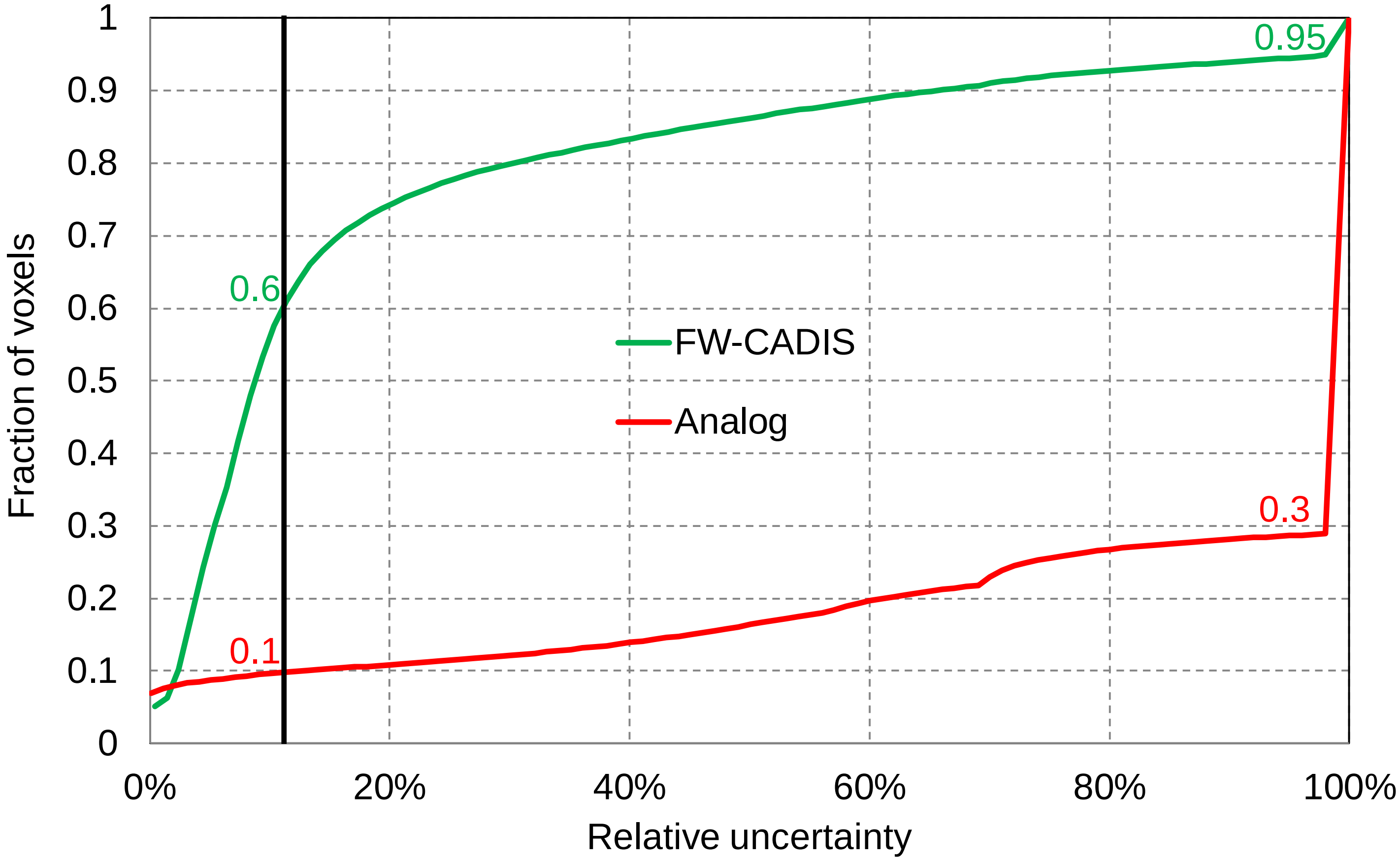
Photons



Total neutron flux cumulative distribution functions (50 days)

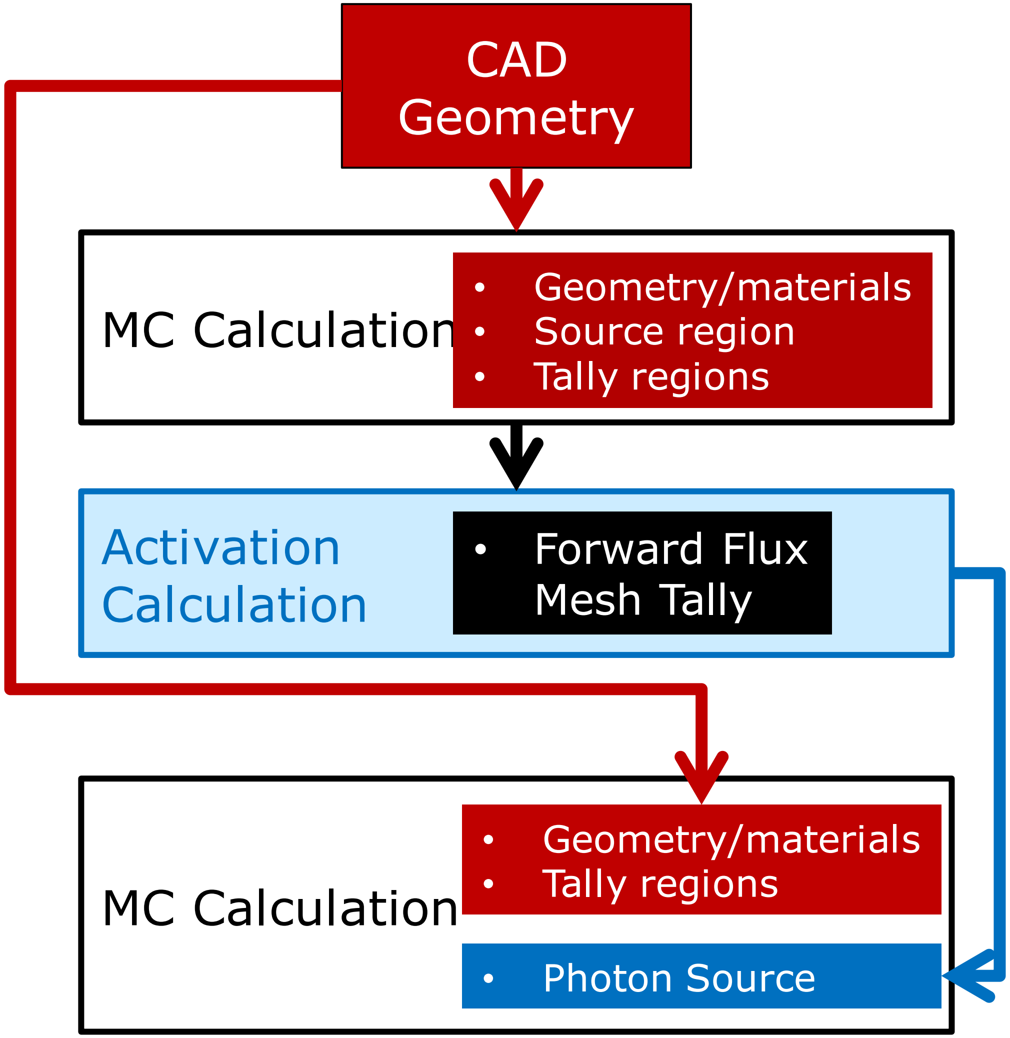


Total gamma flux cumulative distribution functions (50 days)



Next Steps: Human Efficiency

- 3-D Activation
  - Automated material mesh generation from CAD
  - Efficient mesh-based photon source sampling



Summary of Research Directions

- Common Domain Solution Coupling
  - Neutronics-Neutronics coupling
    - Hybrid acceleration of shielding
    - Hybrid acceleration of source convergence
  - Neutronics-"other physics" coupling
    - N source term
    - N feedbacks
    - Activation dose/depletion
      - Uncertainty propagation
- Advanced mesh tallies
  - Alternative tally estimators
  - $hp\sigma$-adaptivity

CAD-Based Neutronics Brings New Opportunities/Challenges

- Fundamental capability in production use for fusion shielding applications
  - Robustness improvements
    - Goal: Guarantee no lost particles
  - Performance improvements
    - Goal: Users don’t care about performance penalty
  - Feature enhancement
    - Goal: Extend utility of Monte Carlo radiation transport

Produced by University Communications

Questions?

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