UK Atomic Energy Authority

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CAD, CSG, Workflows and all

WG47 - Contributed Talk

Official

Contents

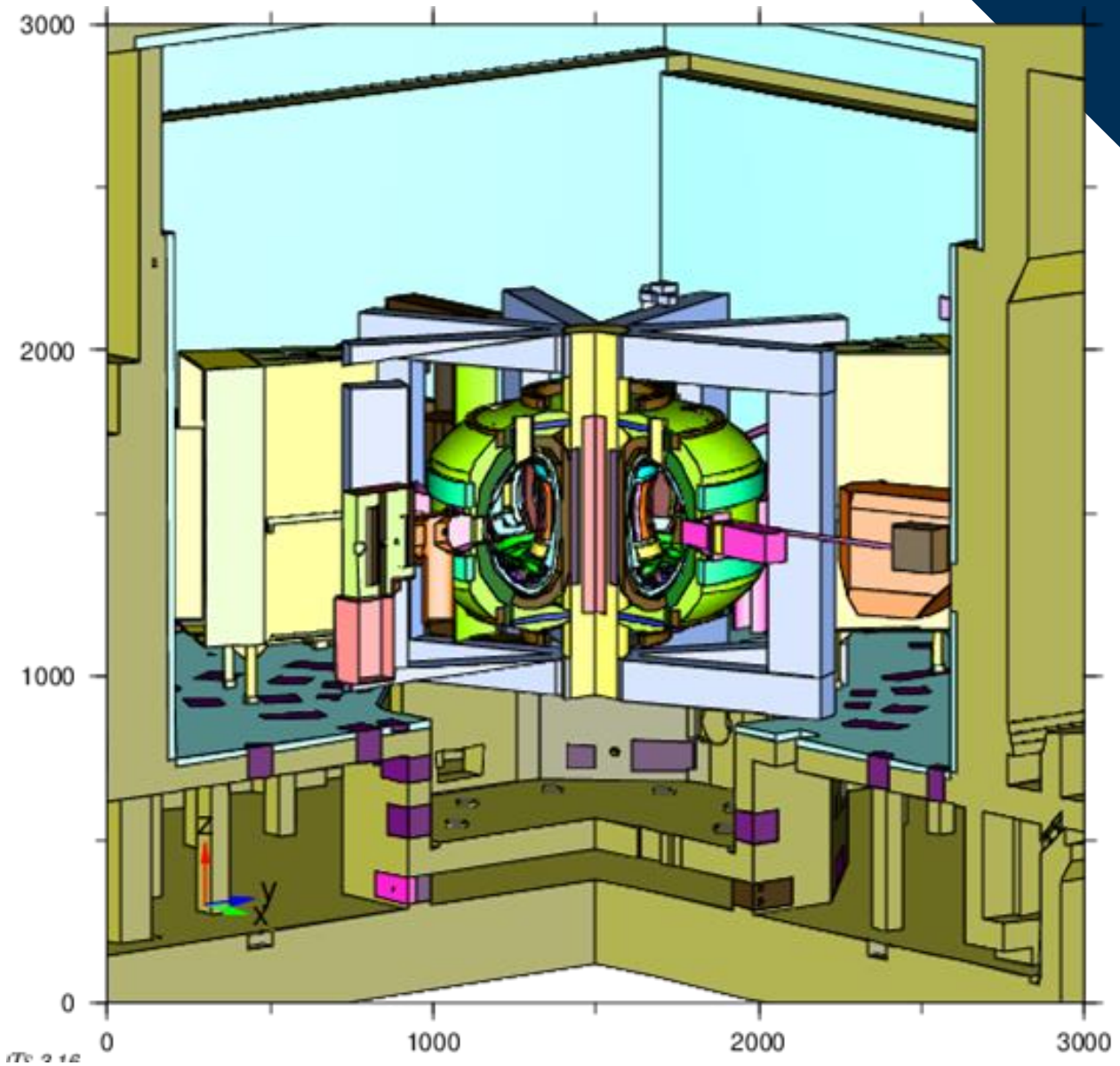
- Introduction
- csg2csg (and examples)
- mcnp2cad
- CAD based radiation transport
- Potential workflows
- Questions

Introduction

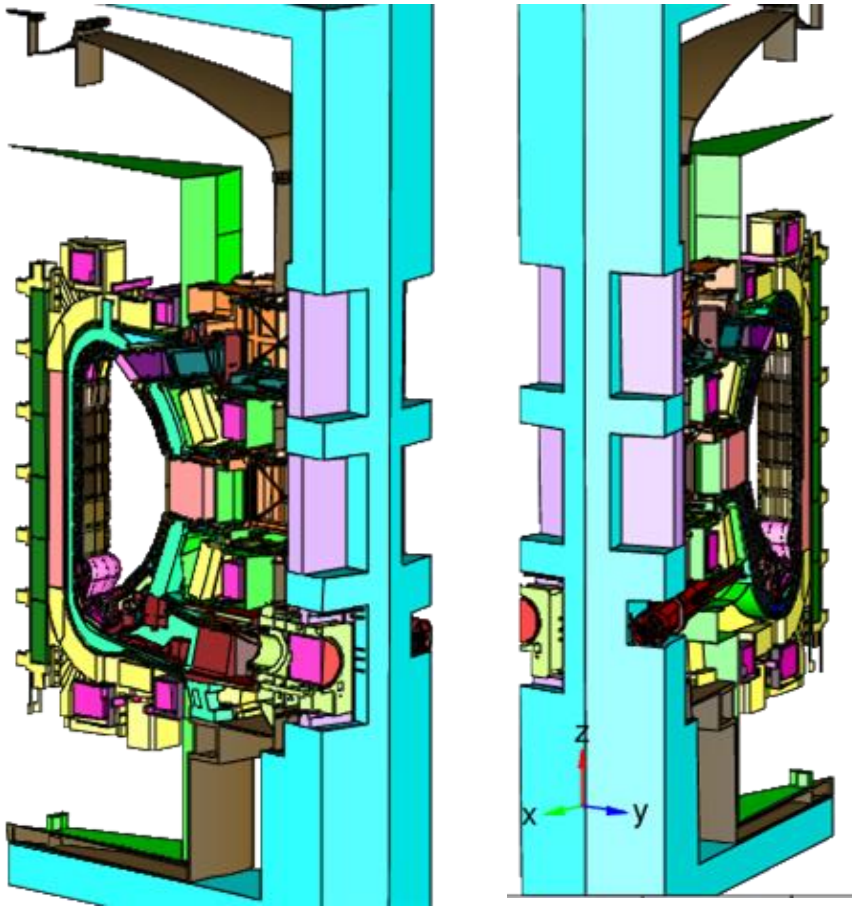
- SINBAD has been around for quite some time now
  - I first used it in 2005
- Times are changing
  - New Monte Carlo codes
  - New cross section sets
  - New experiments
  - CAD based routes
  - Version control!
  - Provenance
  - Massive increase in computing capacity

csg2csg

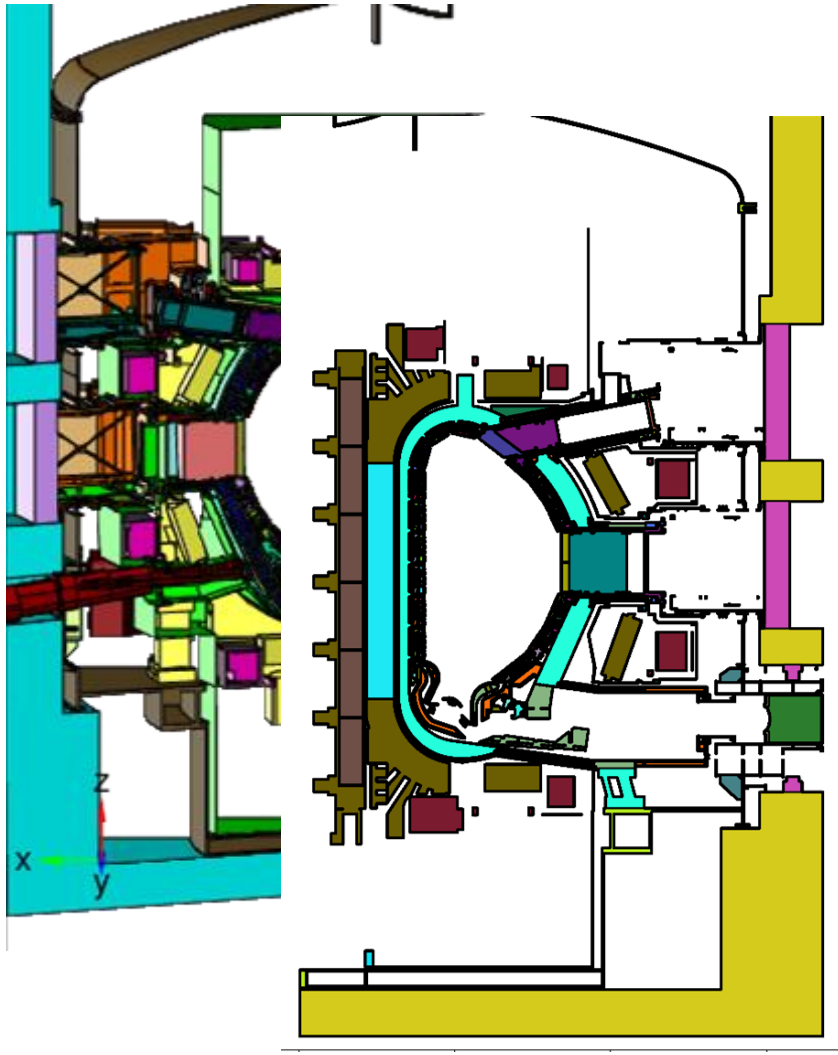
- Anytime one wants to trial another MC code, we take our favourite geometry which encapsulates the problem you're interested in, but aaaah aghast, the syntax isn't the same, oh and the materials are defined differently, one can't specify isotopes…… I haven't got time
- `csg2csg` is a minimal dependency Python3 code that ingests MC CSG geometry and exports it to another format (MCNP->FLUKA/OpenMC/PHITS/Serpent2)



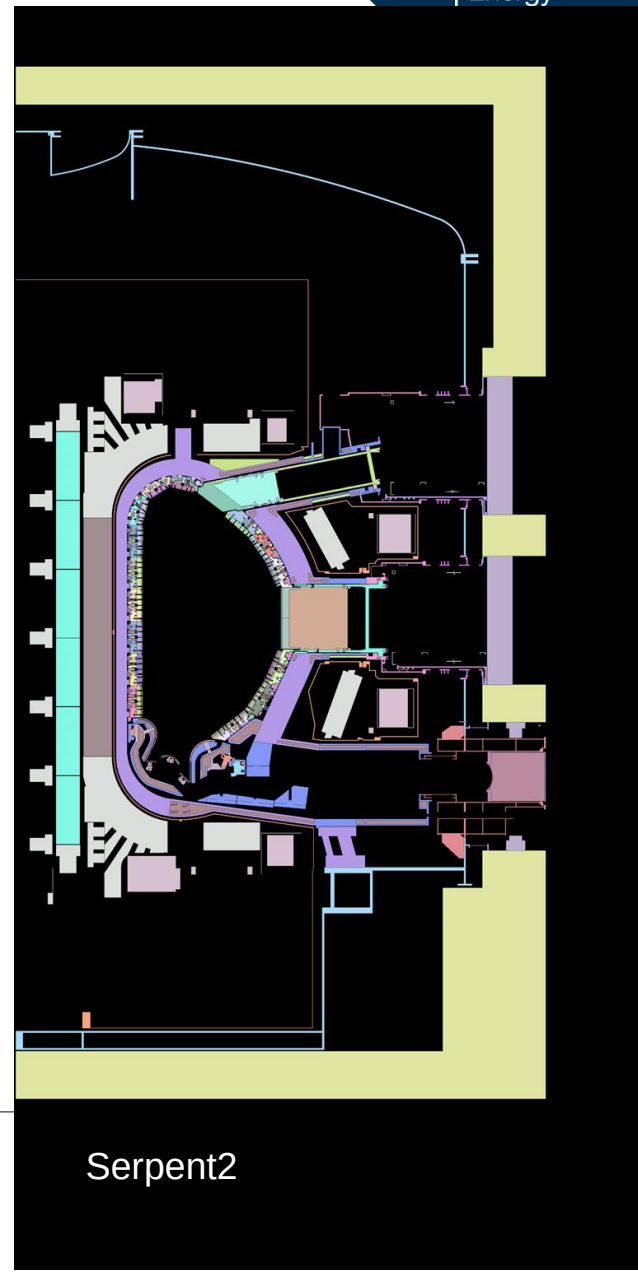
Example C-Model



PHITS317



OpenMC



Serpent2

csg2csg

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- Very much a work in progress
- Feel free to try it

```
git clone https://github.com/makeclean/csg2csg
```

- Or you can pip install it directly

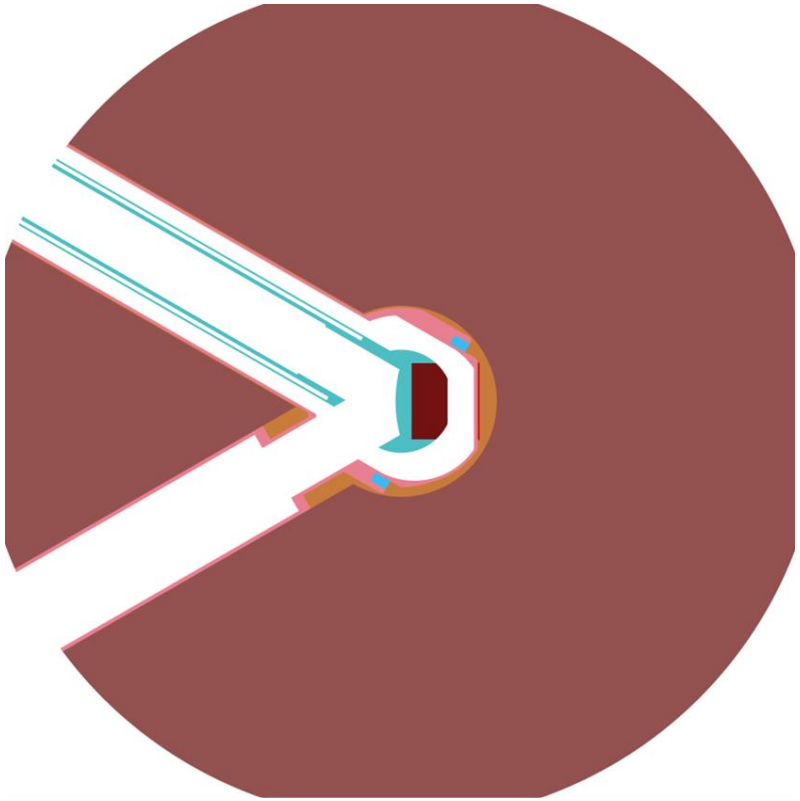
```
pip install csg2csg --user
```

- Similar in spirit to t4_geom_convert which converts MCNP to Tripoli4 format

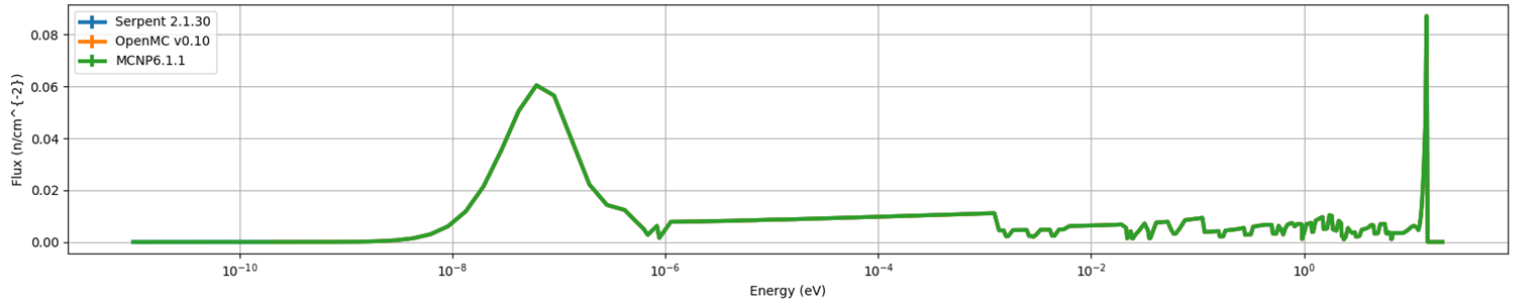
  https://github.com/arekfu/t4_geom_convert

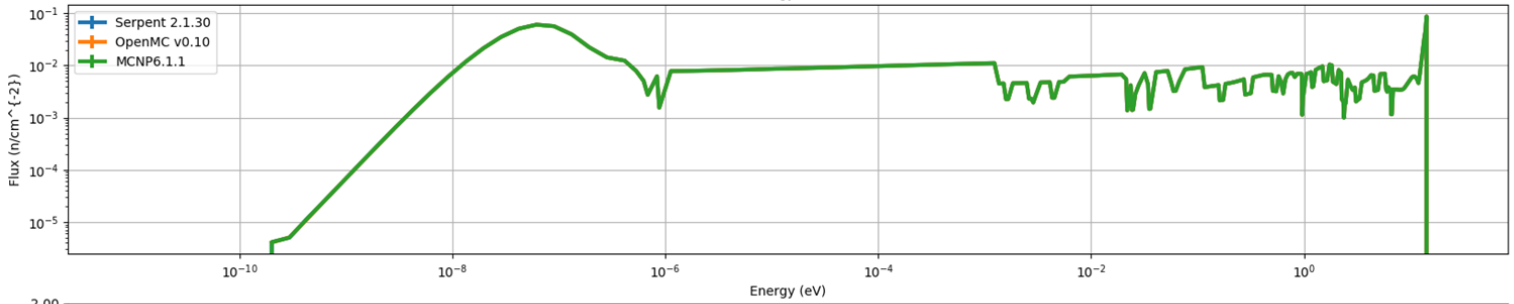
- Hope to take inspiration one day and re-order the MCNP into convex zones to allow translation to zonal codes (CSG with no union operator) like McBEND and Tripoli4

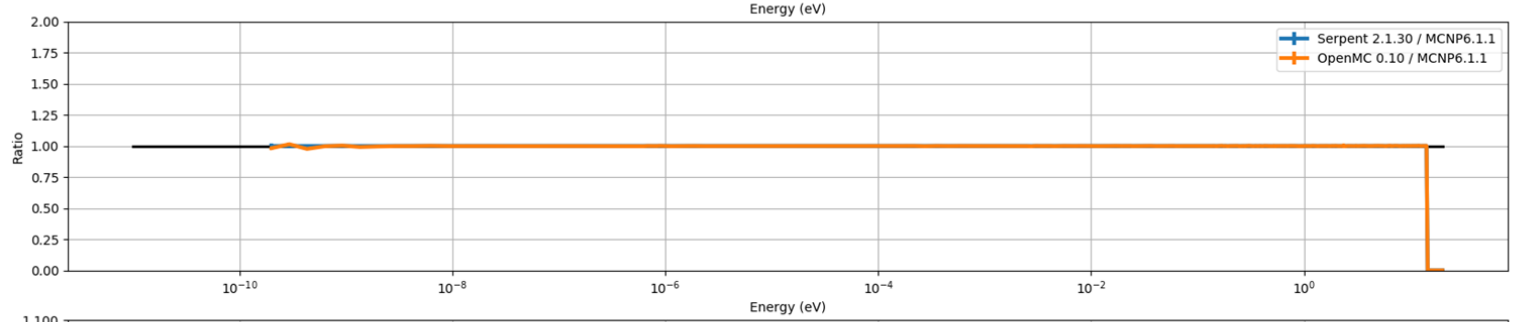
OpenMC KANT Verification

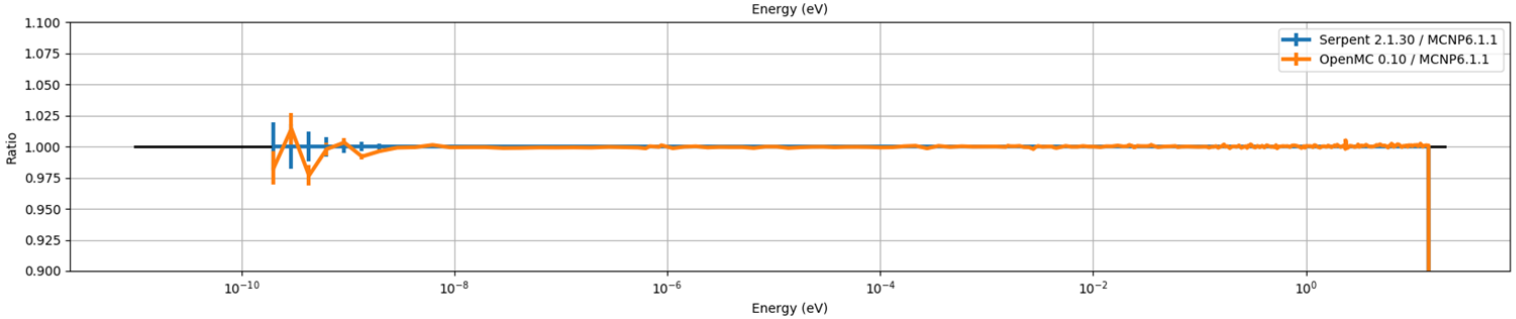


- KANT is a Beryllium sphere with a DT generator embedded inside to provide neutrons

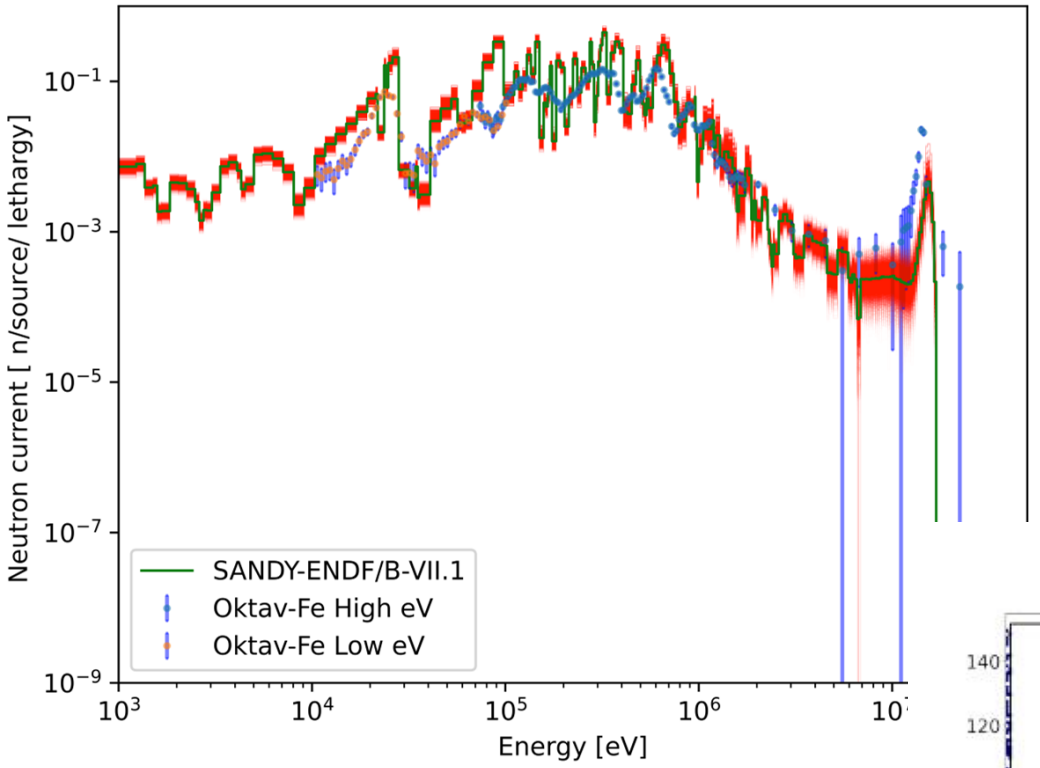


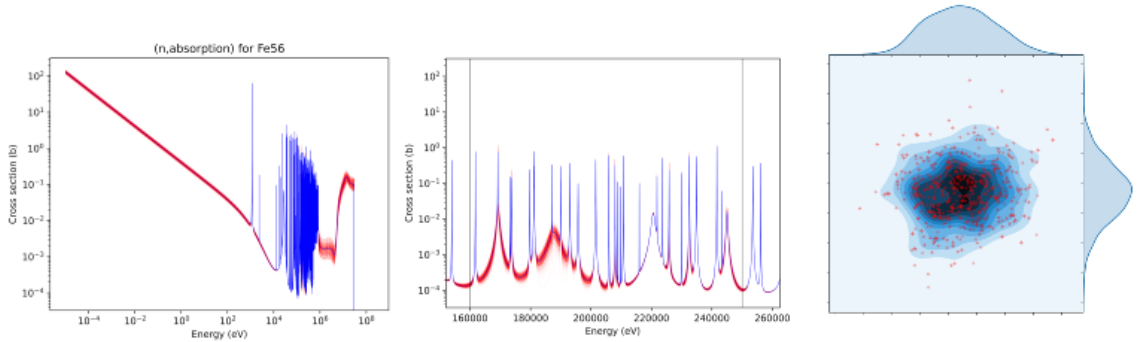




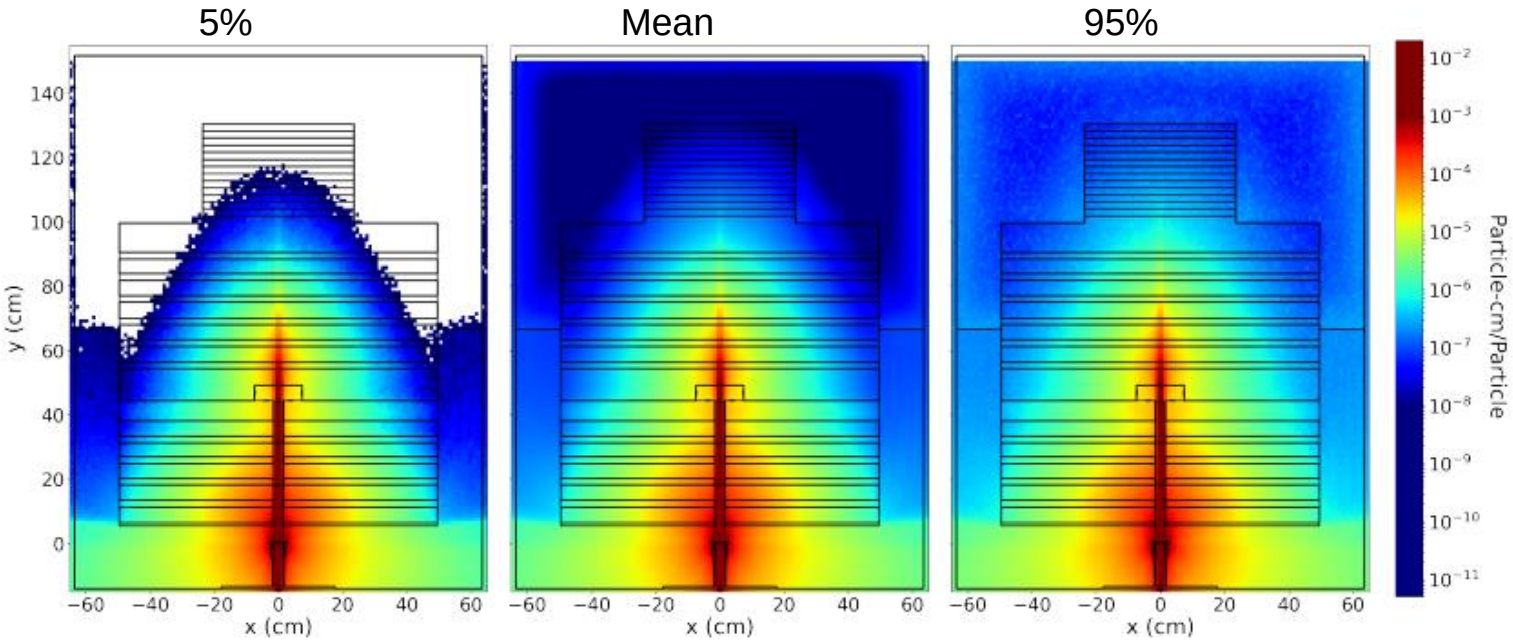


OpenMC UQ Examples





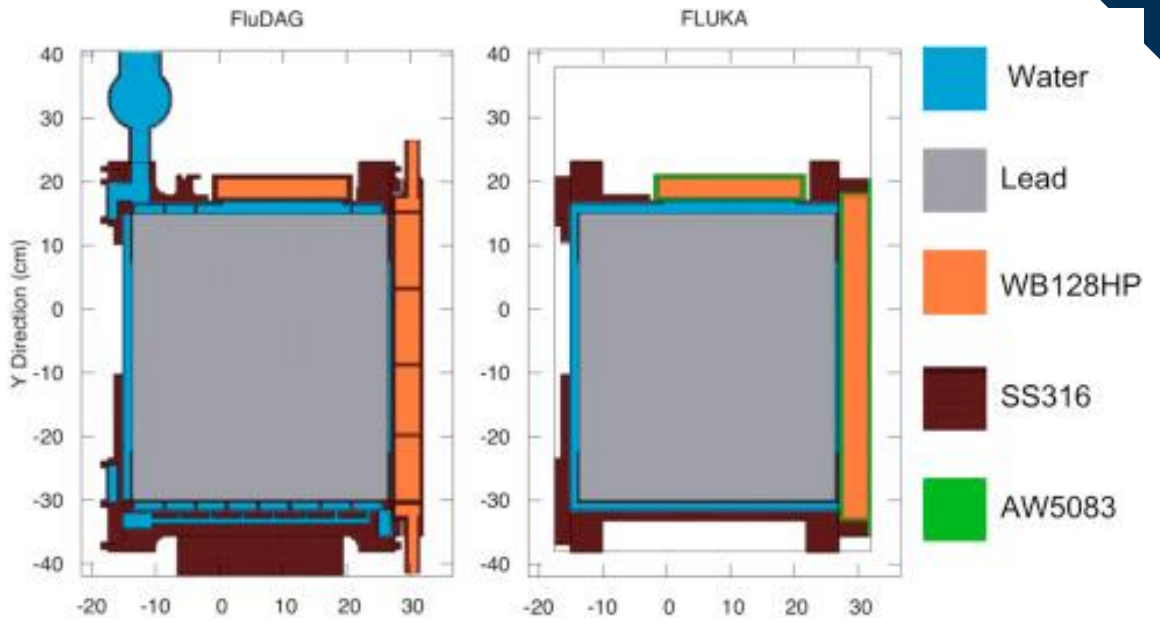
FNG-STR Uncertainty bounds

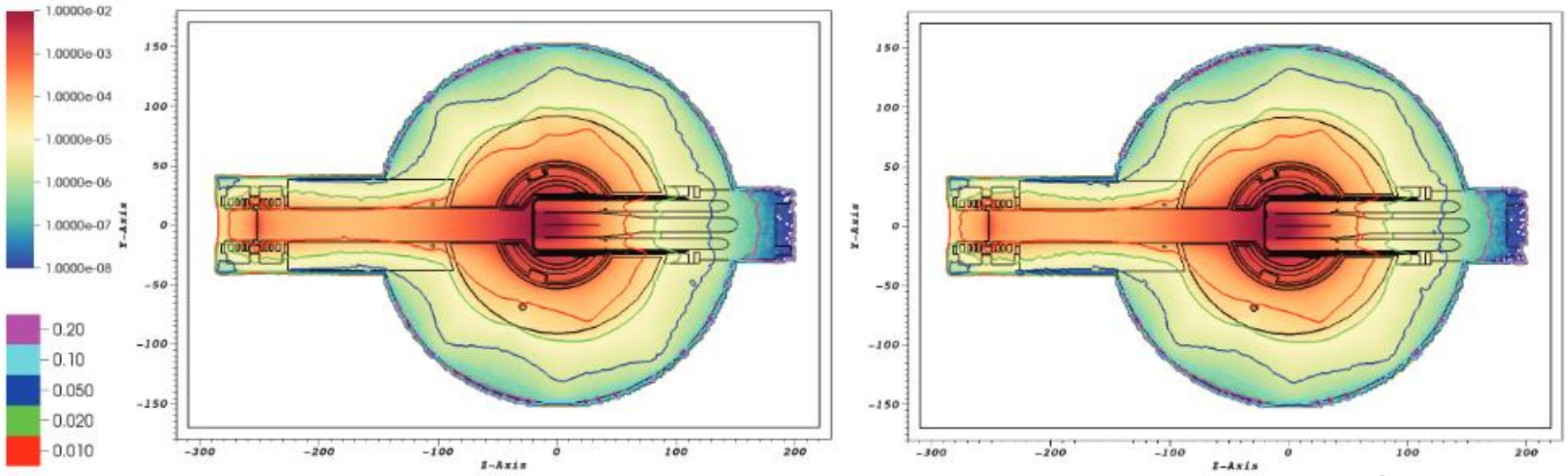


- Using SANDY and TENDL uncertainty data
- Use MCMC to generate cross sections for each nuclide in the problem e.g. 20 nuclides x 500 evaluations
- 10k individual calculations

mcnp2cad

- Tool developed at UW-Madison (but again - open source)
- Can ingest MCNP geometry and spit out a CAD geometry
  - STEP (no metadata)
  - ACIS (including metadata)





SNS geometry translated by mcnp2cad (MCNP geometry left) and DAG-MCNP geometry right

CAD Based Workflows

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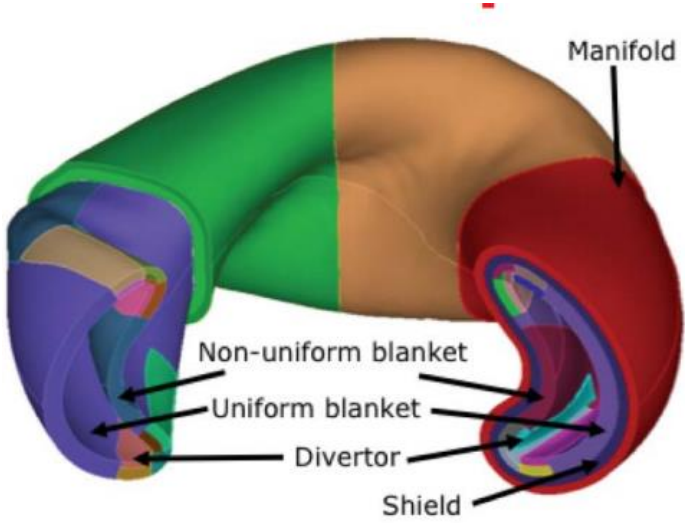
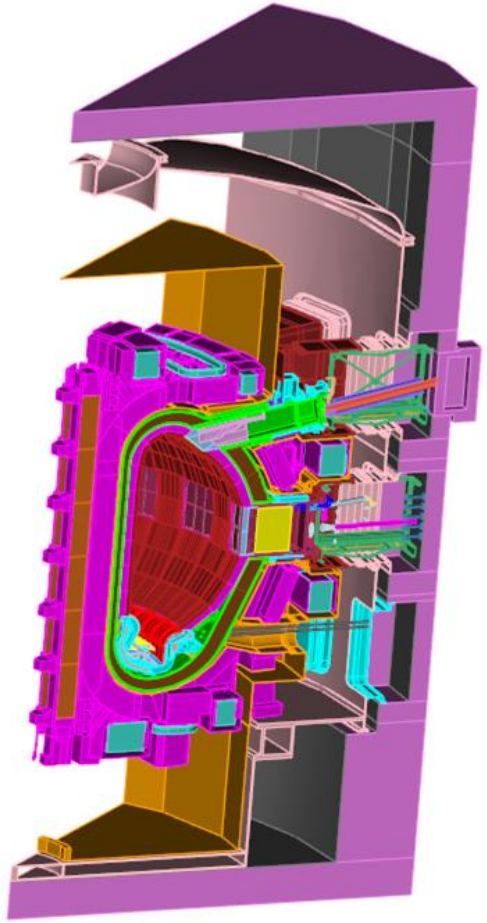
- CAD is desirable as a source of geometry for Monte Carlo calculations for several reasons
  - Allows very complex models to be represented (fidelity,accuracy)
  - Produced for manufacturing purposes (provenance)
  - The model usually already exists (you don't need to make it)
  - User friendly, easier to fix and modify than CSG (effort)
  - Faster analysis turnaround (efficiency)
- CAD model integrity - "cleanliness"
- Several routes for use:
  - Translation - MCAM, McCAD, FastRAD, CATIA-GDML
  - Directly - DAGMC
  - Hybrid - OiNK (Dead? not heard about it in a long time)
- The translation route is hard (impossible?) to script/automate

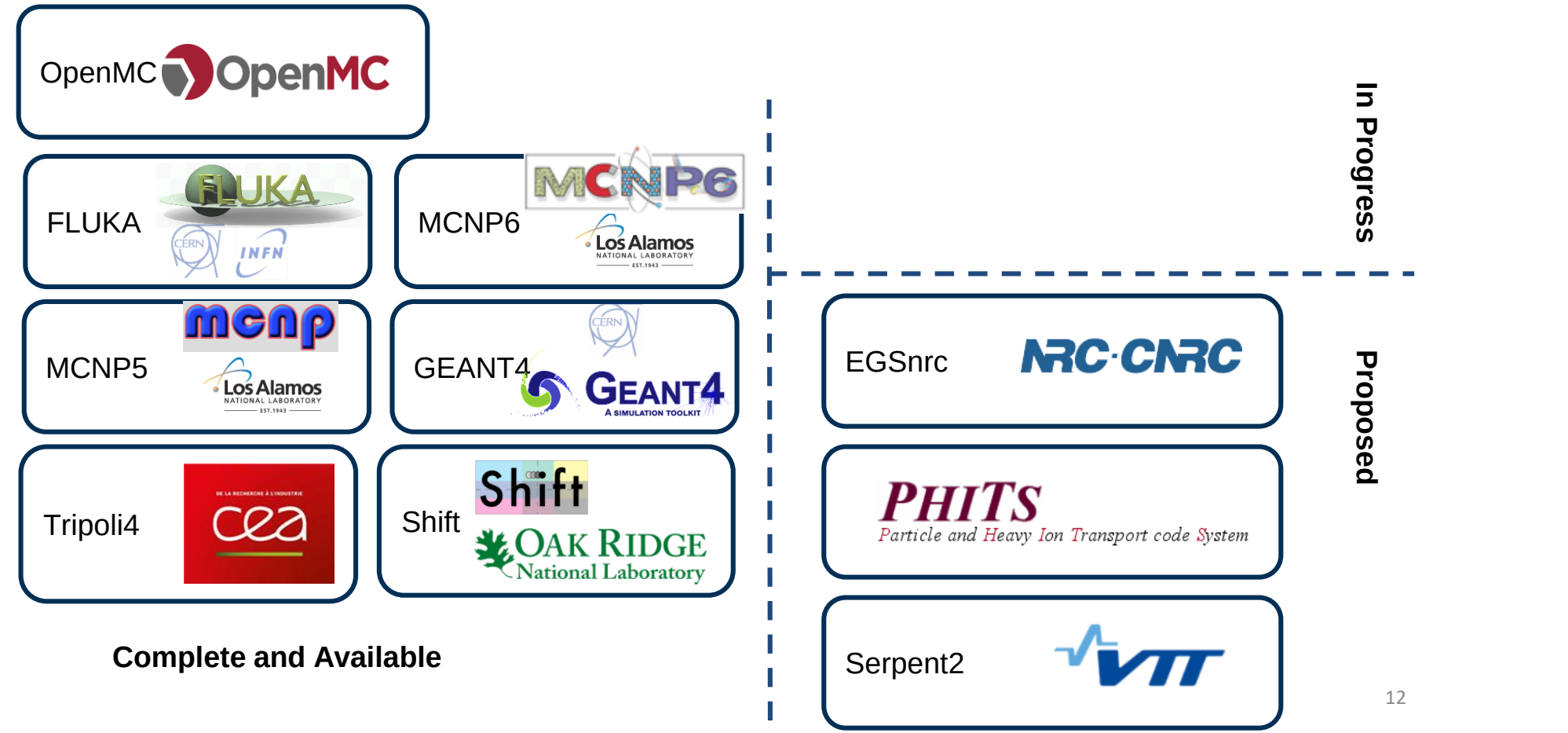
CAD Based Workflows

- Automation (including translation) provides:
  - Reduced human effort
  - Increased quality assurance
  - Direct geometry use provides **richer surface** representation
  - Facilitates coupling to other analysis types through common geometry
- The initial ‘simplification’ from the raw CAD geometry is still human driven, but could be automated

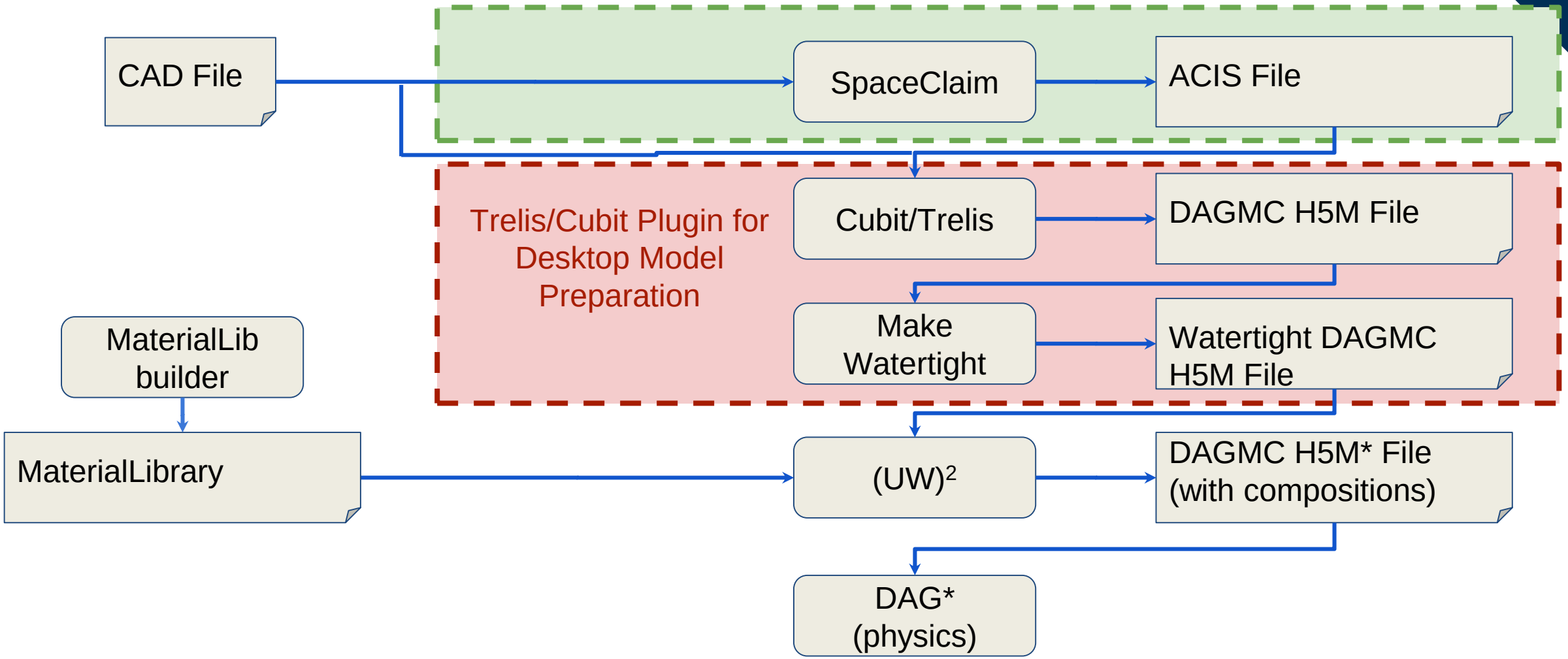




DAGMC - Integration

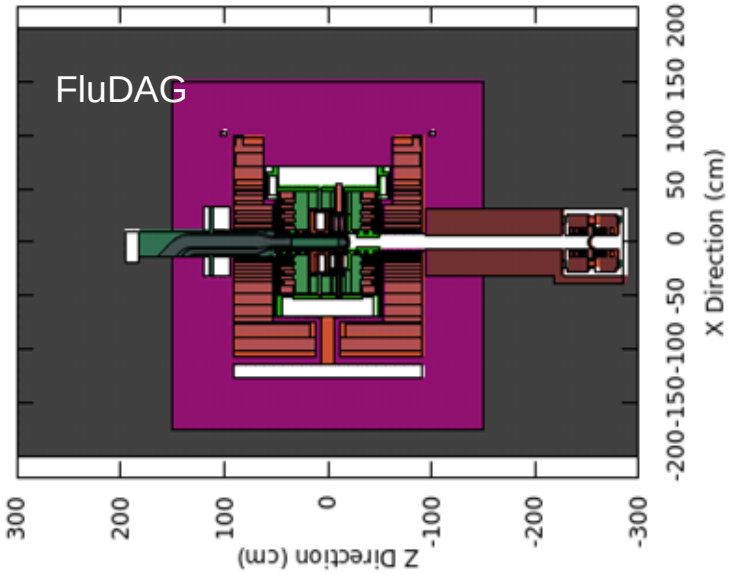


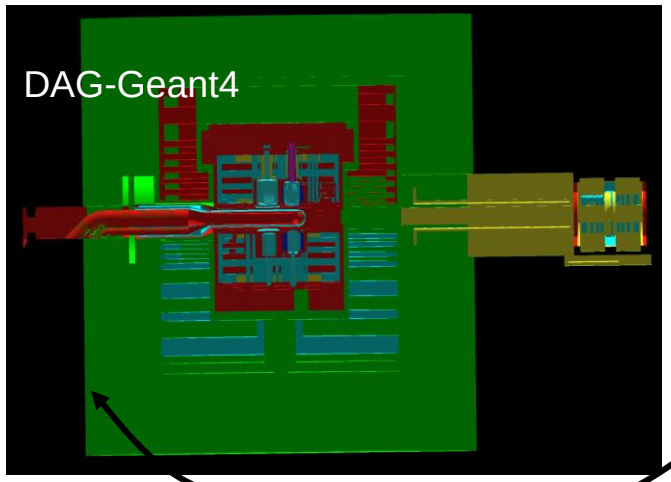
DAGMC Workflow

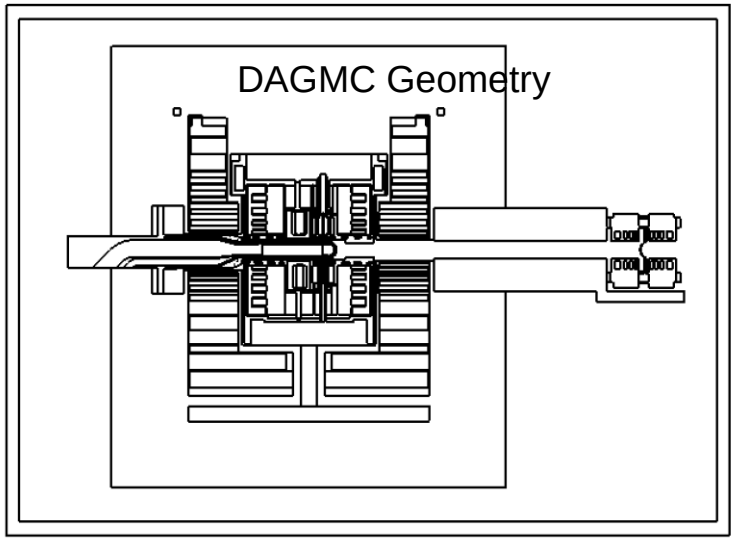


Geometry as a Service

- We have MC code agnostic workflow where materials are encoded in generic form







mat:Mercury
mat:StainlessSteel
mat:ParaHydrogen
mat:Cadmium
….

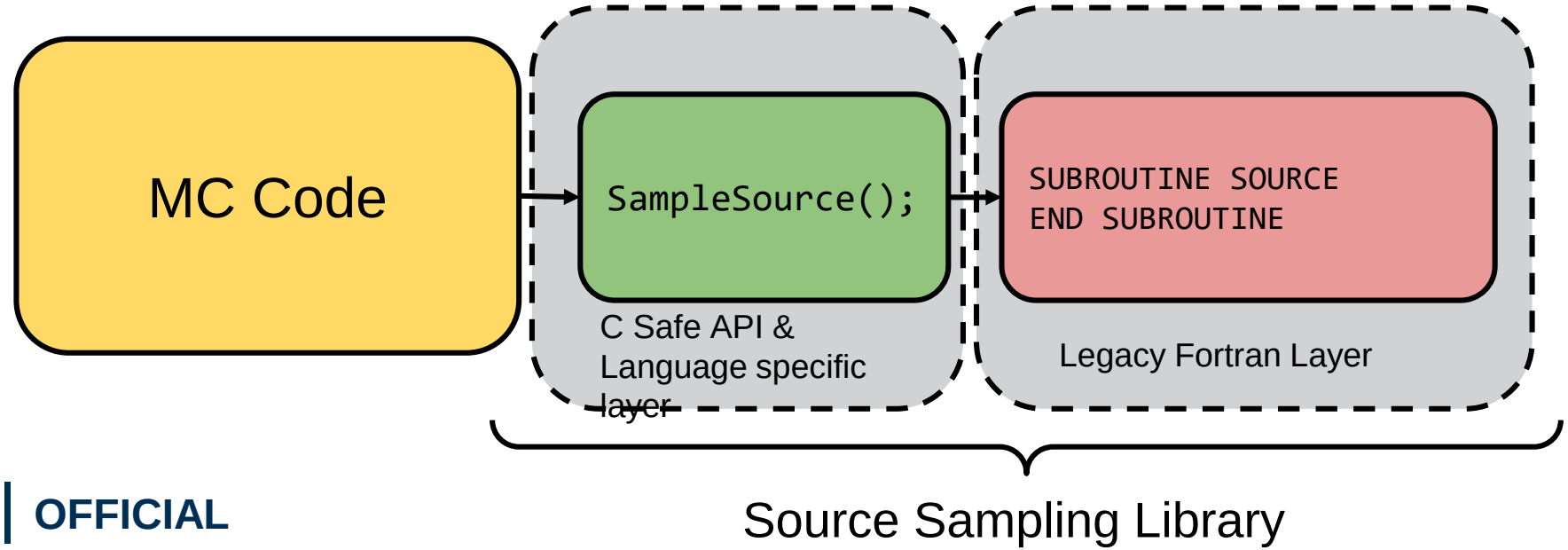
- Deploy the literal same geometry in supported codes - no changes needed

Potential geometry conversion workflows

- For already existent MCNP geometry (e.g. KANT or FNG)
  - MCNP ⟶ `csg2csg` ⟶ OpenMC ⟶ results
  - MCNP ⟶ `csg2csg` ⟶ Serpent2 ⟶ results
  - MCNP ⟶ `csg2csg` ⟶ FLUKA ⟶ results
  - MCNP ⟶ `csg2csg` ⟶ Phits ⟶ results
- For already existent MCNP geometry (e.g. KANT or FNG)
  - MCNP ⟶ `mcnp2cad` ⟶ DAG-OpenMC ⟶ results
  - ⟶ DAG-MCNP6 ⟶ results
  - ⟶ FluDAG ⟶ results
  - ⟶ DAG-Tripoli4 ⟶ results
- Straightforward to get multiple physics results either from CSG or CAD based

Radiation Sources

- If we want to image a world where we treat all MC codes equitably, then the source of most pain is the radiation source
- Most are MCNP SDEF relying upon (a really very good and concise) syntax to define complex radiation sources
  - No other MC code has had the time, money or desire to replace that functionality
- Instead complex sources will need to be de-MCNP'd



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I do not believe that one can validate a Monte Carlo code in isolation, I believe you can only validate a Monte Carlo code with a specific set of nuclear data

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Potential Workflows for New Geometry

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- **Automation is Important**
  - Automation is checkable
  - Automation is repeatable
  - Automation is verifiable
  - Automation is testable
- **Script everything!**
- **We should not rely on trust**
  - It should not take 6 months to repeat a benchmark in a new code
  - The data contained in the benchmark should be unambiguous
- The running of entire benchmark suites should be automatic

Potential Workflows

From an experiment we derive the CAD geometry for the device, the experimental setup data, documents, descriptions and the experimental results

We should recognise that the purpose of the experiment is to provide validation data for simulation, the data therefore should be ready for comparison

There should be no ambiguity in input geometry, source definition, materials description, explicit assumptions on isotopic break down, explicit normalisation instructions

Where you going to get your CAD from?

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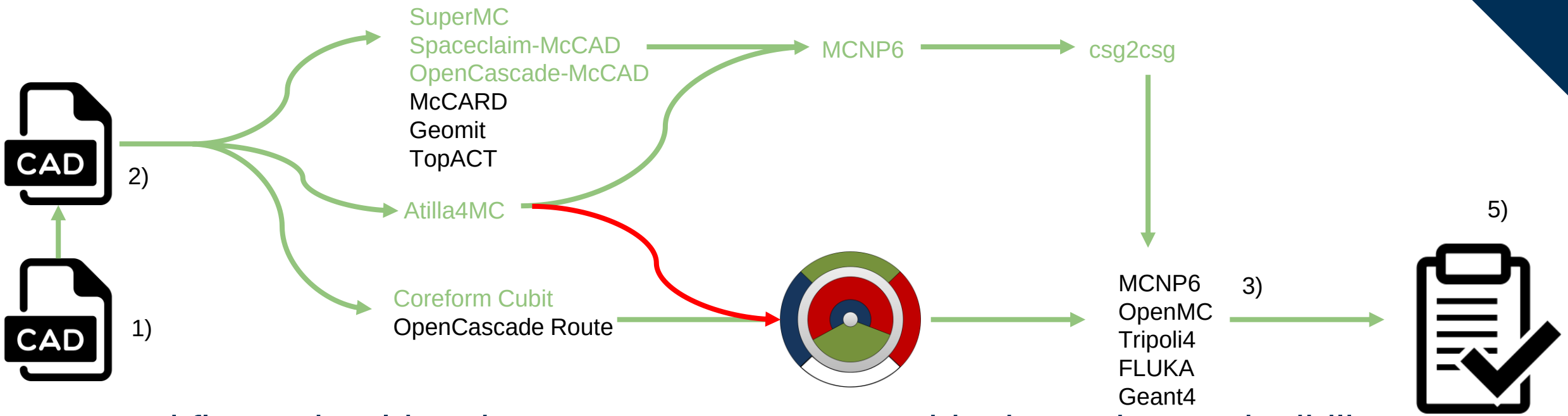
- CAD can come from a number of places
  - Human built from scratch
    - ➢ Traditional CATIA, Solidworks, SpaceClaim etc
  - Programmatically generated
    - ➢ CadQuery, OpenSCAD, (many others)
- Why?
  - Human built CAD can’t be repeated when software packages change
  - Programmatically generated can be re-run when/if bugs are found
- Human built is easier when handling large CAD models
- Programmatic is easier for simpler models
- Either way, depends on your local resources
- **Metadata is critical either way**
- **Proprietary or closed format need to be avoided**

Potential Workflows

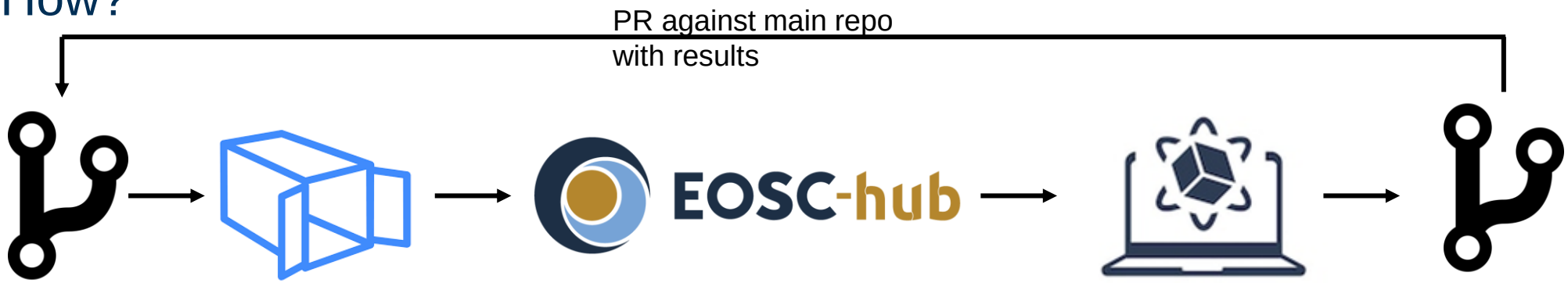


New workflows should embrace provenance, unambiguity and reproducibility

1. Reference CAD Model (before any modification)
2. Reference CAD Model (conversion ready)
3. Reference MC Inputs
4. Reference Cross Sections
5. Reference Outputs

Automation

- Should SINBAD include validation against multiple cross section sets?
  - I think it should
- How?



Git VC

- 30 52 MeV
- ….
- ….
- ….
- Yayoi Fe

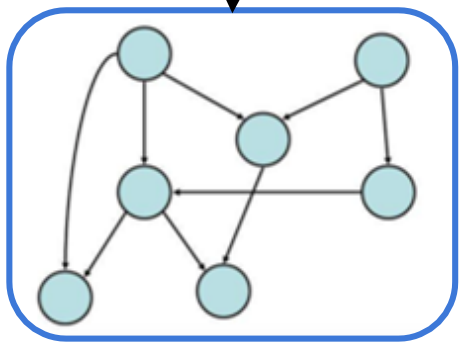
Container

- OpenMC
- FLUKA
- Geant4
- Serpent2?
- PHITS?
- MCNP6
- SHIFT

Cloud or HPC layer

- ENDF/B-VIII
- ENDF/B-VII
- FENDL-3.1d
- JENDL-4.0
- etc

Simulations



Directed Acyclic Graph of jobs

Git VC

- Condor DAGMAN
- Custom job builder
  - PBS Job Array
  - PBS Job Dependency

With DAGMAN could submit entire validation suite as one task which will get churned through by the DAG Manager

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Questions