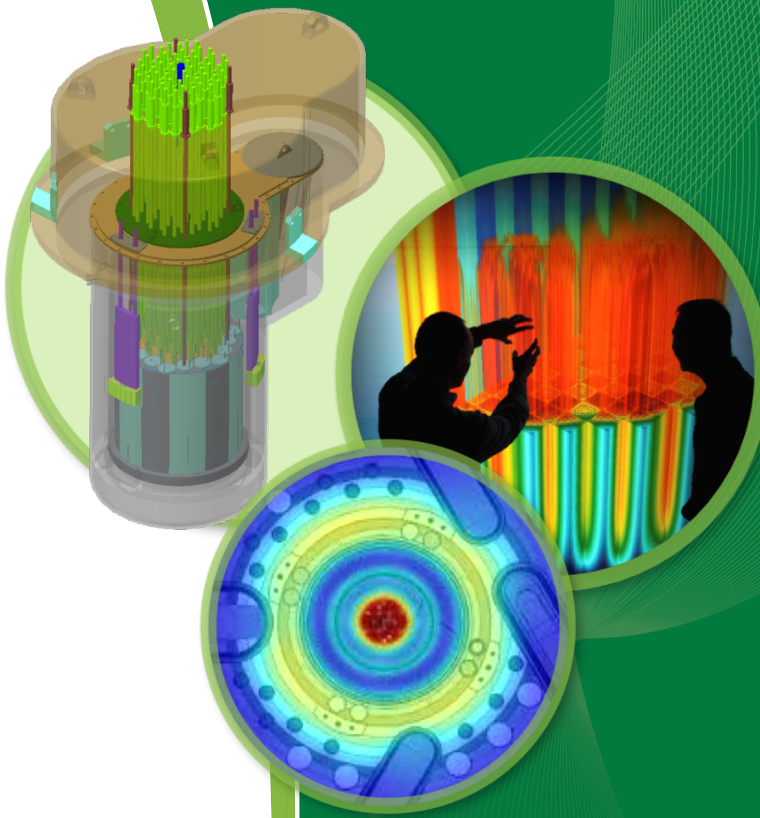
COUPLE/ORIGEN Cross Section Generation for Reactor Physics Applications



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Outline

- Overview of Couple/ORIGEN/OPUS
- Fuel Cycle Applications (cross section vs. recipes)
- Radiation Experiment Applications (Ir-192 production in HFIR)
- Conclusion and Wish List

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Overview of COUPLE/ORIGEN/OPUS

- COUPLE
  - Creates problem specific one group cross sections for ORIGEN using:
    - 44, 238, 256 flux spectrum
    - Pre-calculated one group cross sections
  - Can be coupled to any other code that provides the above information include MCNP and MC2-3
  - CSAS can be used before COUPLE to improve accuracy if desired
- ORIGEN
  - Neutron activation, actinide transmutation, fission product generation, and radiation source term calculation
- OPUS
  - Reads and processes the ORIGEN binary concentration file (f71) into a easy format for scripting

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COUPLE/ORIGEN for fuel cycle applications

- All fuel cycle tools need to represent transmutation (and decay) of materials in reactors
  - This is the most complex part of the fuel cycle model, therefore getting it “right” is vital to the accuracy of the model
- Two methods for calculating reactor inventories includes:
  - pre-calculated recipes
  - cross sections
- Recipes are tabulated sets of discharge compositions for a given fuel irradiation history
- Recipes work well for modeling fuel cycles:
  - with fixed input and output compositions
  - already at equilibrium when compositions do not vary significantly
- Cross Sections can be calculated using COUPLE
- Recipes and Decay can be calculated with ORIGEN

Cross sections for fuel cycle analysis

- Output streams in the reactor models are dynamic and changes based on input stream radionuclide composition and internal depletion calculations.
- Some simulators can also interpolate cross sections based on reactor-, cycle-, and scenario-specific production and destruction routes
- Interpolation can capture the effects of changes in the neutron flux spectrum and associated magnitude of isotopic concentrations
- Utilization of cross sections allow for adding additional functions such as:
  - Pu equivalence
  - radioactive decay

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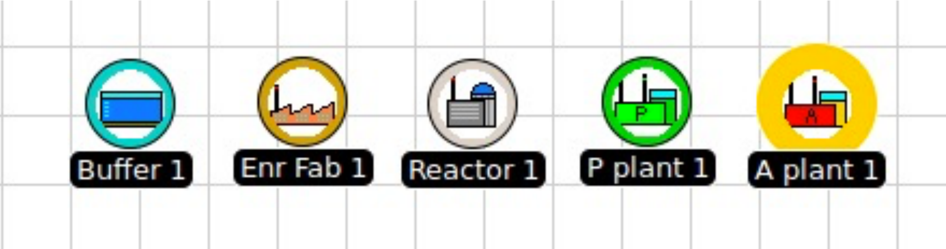
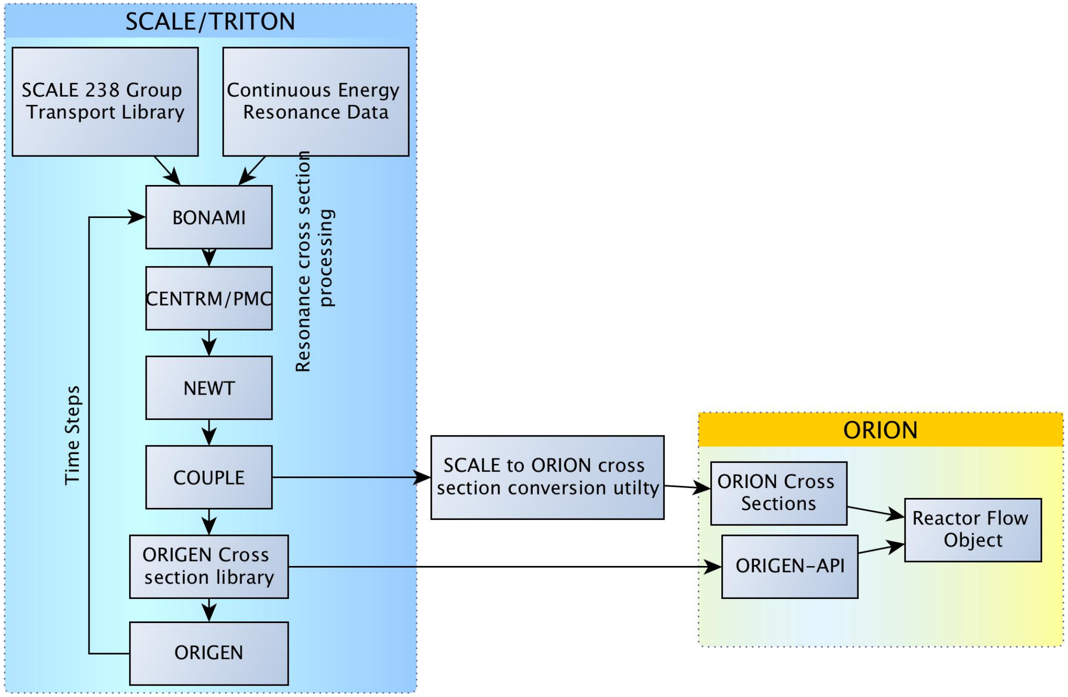
ORION: one tool being used to help answer the big questions

- ORION - a nuclear fuel cycle simulator developed at UK NNL
  - Simulate full range of nuclear-related facilities e.g.:
    - interim and long-term storage locations
    - fabrication and enrichment plants
    - reprocessing facilities
    - reactors
  - Tracks over 2,500 nuclides
  - Models decay and in-reactor irradiation
  - Can use ORIGEN for depletion analysis

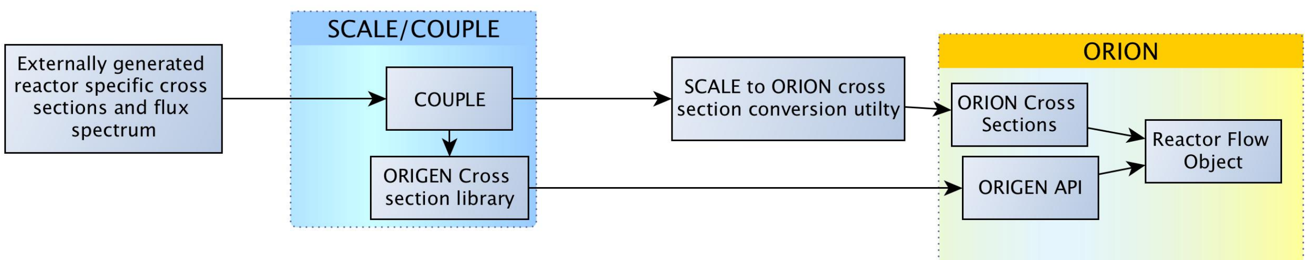


Generating cross sections for use in ORION

- Two methods have been developed for generating cross section for ORION:
  - Converting cross section results from COUPLE into FISPIN format
  - Using ft71 files generated from COUPLE with the ORIGEN-API within ORION

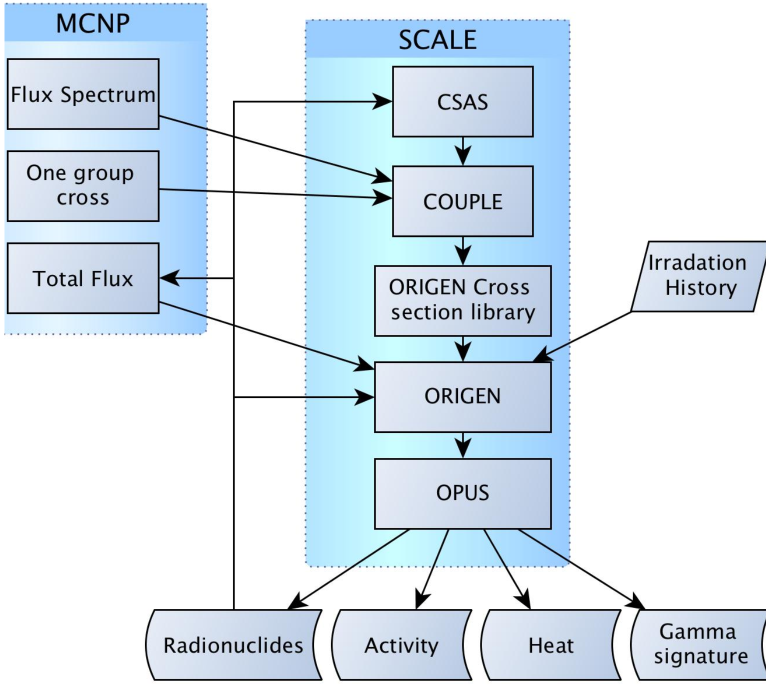


- Couple has been used to generate fuel cycle cross sections for: LWR, MOX , SFR, and MSR



Decay heat from the activation of experiments in HFIR using COUPLE/ORIGEN

- MCNP/SCALE
  - MCNP used to calculate for each cell of interest:
    - Flux Spectrum
    - Subset of one group cross sections
    - Total Flux
  - COUPLE uses flux spectrum and one group cross sections to create ORIGEN cross section library
  - ORIGEN uses total flux from MCNP for irradiation and decay of the sample
  - OPUS extract the data into an easy to process format
  - Radionuclide information from OPUS/ORIGEN is fed back into the MCNP code and process repeats for each time step.
  - Final results include radionuclide, activity, heat, and gamma signature



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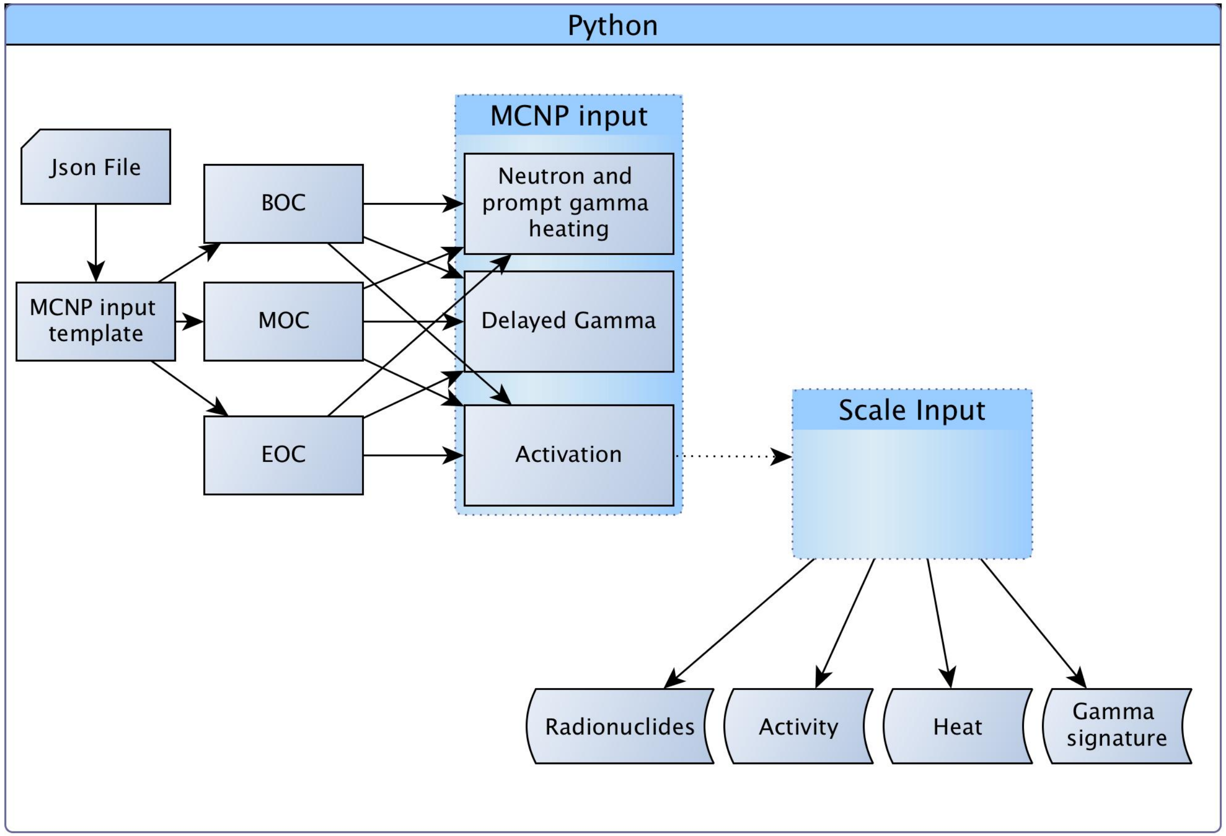
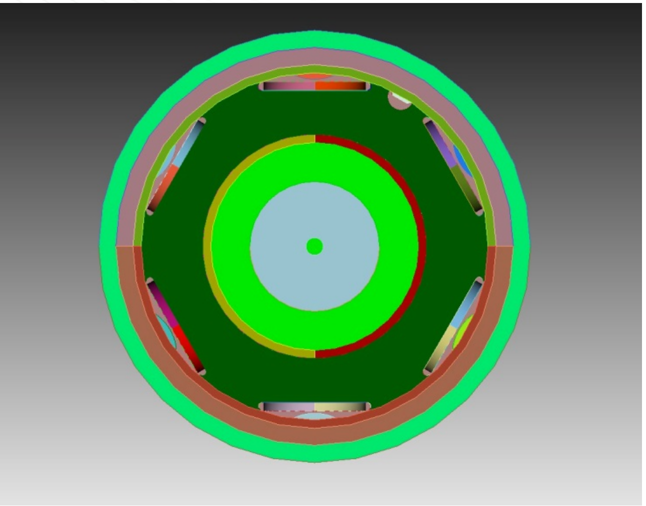
Scripting codes such as Python can be used to automate a lot of the steps

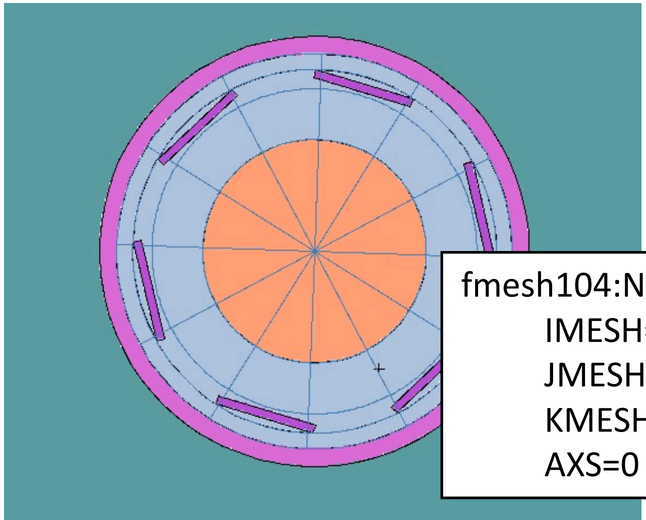
- Scripting languages can be used to help accelerate the neutronic modeling process until the tools are built into the code.

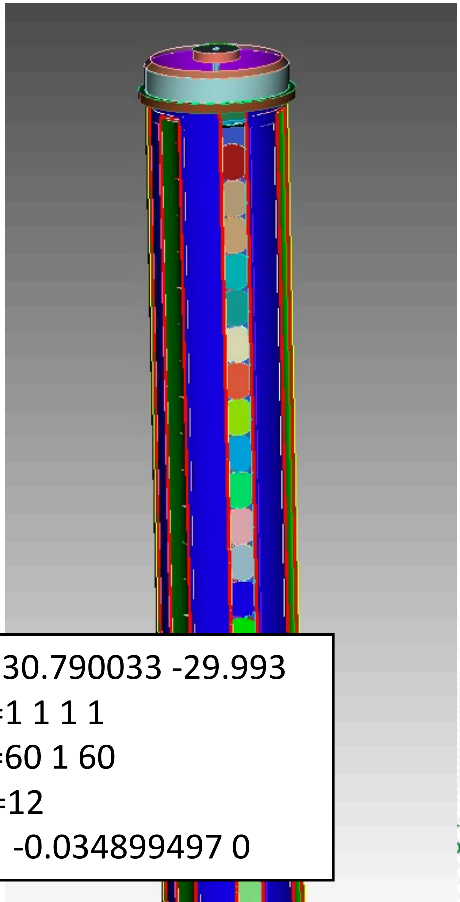


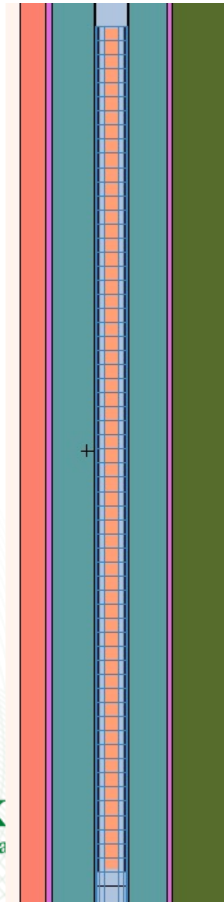
MCNP mesh for the Ir-192 model

- In MCNP5 fmesh can be used to calculate flux, energy disposition, and other important parameters in a much finer resolution without having to explicitly define each region



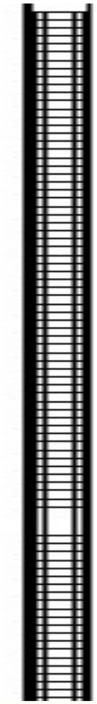




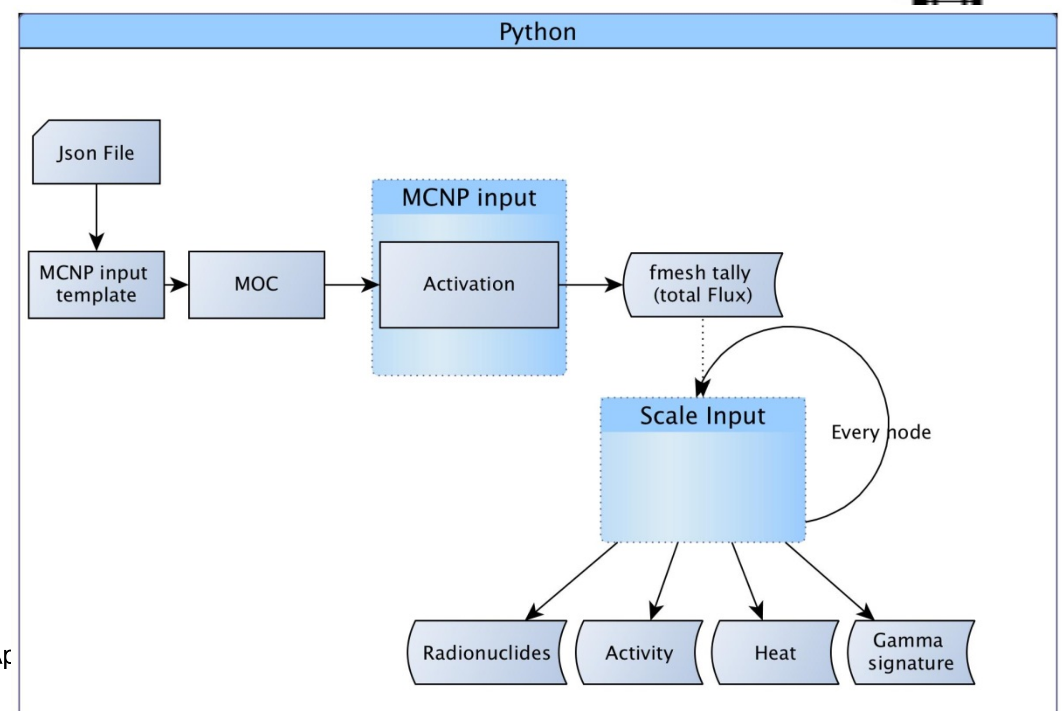


```
fmesh104:N GEOM=cyl          ORIGIN=9.211016  30.790033 -29.993
      IMESH=0.33 0.48 0.537 0.584            IINTS=1 1 1 1
      JMESH=28.33  30.48  58.81              JINTS=60 1 60
      KMESH=1                                KINTS=12
      AXS=0 0 1        VEC=0.999390827           -0.034899497 0
```

Mesh based depletion

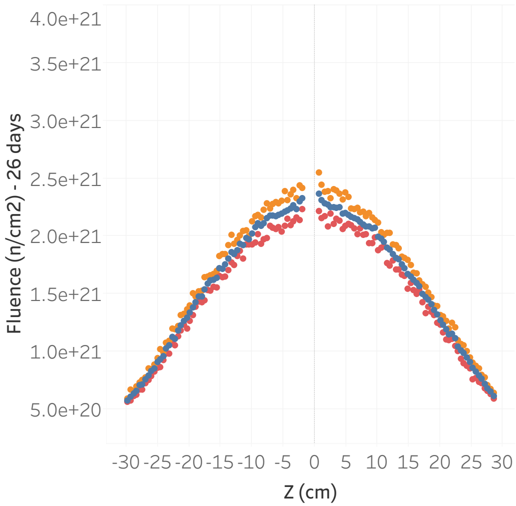


- Information from the flux tally is automatically used to create a SCALE input (over 700 depletion calculations)
- Results are saved to a database for additional analysis and visualization.
- Information for every region in the mesh includes:
  - radionuclides
  - activity over time
  - heat rates during irradiation
- Results can be used for:
  - Experiment optimization
  - Safety calculation
  - Transportation calculation

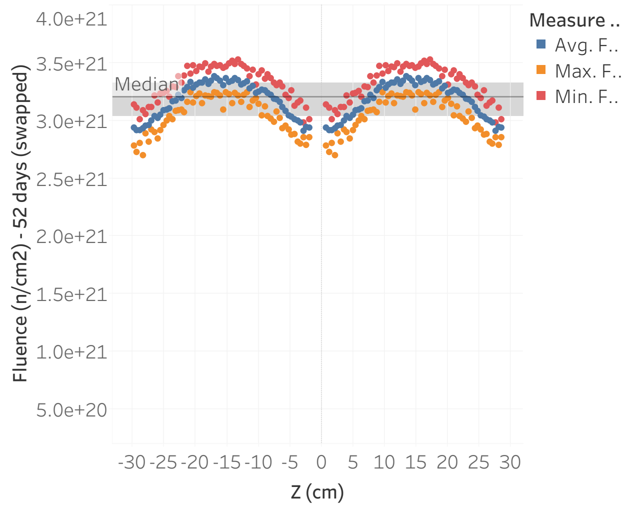


Results from mesh based depletion

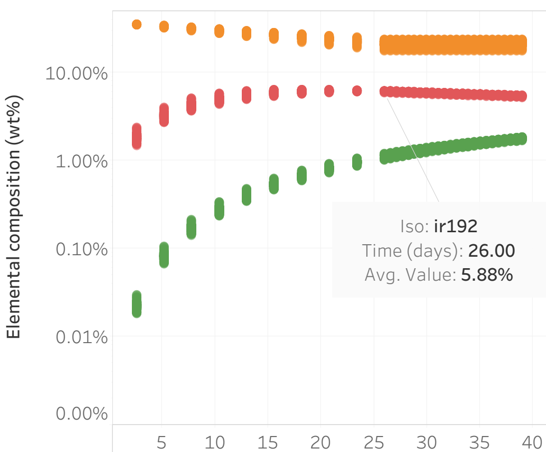
- Initially thought higher fluence would mean more Ir-192 production
- Also thought swapping would produce a more uniform fluence and as such a consistent distribution of Ir-192
- However, from the mesh based depletion approach at was determined one capsule in the center of the experiment produced better results than two targets irradiated for two cycles
- May be due to the high cross section of Ir-192 along with its short half-life



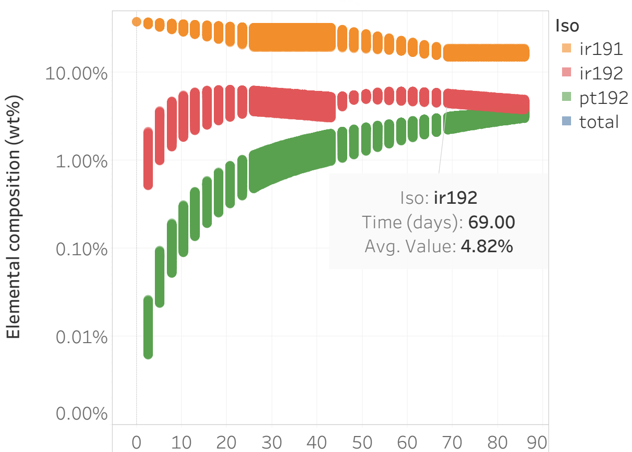
Fluence after once cycle



Fluence after two cycles with targets swapped



Isotopic composition for center position after 1 cycle



Isotopic composition after two cycles with targets swapped

Future Work

- Further understand when using cross sections versus recipes make a significant difference in fuel cycle analysis
- Use ORIGEN to create radiation source term for use in MCNP to determine what fracture of gamma rays are absorbed in the sample vs being absorbed outside the experiment

My wish list for the SCALE community

- Create a way to combine multiple COUPLE generated cross sections files into one ft71 file
- Create a github site to help develop python processing tools for people among SCALE user group to help develop