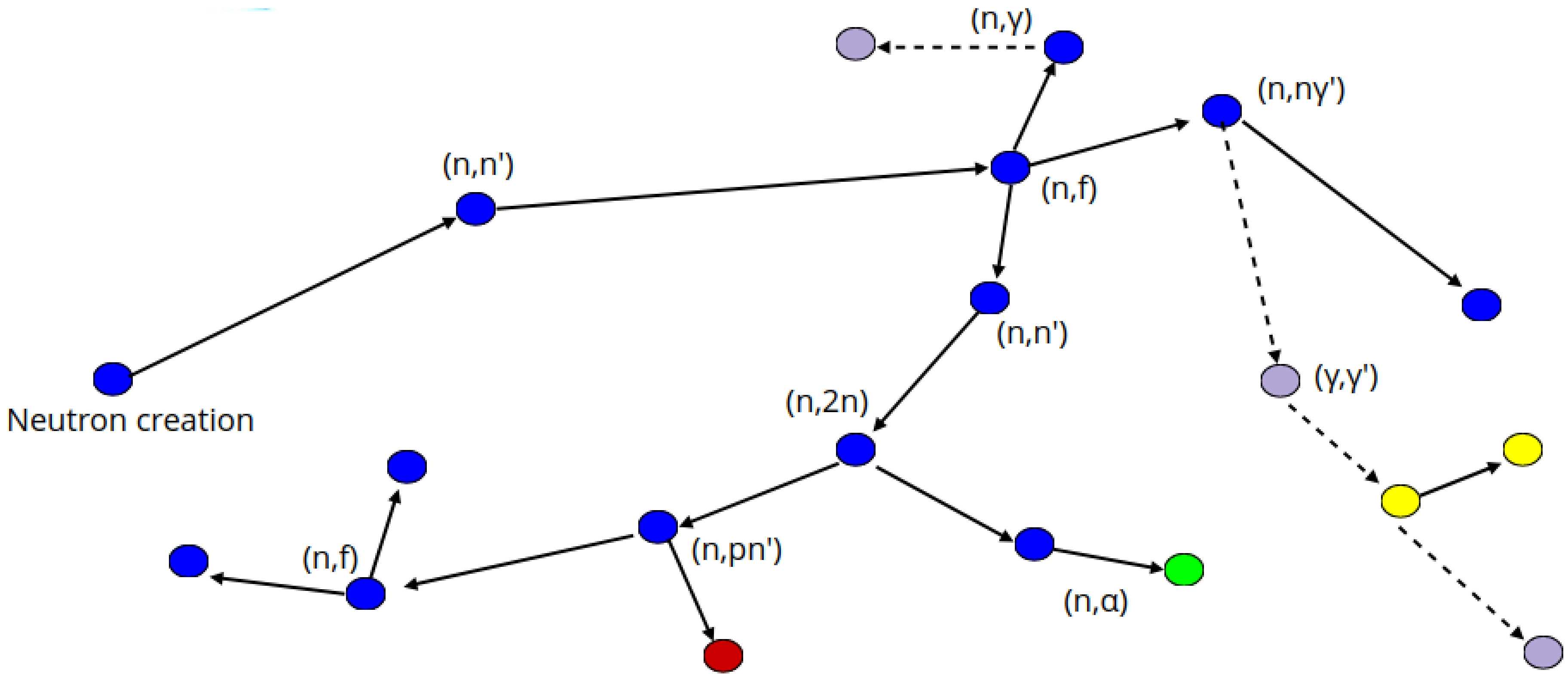
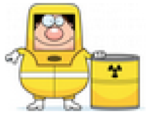
Fusion Neutronics Workshop

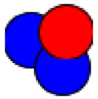


Why is neutronics useful

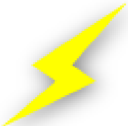


- Radioactivity - Neutrons activate material, making it radioactive leading to handling and waste storage requirements.

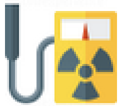
- Hazardous - Neutrons are Hazardous to health and shielded will be needed to protect the workforce.



- *Produce fuel* - Neutrons will be needed to convert lithium into tritium to fuel the reactor.



- *Electricity* - 80% of the energy release by each DT reaction is transferred to the neutron.



- *Structural integrity* - Neutrons cause damage to materials such as embrittlement, swelling, change conductivity …
- *Diagnose* - Neutrons are an important method of measuring a variety of plasma parameters (e.g. Q value).

Topics Covered Half Day Course

- Neutron and Photon interaction cross sections
- Material creation
- Particle sources
- Constructive Solid Geometry (CSG)
- Tallies (heat, tritium breeding ratio, damage, flux)
- Neutron activation

Getting started

- 🐳 Install Docker
- 🔽 Download the docker image
- 🏃 Run the docker image
- 🔗 Navigate to the URL in the terminal

Detailed instructions are on GitHub

Containers

Install single package (Docker) and avoid installing a few hundred packages.

- Portable
- Reproducible
- Security
- Isolation
- Deployable

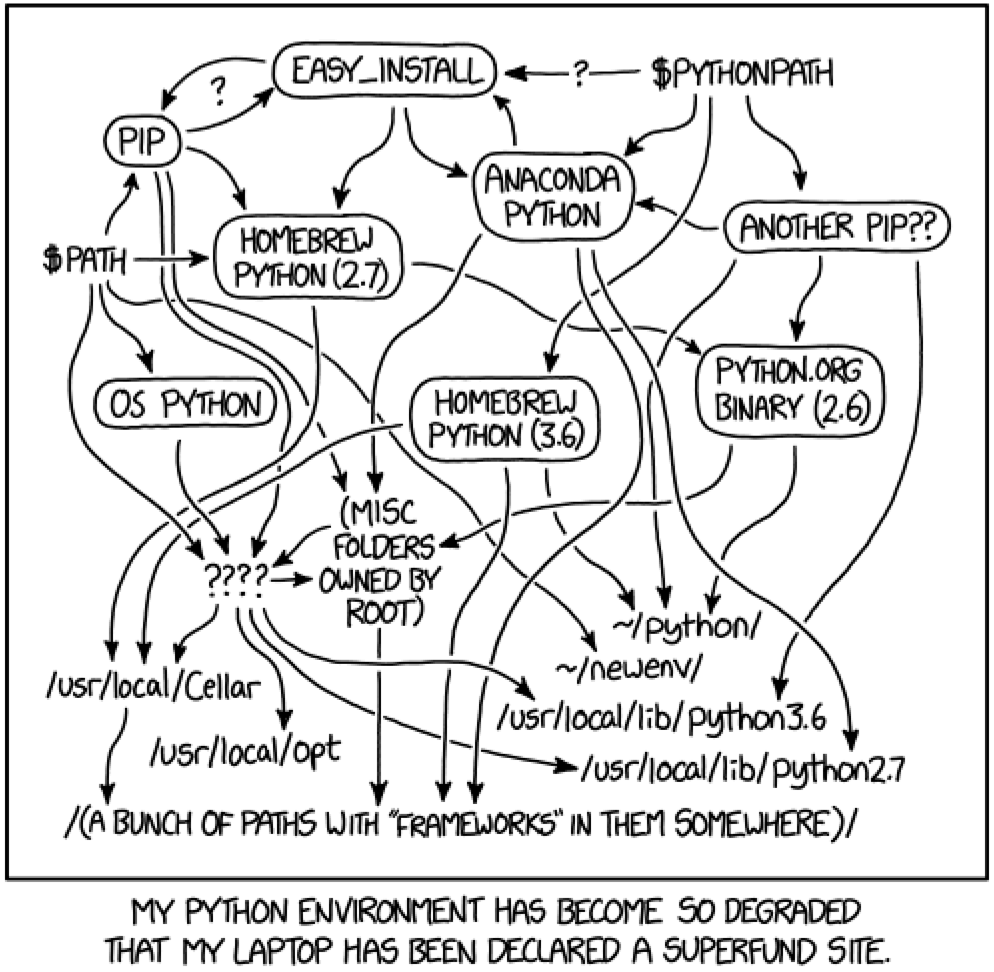
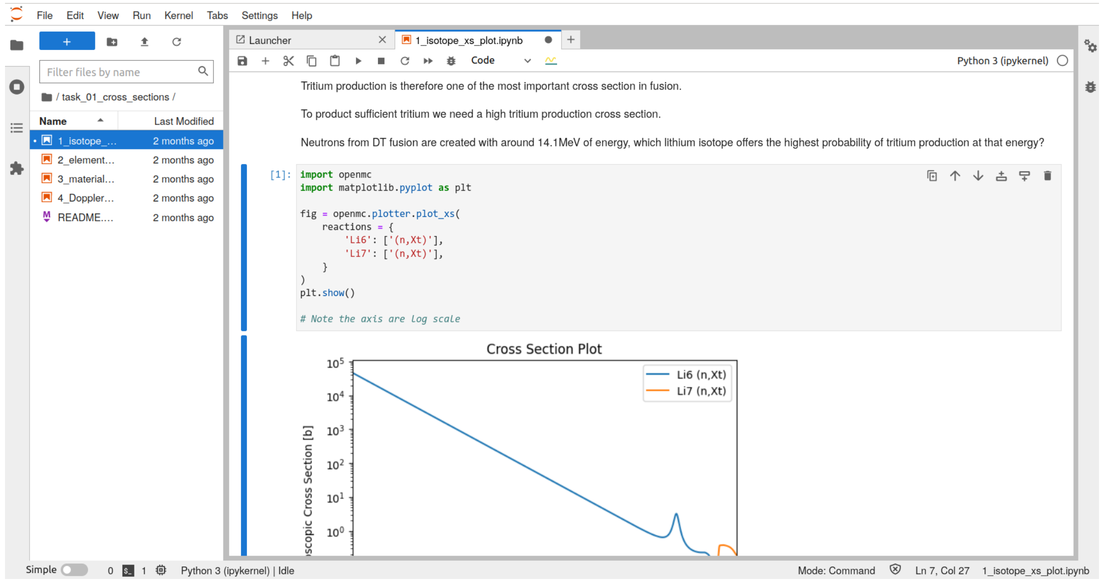


image source xkcd.com

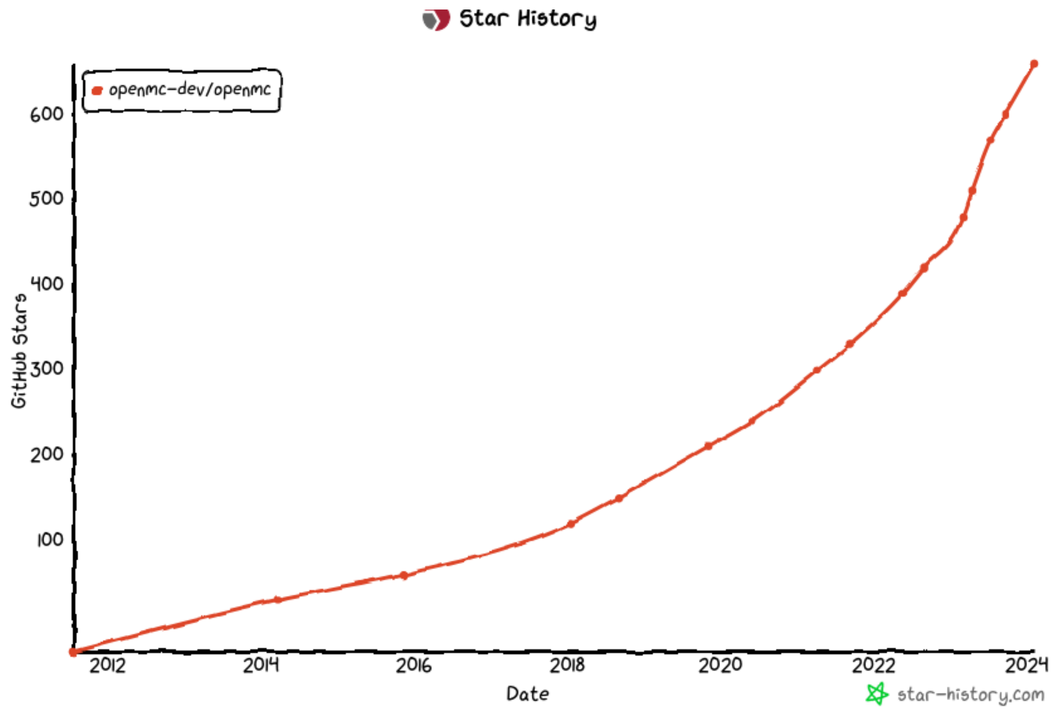
Tasks

- Collection of Jupyter notebooks
- Separate task folder for each topic
- Learning outcomes for each task
- Simulation outputs include:
  - numbers
  - graphs
  - images
  - 3D visualization.



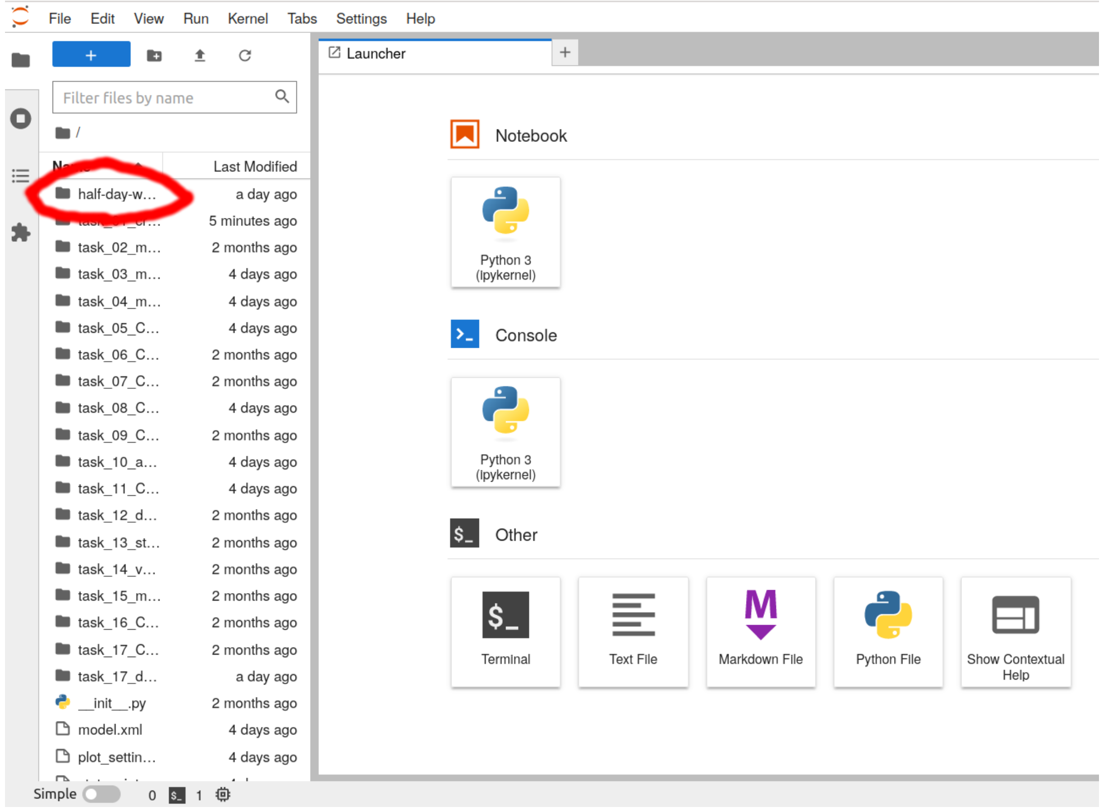
OpenMC

- Increasing adoption in fusion
- Supportive community
- GitHub repository
- Permissive license (MIT)
- Python API, C++ backend
- Scales to 100,000+ cores
- CPU and GPU version
- Online documentation
- Excellent fusion specific workshops



Getting started

1. Run the docker image `docker run -p 8888:8888 ghcr.io/fusion-energy/neutronics-workshop`
2. Double click on the `half-day-workshop` folder circled in red.



Timetable

- 9.00 Introduction presentation
- 9.10 Plotting cross sections
  - task_01_isotope_xs_plot
  - task_02_element_xs_plot
  - task_03_material_xs_plot
- 9.40 Making materials
  - task_04_example_materials_from_isotopes
  - task_05_example_materials_from_elements
- 9.55 Geometry
  - task_06_simple_csg_geometry
- 10.15 Break ☕
- 10.30 Plotting particles
  - task_07_point_source_plots
  - task_08_ring_source
  - task_09_plasma_source_plots
- 11.05 Tritium Breeding Ratio (TBR)
  - task_10_example_tritium_production
- 11.15 Damage (DPA)
  - task_11_find_dpa
- 11:30 Break ☕
- 11:45 neutron photon spectra
  - task_12_example_neutron_spectra_on_cell
  - task_13_example_photon_spectra
- 12.15 mesh tallies
  - task_14_example_2d_regular_mesh_tallies
- 12.30 activation
  - task_15_full_pulse_schedule
- 12.45 Putting it all together
  - task_16_optimal_design

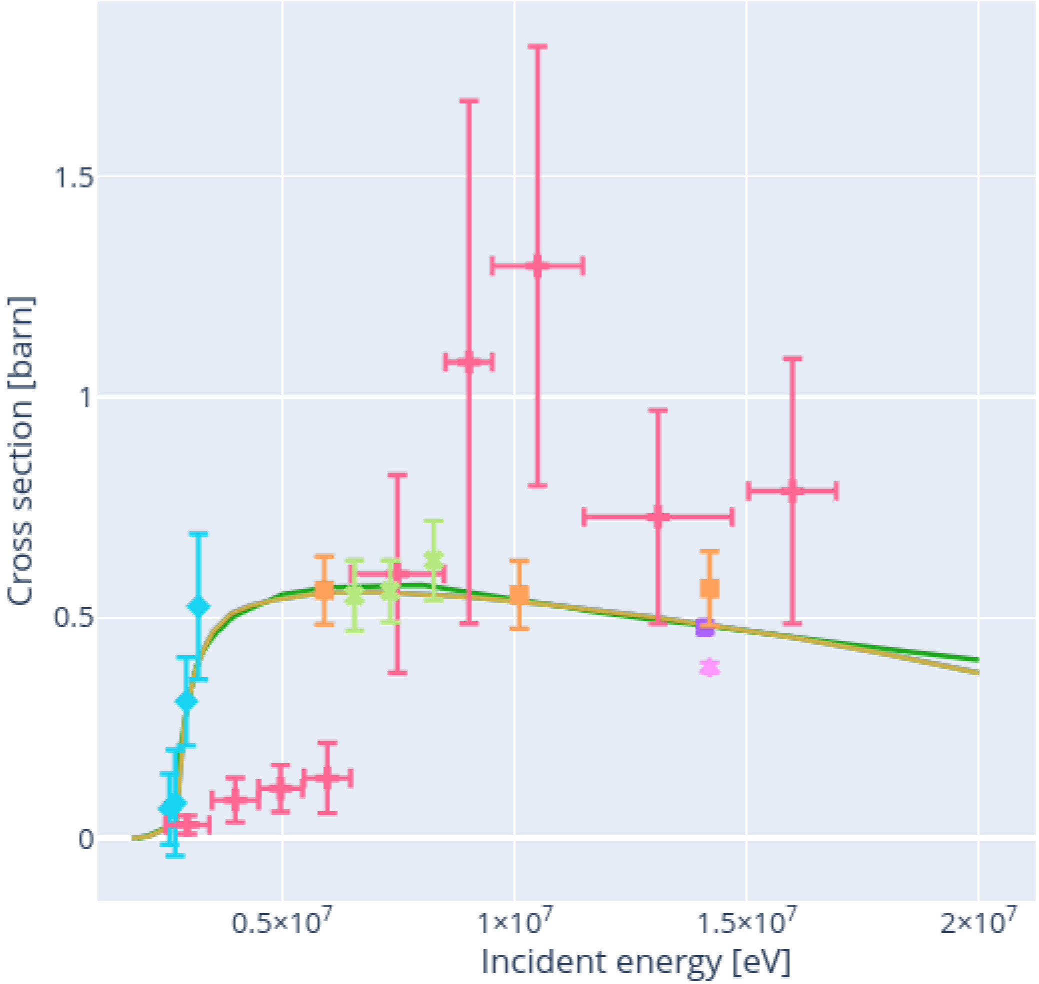
Microscopic Cross Sections

- Probability of interaction is characterised by the microscopic cross-section (σ). It is the effective size of the nucleus.
- Cross section data is key to the neutronics workflow and provide us with the likelihood of a particular interaction.
- Cross sections can be measured experimentally with monoenergetic neutrons.

Experimental data

Availability of experimental data varies for different reactions and different isotopes.

Typically the experimental data is then interpreted to create evaluation libraries, such as ENDF, JEFF, JENDL, CENDL.



Source IAEA nuclear data services

Cross section reactions

Cross section evaluations exist for:

- different nuclides
- different interactions.

A list of reactions available in OpenMC is here

For example:

- Be9(n,2n)2He would be a neutron interaction with beryllium 9 which results in 2 neutrons and 2 helium nuclei.
- Li6(n,Xt) would be a neutron interaction with lithium 6 nuclei which results in a tritium and X is a wildcard.

Reaction rate

- The reaction rate (RR) can be found by knowing the number of neutrons per unit volume (n), the velocity of neutrons (v), the material density (p), Avogadro's number (N_a), the microscopic cross section at the neutron energy (σ_e) and the atomic weight of the material (M).
- This reduces down to the neutron flux (ϕ), nuclide number density (N_d) and microscopic cross section\sigma_{e}.
- This can be reduced one more stage by making use of the Macroscopic cross section (Σ_e).

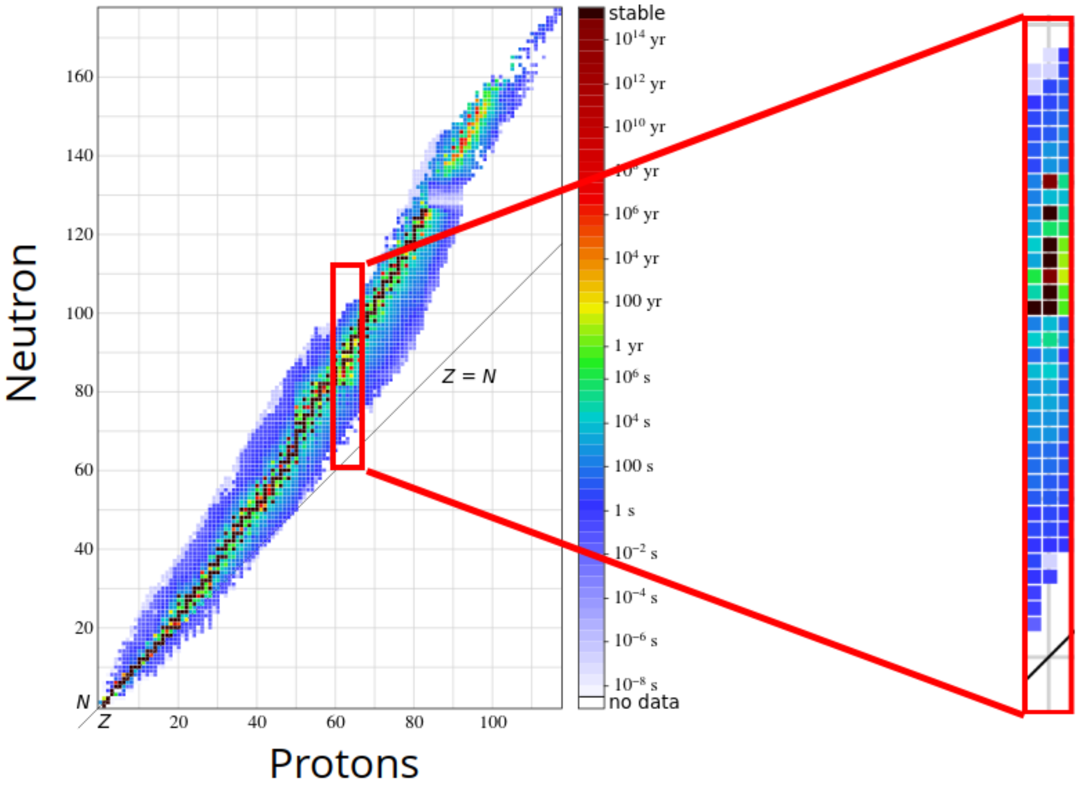
$$RR = \frac{nv\rho N_a \sigma_e}{M} = \phi N_d \sigma_e = \phi \Sigma_e$$

Now complete tasks 1, 2 and 3 in the half day workshop

Making materials

Neutronics codes require the isotopes and the number density.

This can be provided with different combinations of density units, isotope/element concentration and weight or atom fractions.



Making materials - nuclides

Simple material construction from nuclides.

```
mat2 = openmc.Material()
mat2.add_nuclide('Li6', 0.0759*2)
mat2.add_nuclide('Li7', 0.9241*2)
mat2.add_nuclide('O16', 0.9976206)
mat2.add_nuclide('O17', 0.000379)
mat2.add_nuclide('O18', 0.0020004)
mat2.set_density('g/cm3', 2.01)
```

Making materials - elements

Simpler material construction from elements.

```python
import openmc

mat1 = openmc.Material()
mat1.add_element('H', 2)
mat1.add_element('O', 1)
mat1.set_density('g/cm3', 2.01)
```

Making materials - enrichment

Simple enriched material construction from elements.

```
import openmc

mat1 = openmc.Material()
mat1.add_element('Li', 4, enrichment_target='Li6', enrichment=60)
mat1.add_element('Si', 1)
mat1.add_element('O', 4)
mat1.set_density('g/cm3', 2.01)
```

Now complete tasks 4 and 5 in the half day workshop

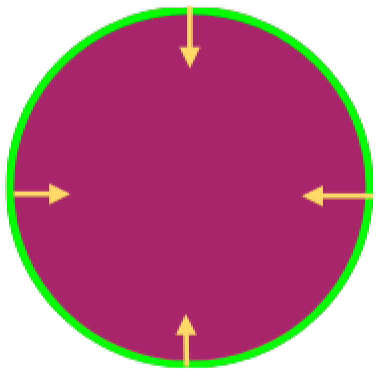
Making Geometry

The simplest geometry is a single surface and a cell defined as below (-) that surface.

```python
import openmc

surface_sphere = openmc.Sphere(r=10.0)
region_inside_sphere = -surface_sphere
cell_sphere = openmc.Cell(region=region_inside_sphere)

cell_sphere.fill = steel
```



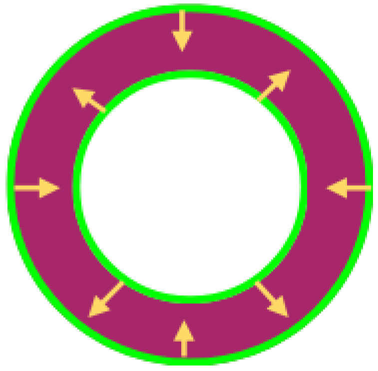
Making Geometry

Cells can also be constrained by multiple surfaces. This example is above (+) one surface and (&) below (-) another

```python
import openmc

surf_sphere1 = openmc.Sphere(r=10.0)
surf_sphere2 = openmc.Sphere(r=20.0)
between_spheres = +surf_sphere1 & -surf_sphere2
cell_between = openmc.Cell(region= between_spheres)

cell_sphere.fill = steel
```

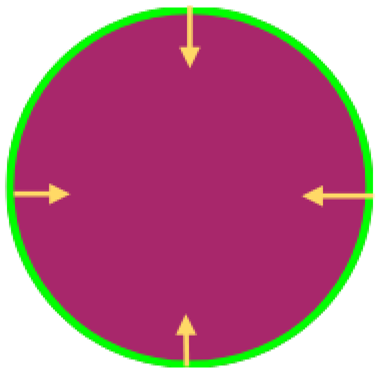


Edge of the model

The outer most surface of the model should have a `boundary_type` set to `"vacuum"` to indicate that neutrons should not be tracked beyond this surface.

```
import openmc

surf_sphere = openmc.Sphere(r=10.0, boundary_type="vacuum")
between_spheres = -surf_sphere
cell_between = openmc.Cell(region= between_spheres)
```



Surfaces available

Constructive Solid Geometry (CSG) [implementation in OpenMC] has the following surface types.

- XPlane, YPlane, ZPlane, Plane
- XCylinder, YCylinder, ZCylinder
- Sphere
- XCone, YCone, ZCone,
- Quadric
- XTorus, YTorus, ZTorus

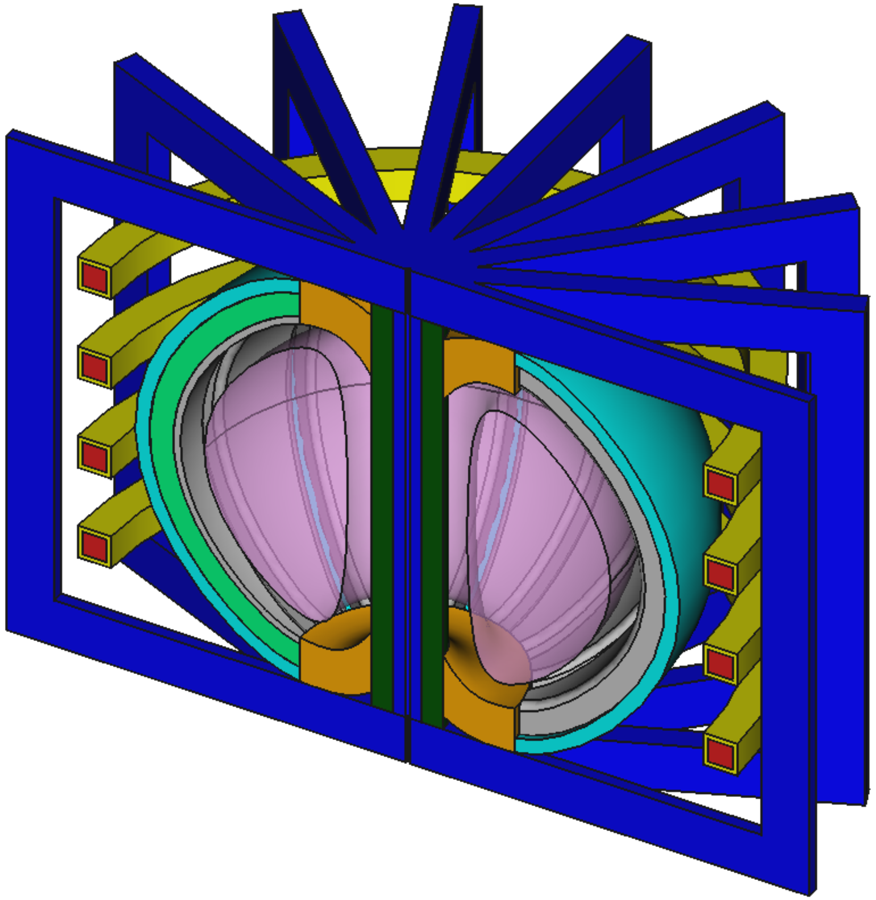


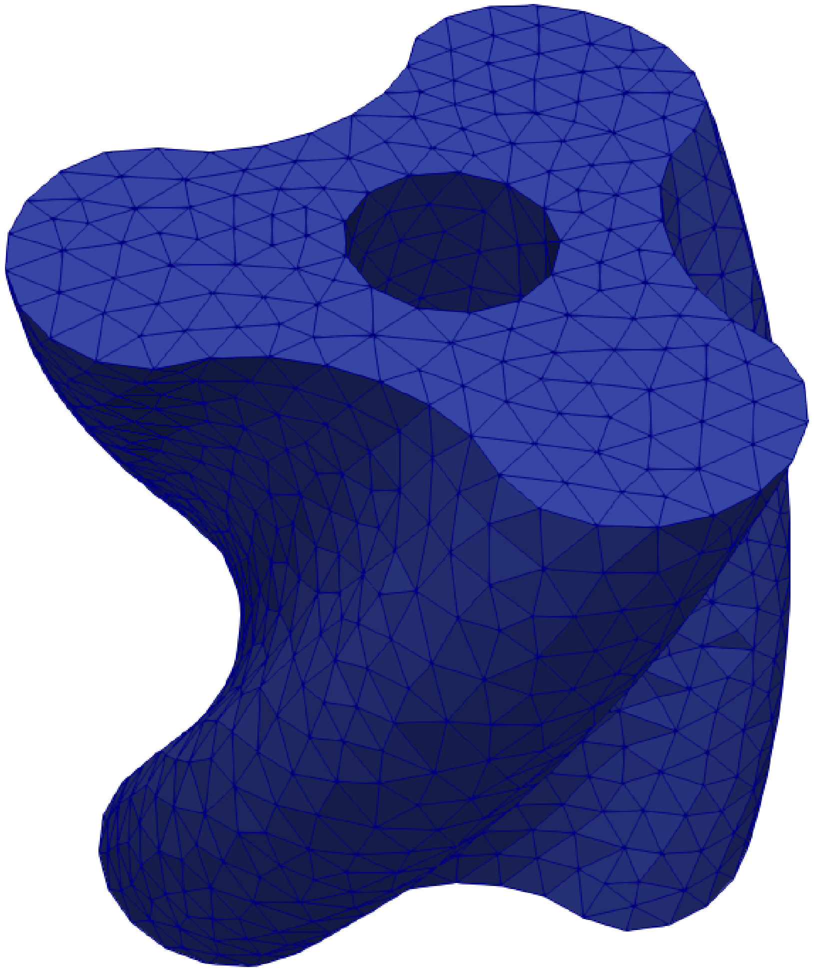
Image source Paramak

More complex geometry

OpenMC also supports:

- boolean operations like union, intersection and complement.
- rotations and translations
- nested geometry with universes
- different surface types (e.g reflective for sector model)

For more complex 3D geometry DAGMC can be used which makes use of a meshed geometry to transport particles.



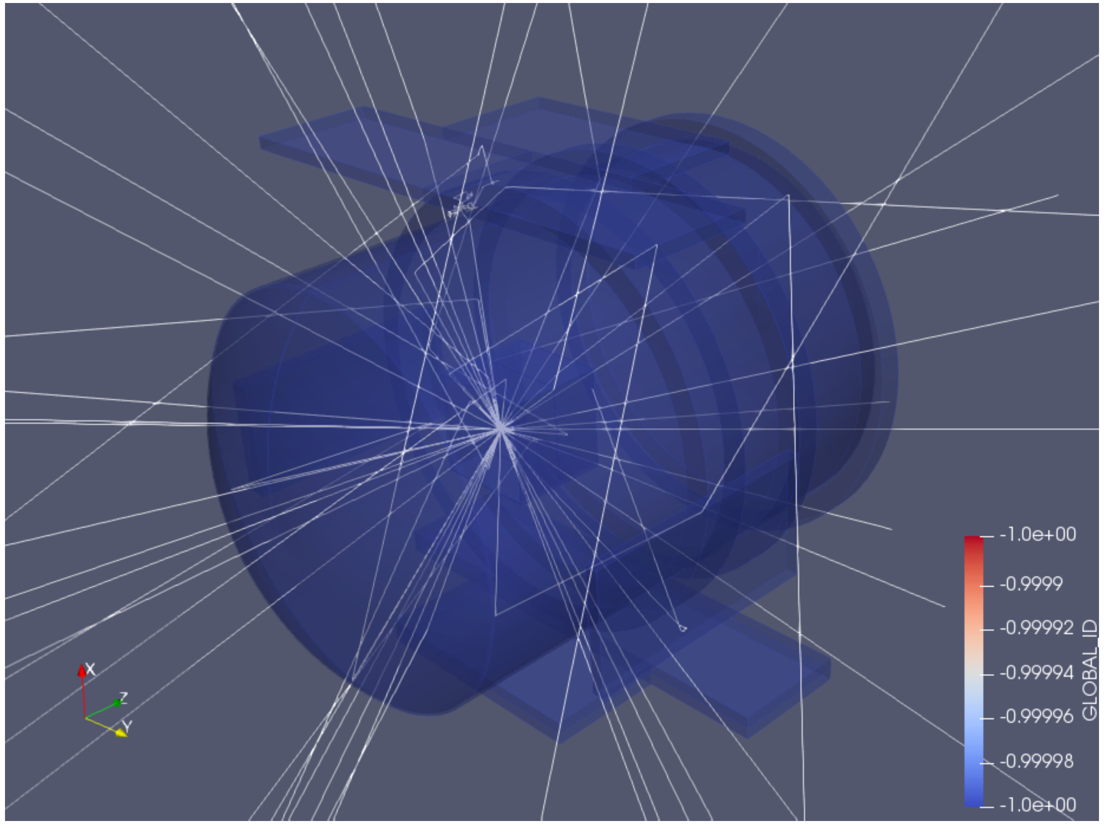
Now complete task 6 in the half day workshop

Plotting particles

Neutron and photon sources have distributions for:

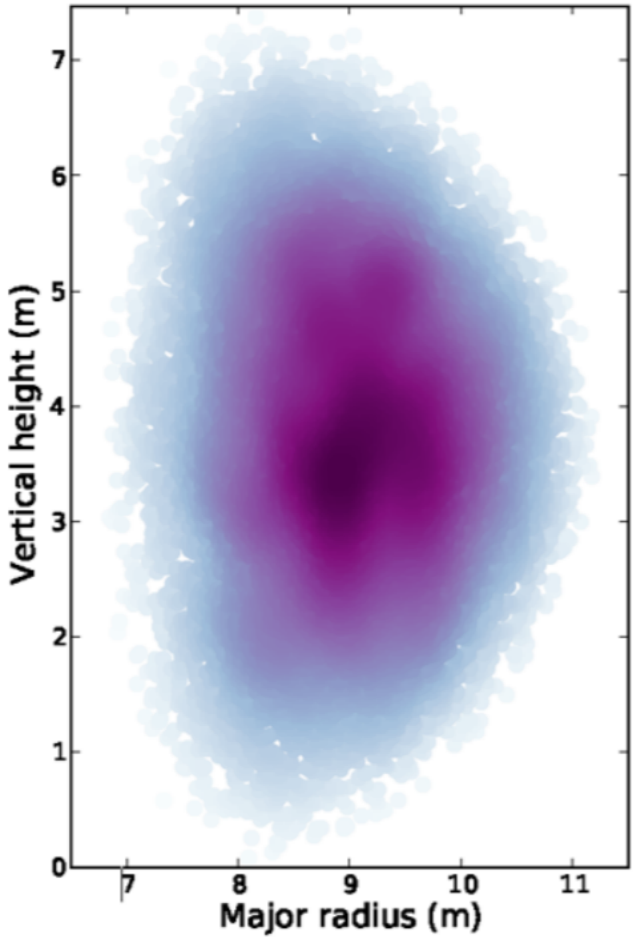
- space
- energy
- direction

Visualization of the source term helps check the simulation is correct



Spatial distribution of MCF and ICF sources

The spatial distribution of MCF plasma covers a larger area compared to ICF'



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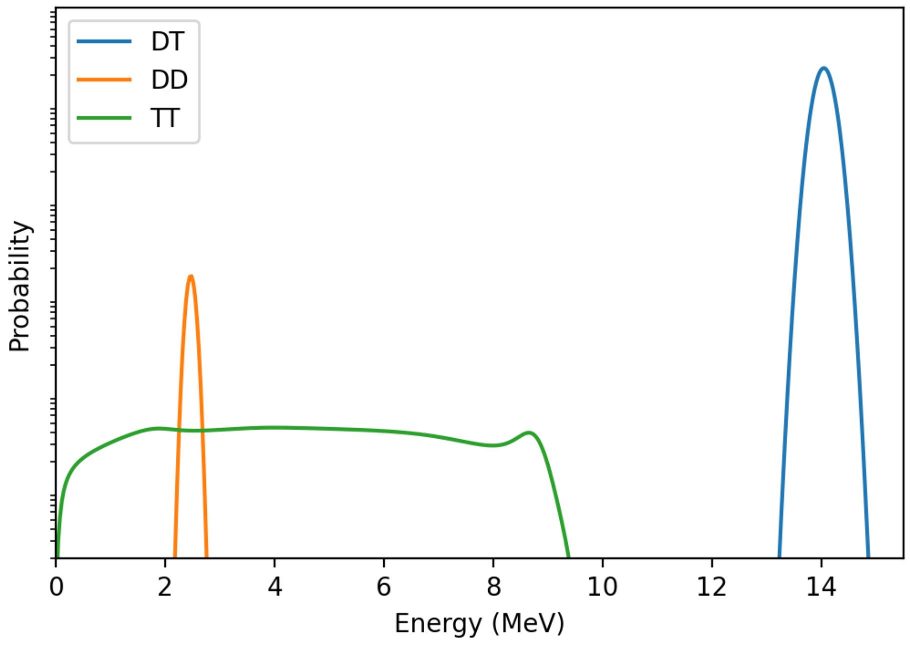
Energy distribution MCF and ICF sources

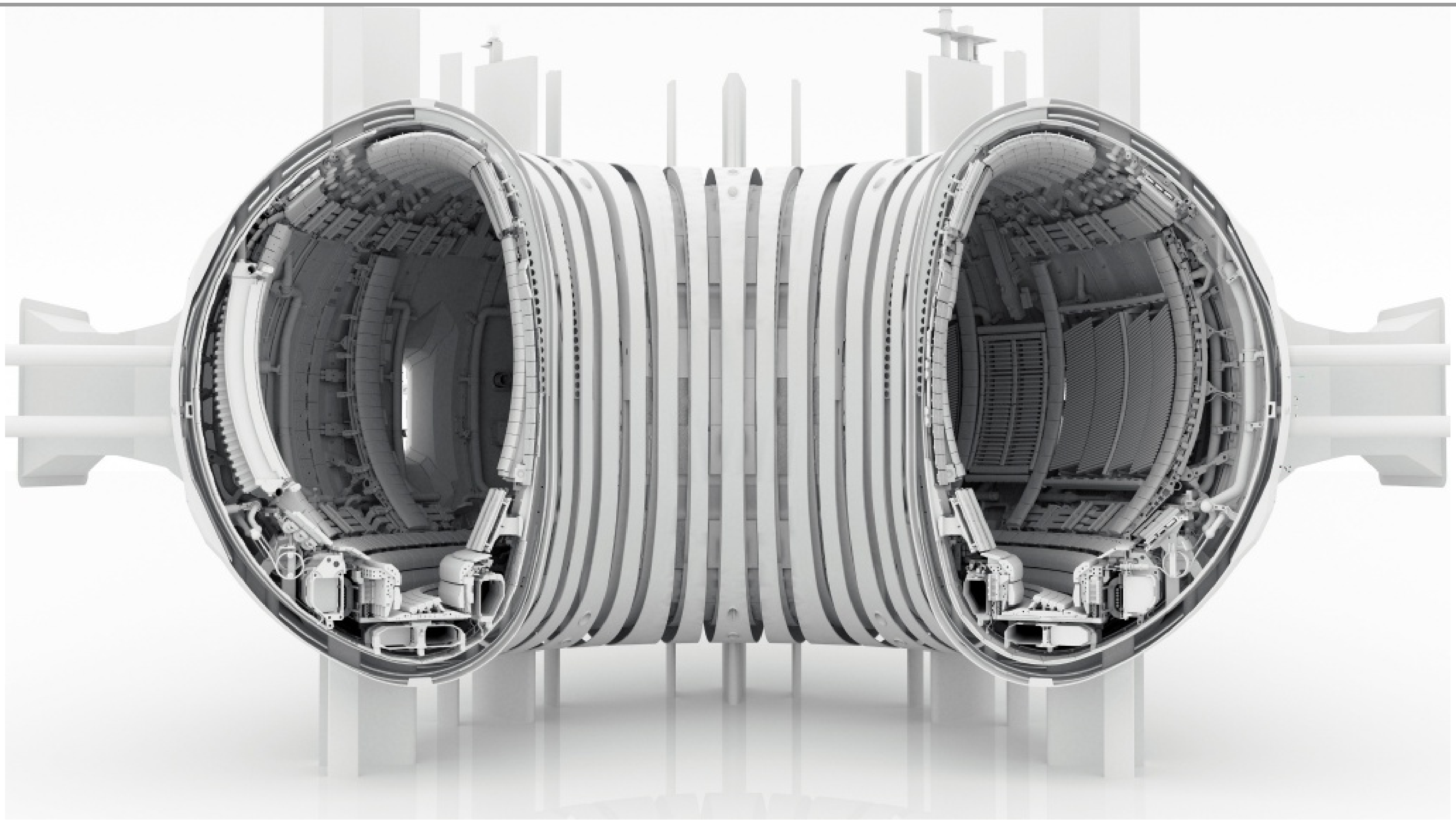
The energy distribution of MCF has less neutron scattering compared to ICF. Neutrons are:

- up scattered through collisions with alpha particles
- down scattered through collisions with DT nuclides
- plot shows initial neutron energy from a 50:50 DT plasma



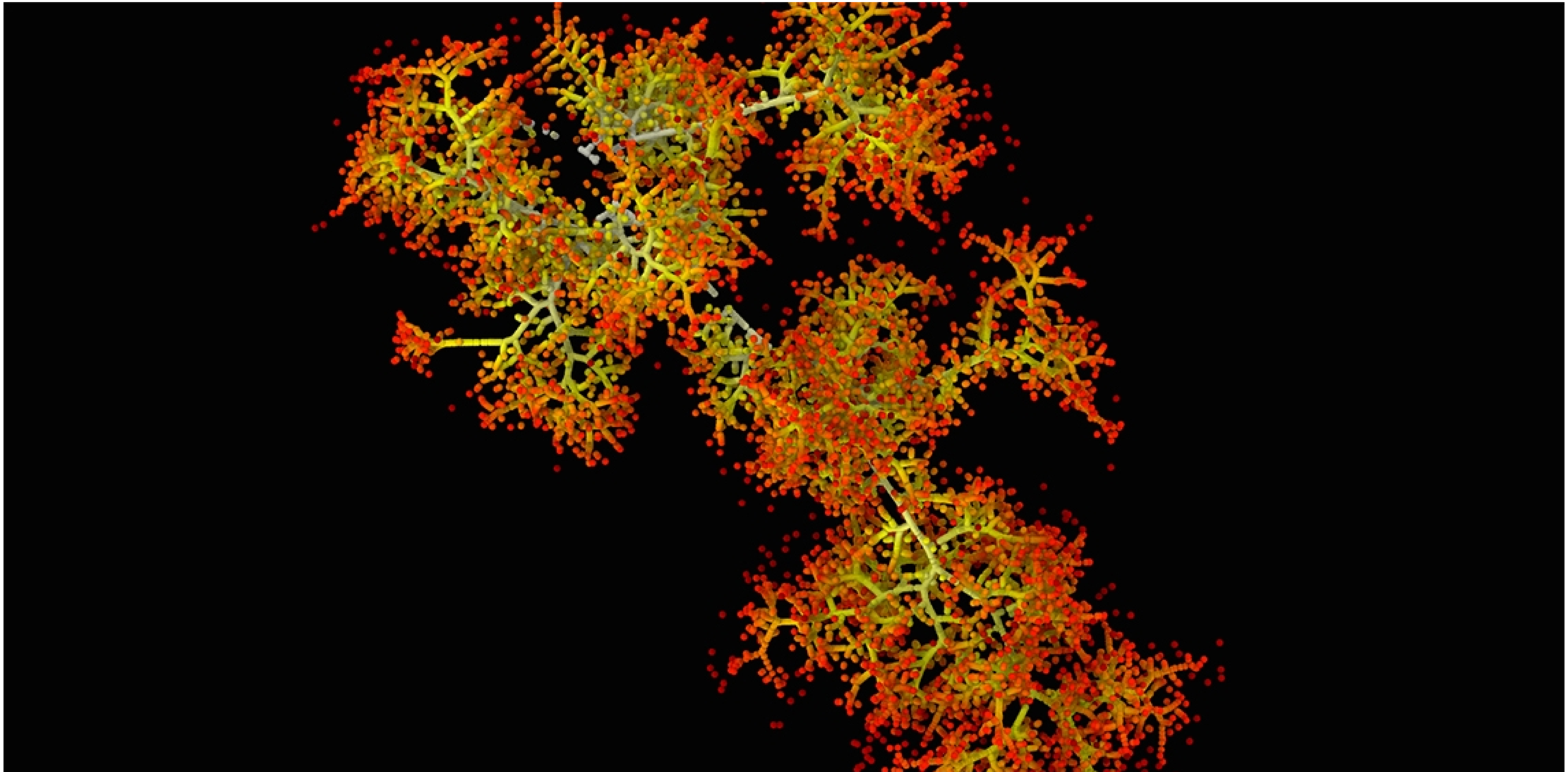
Now complete tasks 7, 8 and 9 in the half day workshop

Tritium Breeding Ratio



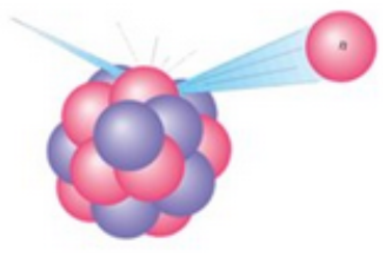
Now complete task 10 in the half day workshop

Damage tallies



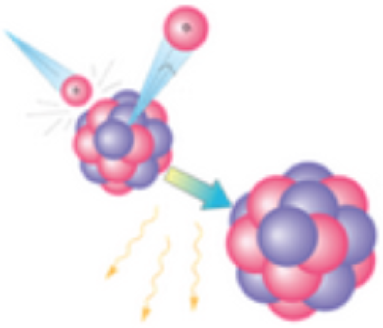
Now complete task 11 in the half day workshop

Neutron scattering



- (n,n)
- Neutron collides with the nucleus
- Neutron scatters of the nucleus losing energy
- Energy gained by the nucleus which recoils

image source slb.com



- (n,n'g)
- Neutron capture by the nucleus
- Instantaneously re-emitted with less energy
- Nucleus in excited state
- Relaxes to ground state by emitting gamma rays

Neutron scattering angle

- At low energies the angular distribution is often isotropic
- As the neutron energy increases the scattering typically becomes more forward peaked
- Resonances in the cross section can impact the angular distribution probabilities

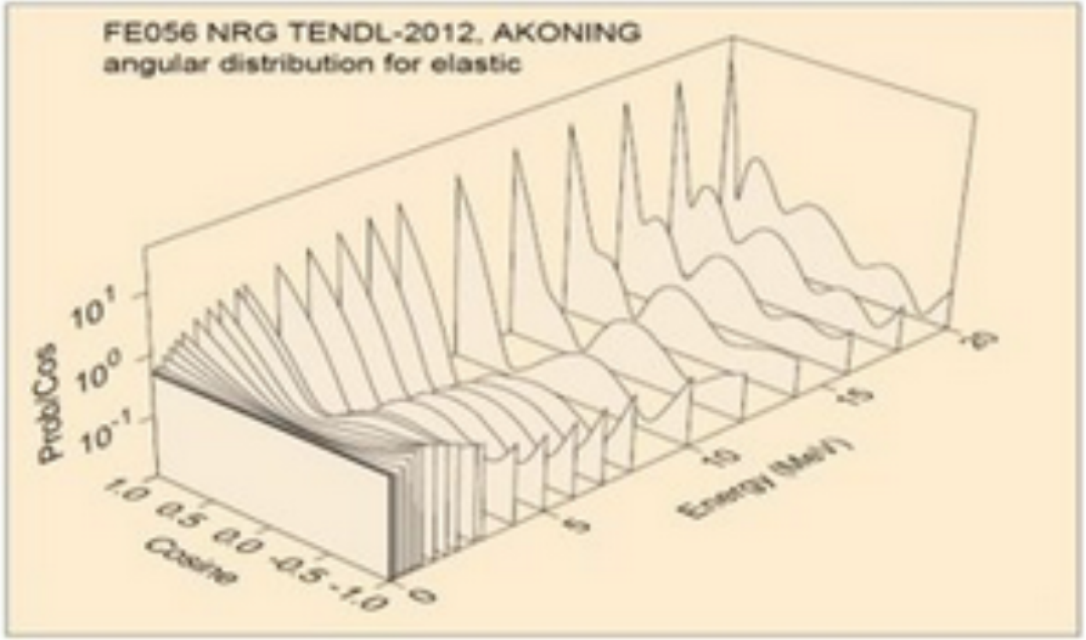
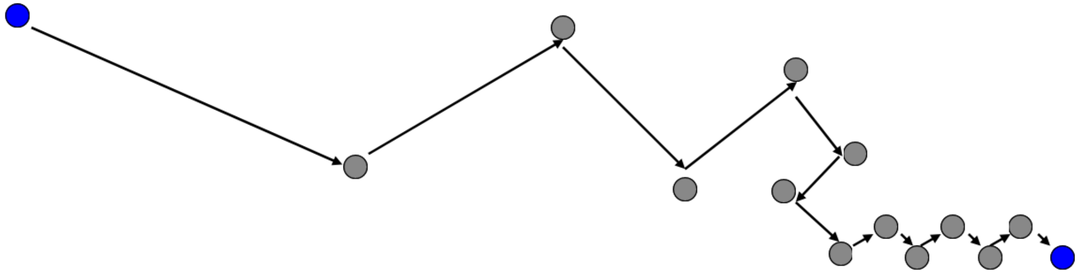
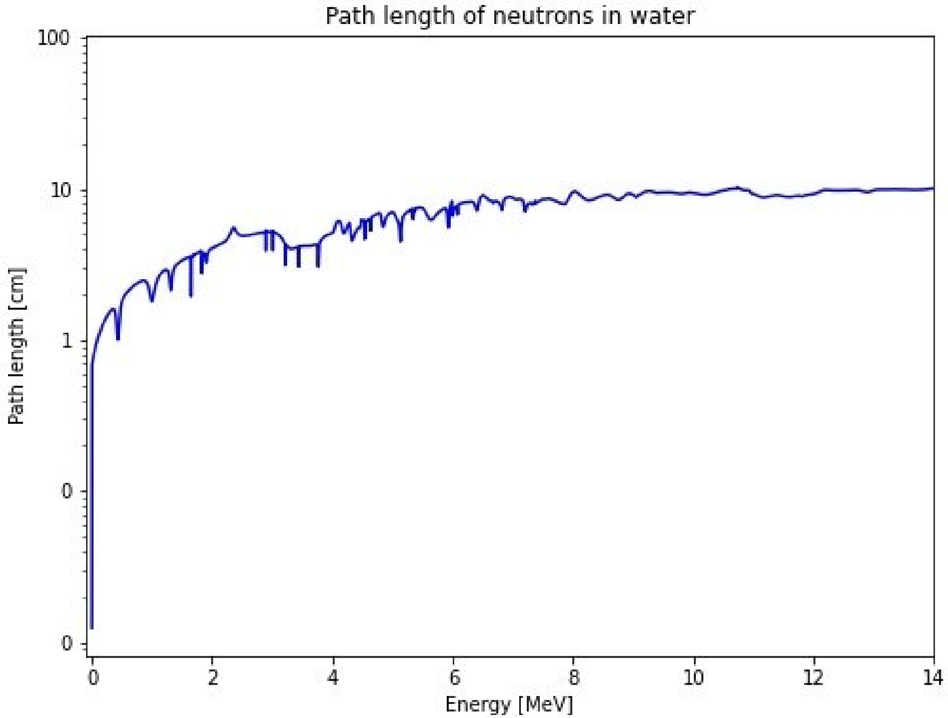


Image source tend.web.psi.ch

Path length

- Path length = 1 / Σ_T
- A 14MeV neutron will lose energy via scattering interactions
- As the neutron energy decreases the path length also decreases
- Path length at thermal energy is more constant





Energy loss

The average logarithmic energy decrement (or loss) per collision (ξ) is related to the atomic mass (A) of the nucleus

$$\xi = 1 + \frac{(A-1)^2}{2A} ln \frac{(A-1)}{(A+1)}$$

	Hydrogen	Deuterium	Beryllium	Carbon	Uranium
Mass of nucleus	1	2	9	12	238
Energy decrement	1	0.7261	0.2078	0.1589	0.0084

Collisions to thermalize

The average number of collisions required to reduce the energy of the neutron from E_0 to E.

$$n = \frac{1}{\xi}(lnE_0 - lnE)$$

If E_0 is 14MeV and E is 0.025eV

	Hydrogen	Deuterium	Beryllium	Carbon	Uranium
Number of collisions to thermalize	20	25	85	115	2172

Moderating power

We should account for the likelihood of scattering.

The number density of the nucleus (ND) and the microscopic cross section (σ) combine to produce the macroscopic scattering cross section (Σ)

$$\Sigma_s = N_D \sigma_s$$

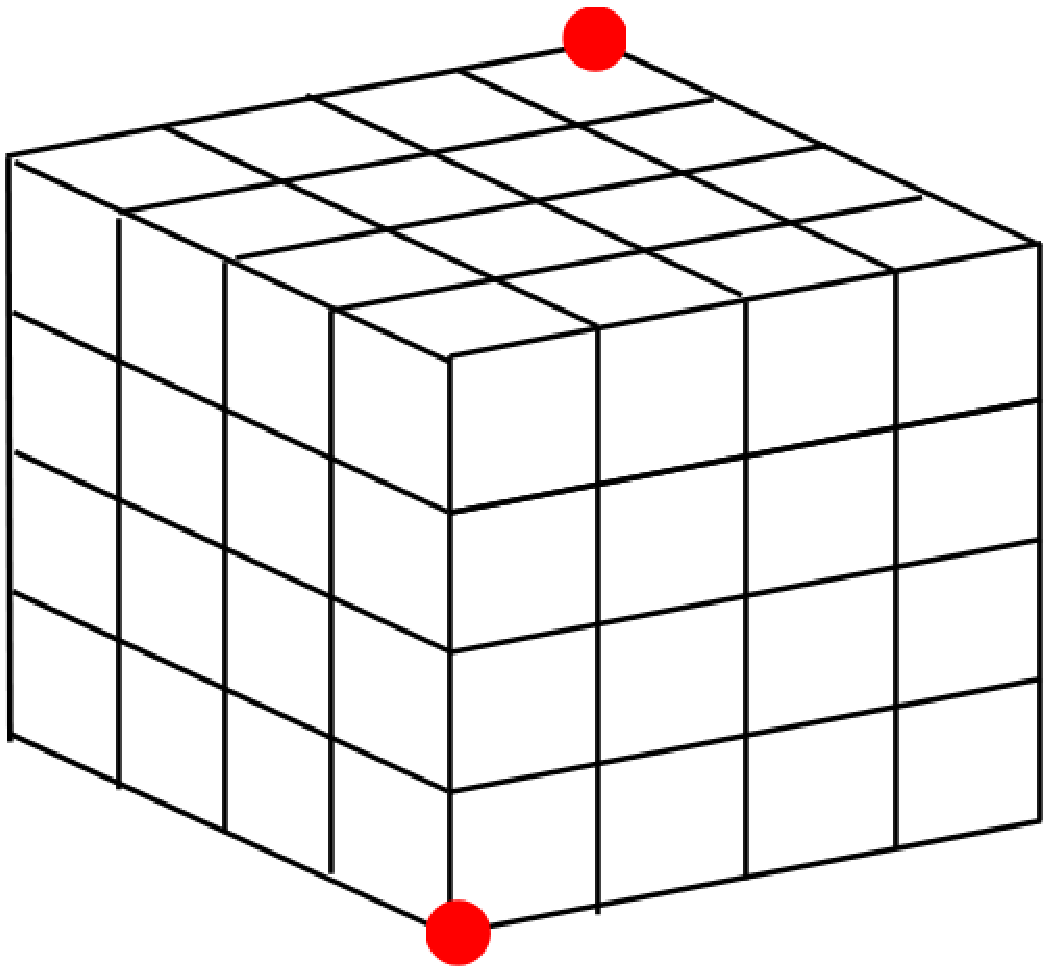
$$Moderating\ power = \xi \Sigma_s$$

	Hydrogen	Deuterium	Beryllium	Carbon	Polyethylene
Moderating power	1.28	0.18	0.16	0.064	3.26

Now complete tasks 12 and 13 in the half day workshop

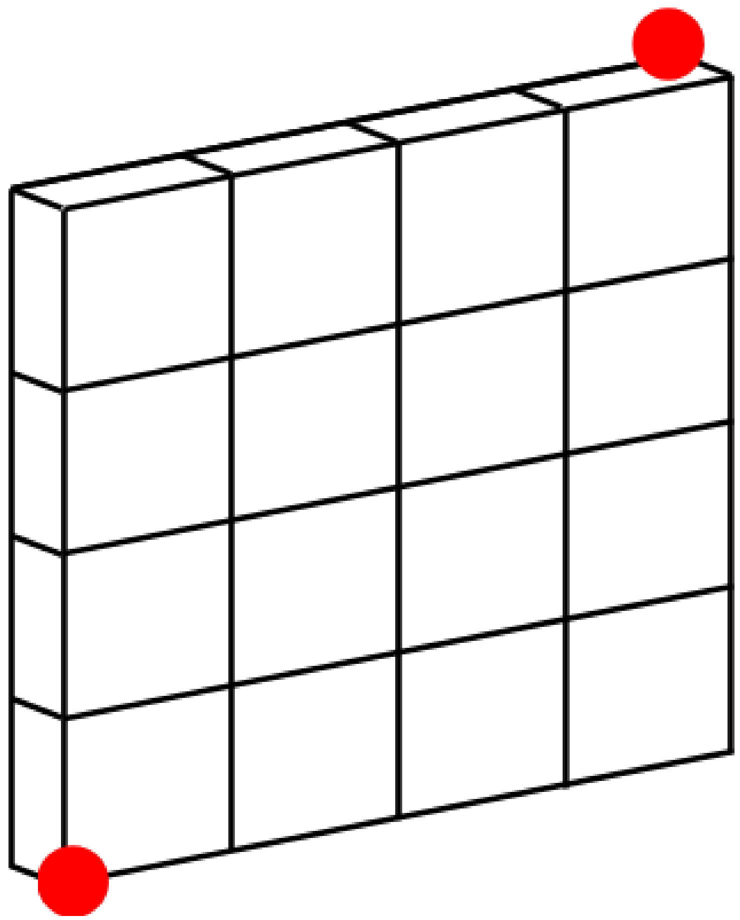
Mesh tallies

- A grid of voxels / mesh elements can be overlaid on a geometry and the neutron response can be tallied in each voxel.
- The mesh is typically 3D and defined with a top right and lower left coordinate.



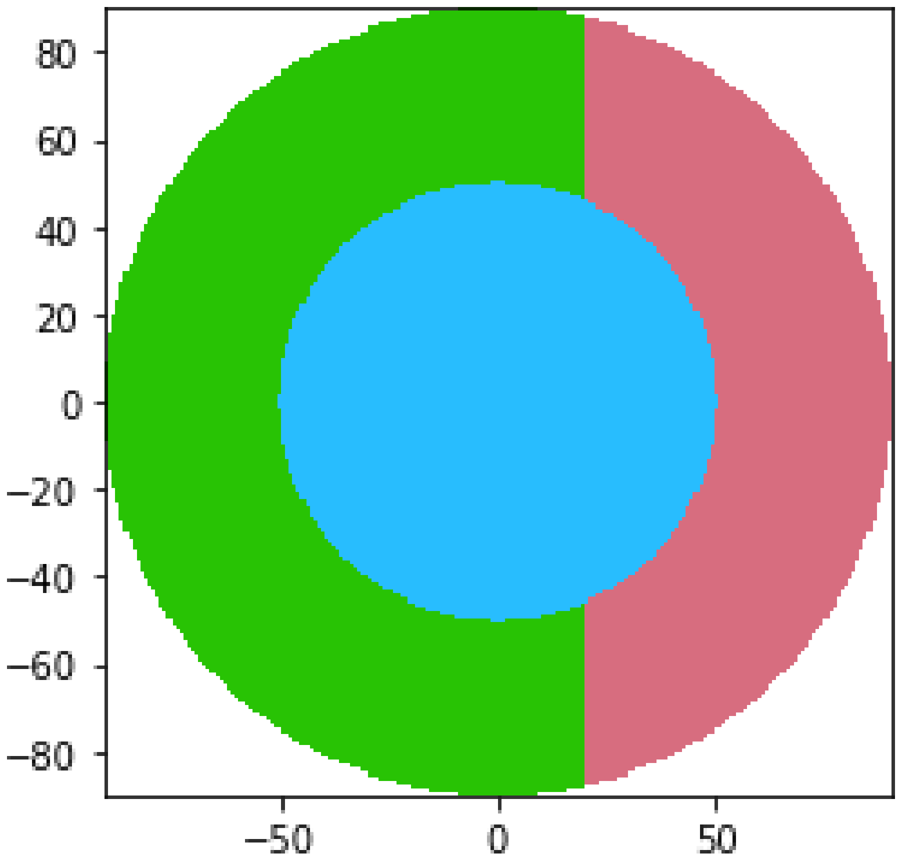
Mesh tallies

- For our example we have a grid of voxels with only 1 voxel in one direction.
- This allows a pixel image of the tally result to be easily plotted.



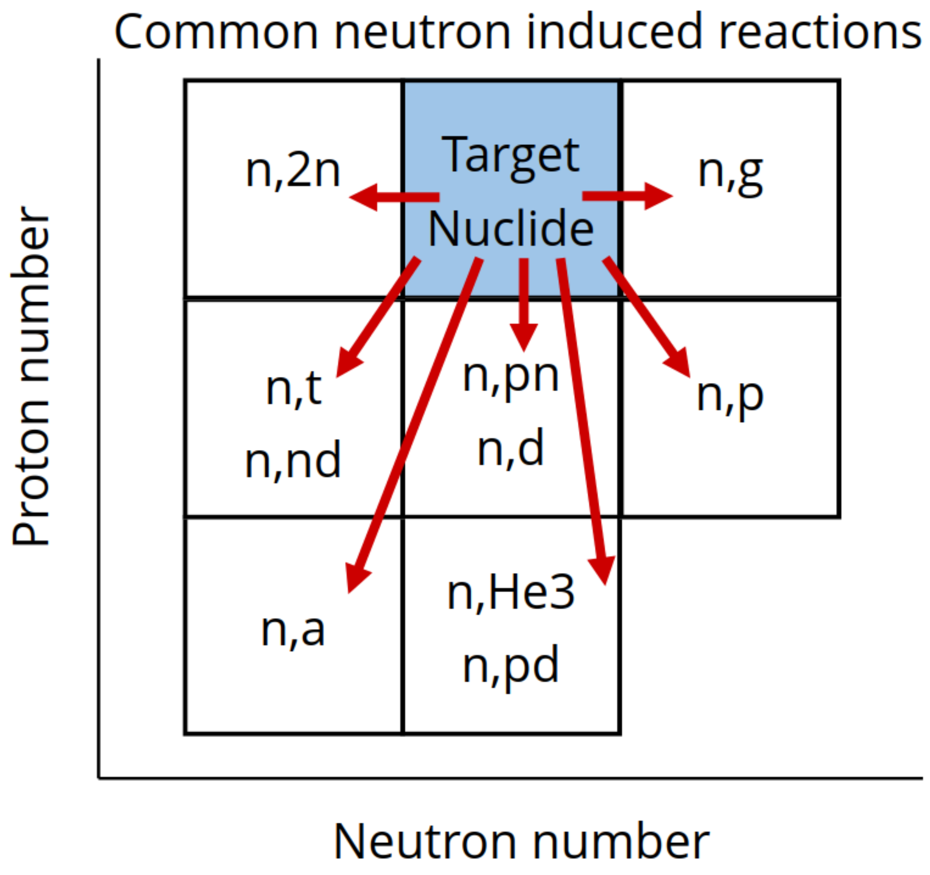
Mesh tallies geometry

- The geometry makes use of a two spheres and a plane surface type.
- The materials in each region respond very differently to neutrons
- The task has mesh tallies with different scores and plotting to visualize the result



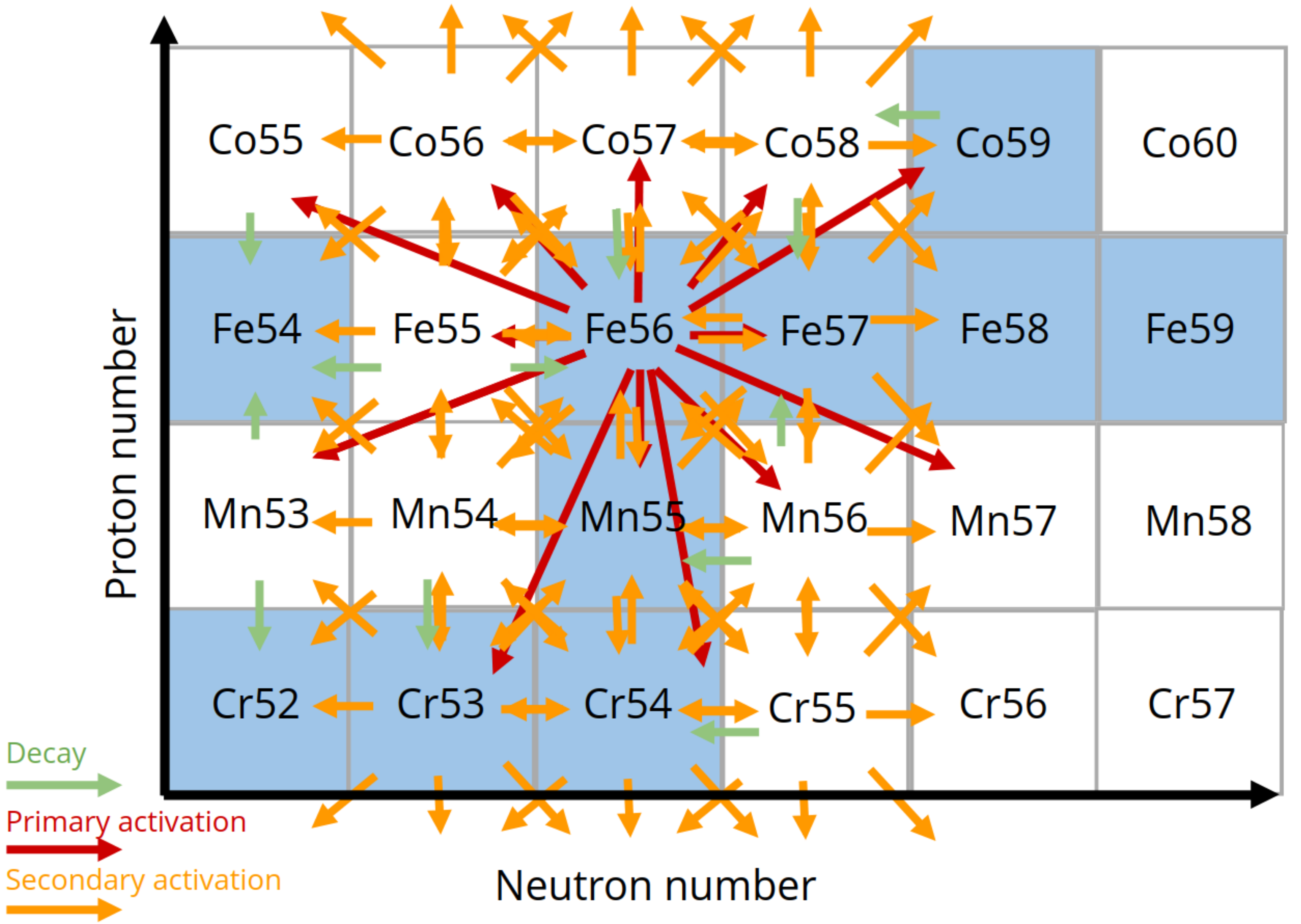
Now complete task 14 in the half day workshop

Activation reactions



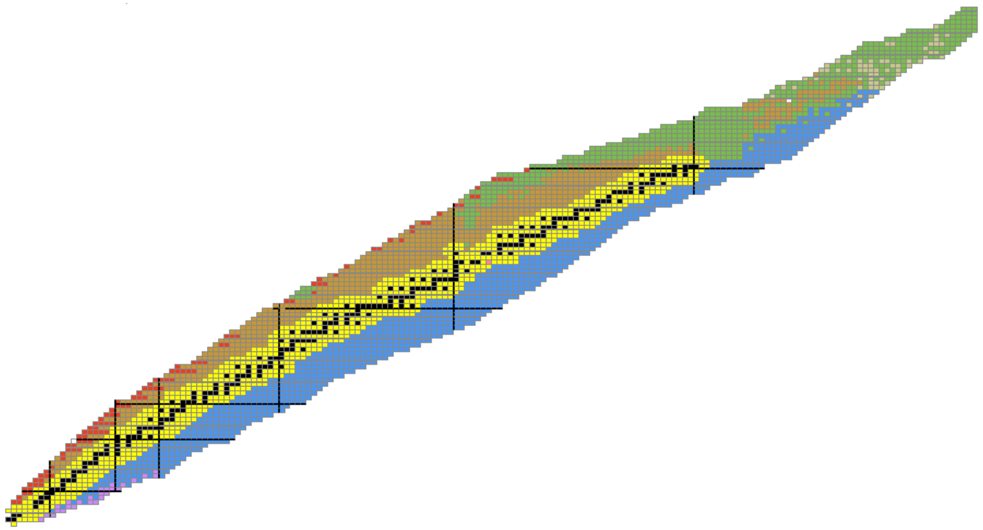
n = neutron
g = gamma
t = tritium
p = proton
d = deuterium
He = helium

Activation pathways

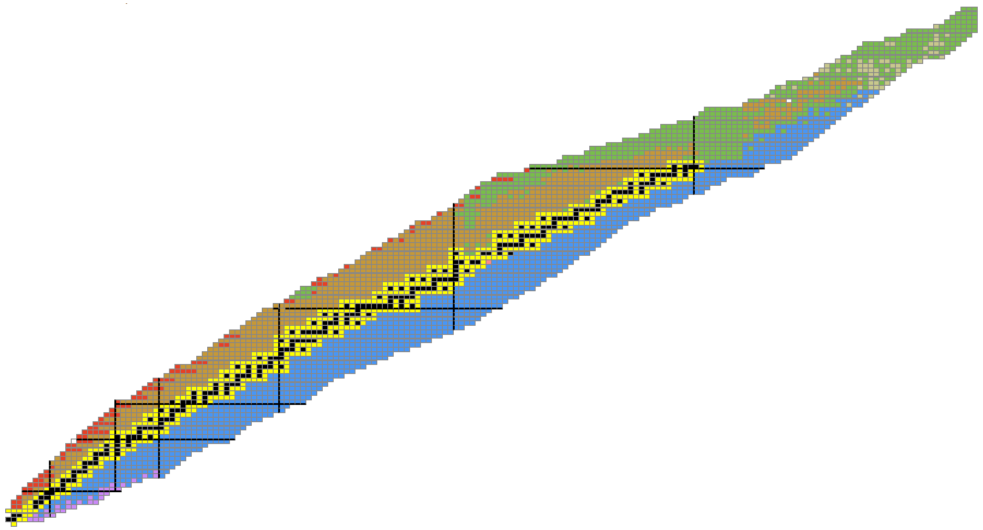


Activation products

- High energy neutron activation

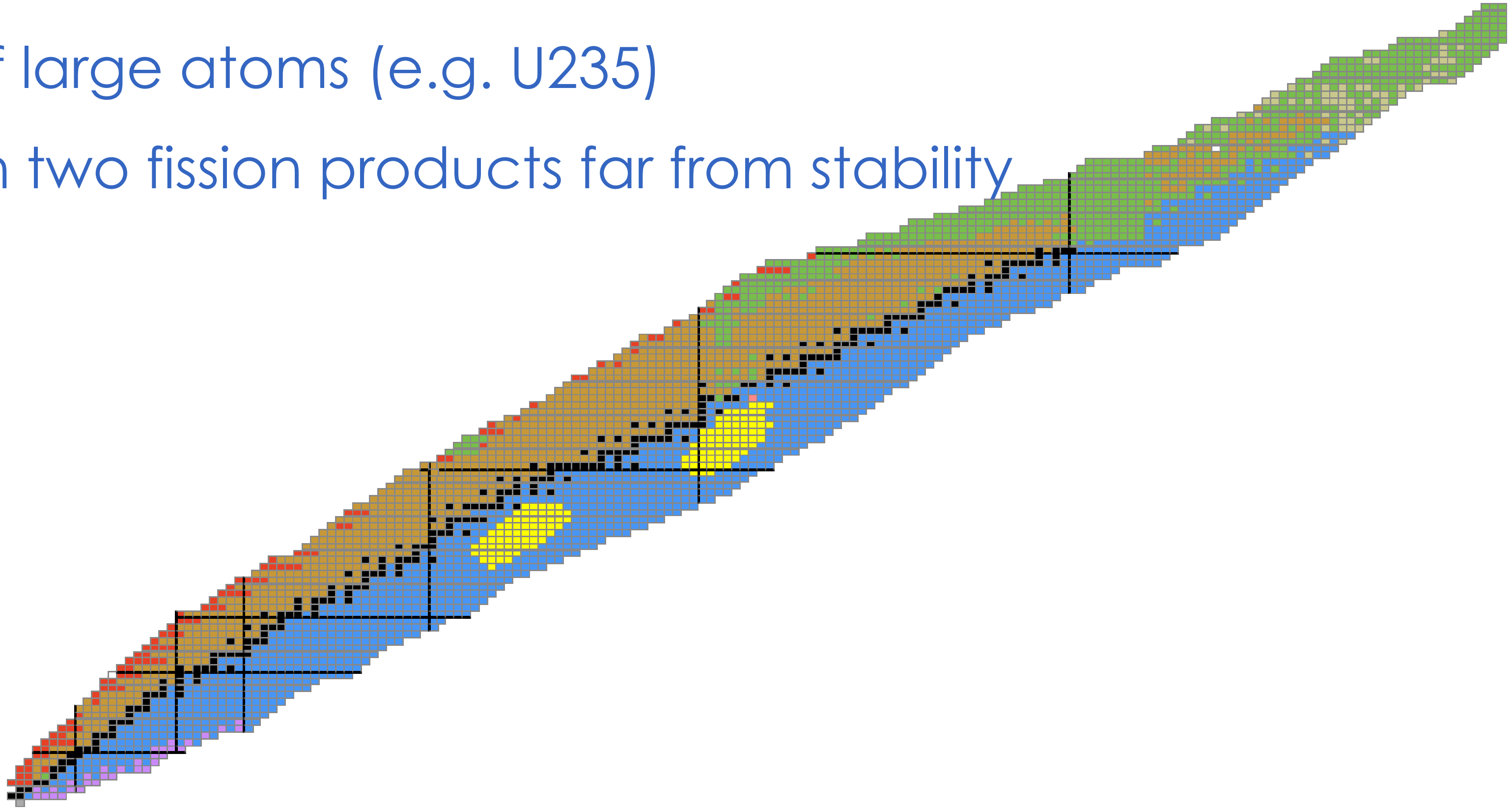


- Low energy neutron activation



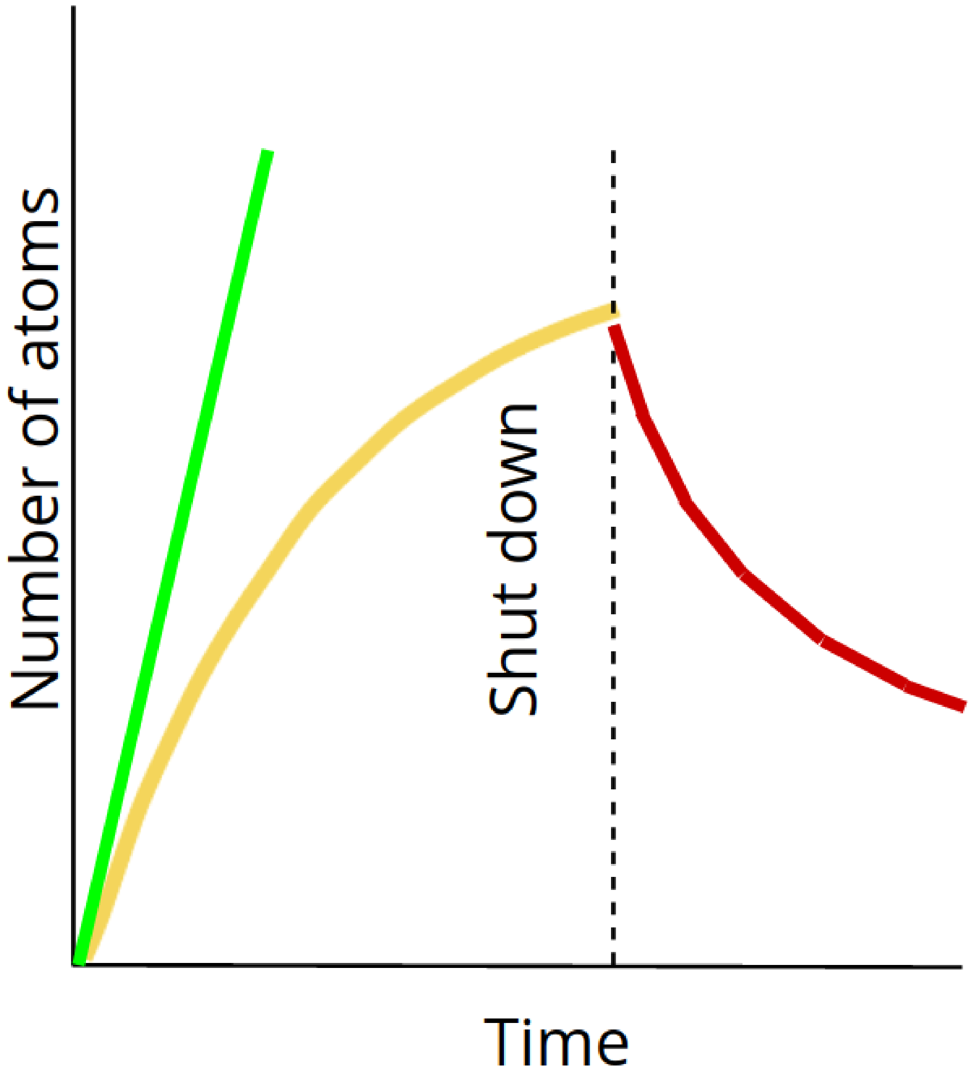
Activation products from fission

- Fission of large atoms (e.g. U235)
- Results in two fission products far from stability



Build up and saturation

- New isotopes created during irradiation
- Radioactive isotopes decay and will eventually reach a point where decay rate is equal to activation rate.
- Decay is more noticeable once the plasma is shutdown.
- The activity is related to the irradiation time and the nuclide half life.



Now complete task 15 in the half day workshop

Summary task

Replace the "`your code here`" sections to make the best reactor.

Chose the best options from a selection of materials.

Refine the design to:

- maximize Tritium Breeding Ratio (TBR)
- maximize blanket heating
- minimize damage to the conductor

Now complete task 16 in the half day workshop