Mads Bertelsen, ESS DMSC

McStas Union components

2019 CSNS McStas School

Session overview

- Introduction of concentric keyword for sample environment simulation
- Introduction to the Union components for advanced sample environment simulation
- Exercise where you build sample environment
- Talk on understanding of Union results and showcase of possibilities
- Exercise on adding loggers to your sample environment
- Last talk with showcase on full instrument simulation

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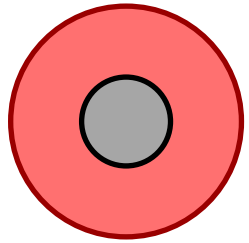
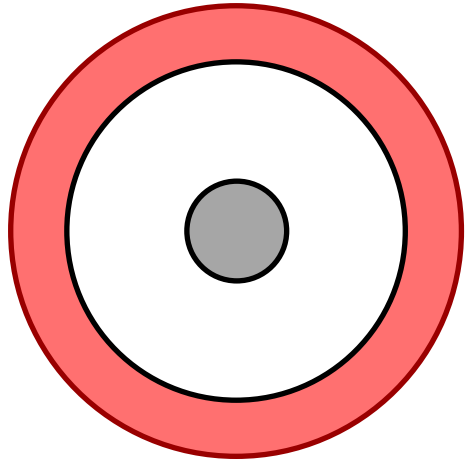
Multiple scattering

- Multiple scattering can happen in all systems
- Adding several materials complicates matters
- In spatially large systems time of flight is affected by multiple scattering





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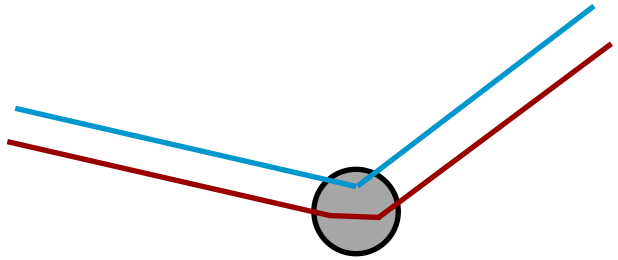
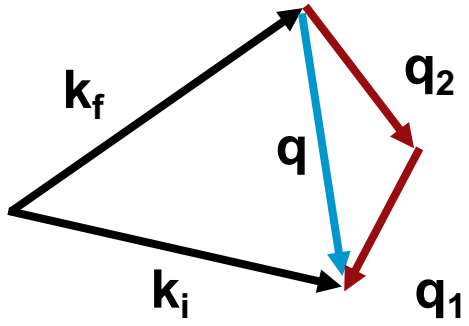
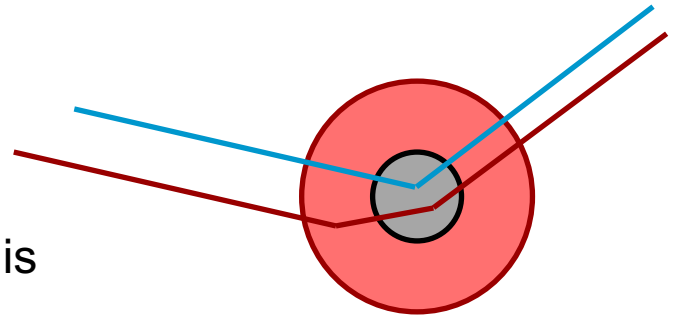
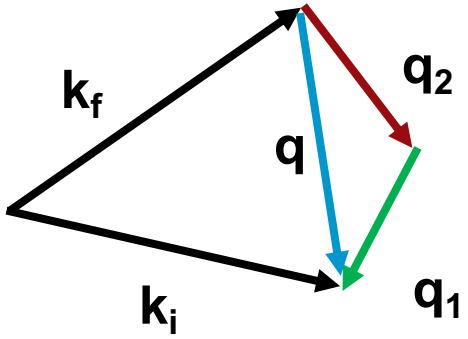
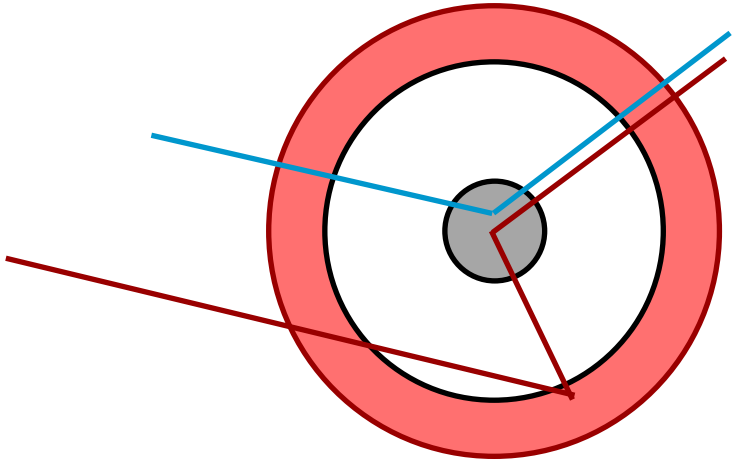
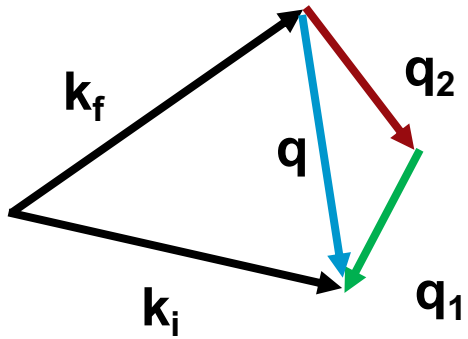






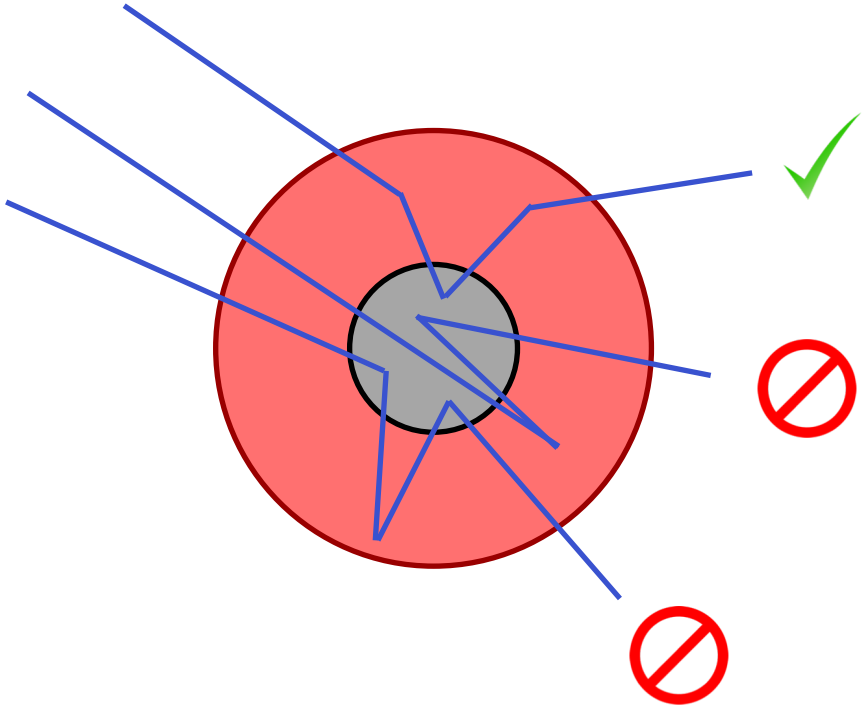


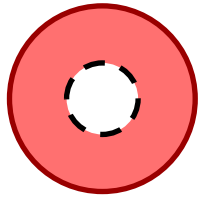




Concentric keyword in McStas

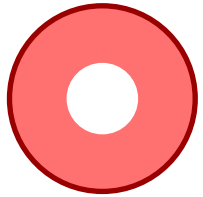
- Simple sample container
- Available in PowderN and Isotropic_sqw





COMPONENT a = Container_1(**concentric=1**, …)
AT (0,0,0) RELATIVE sample_position

COMPONENT b = Sample(…)
AT (0,0,0) RELATIVE sample_positon



COMPONENT c = Container_2(**concentric=0**,…)
AT (0,0,0) RELATIVE Container_1

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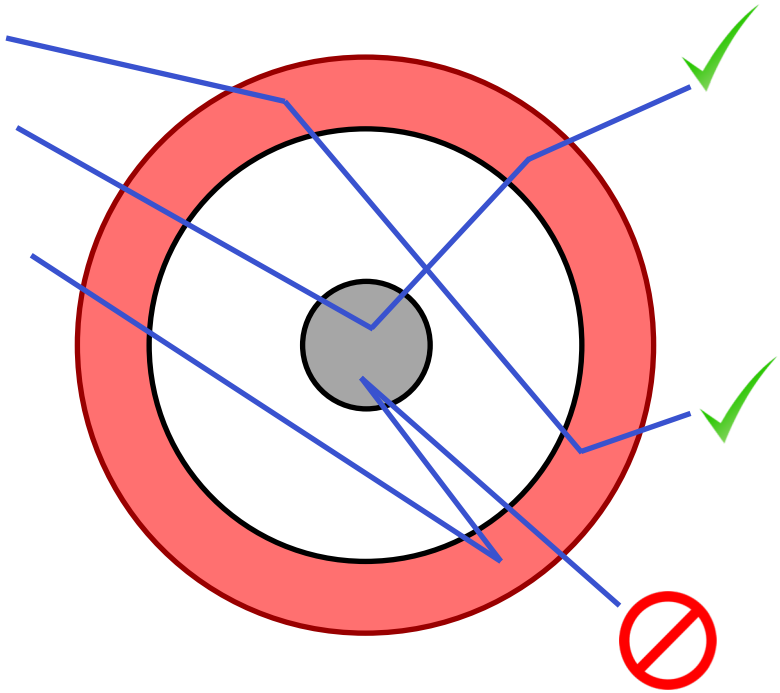
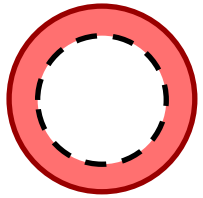
Concentric keyword in McStas

- Sample environment
- Available in PowderN and Isotropic_sqw





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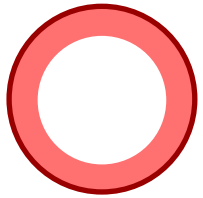
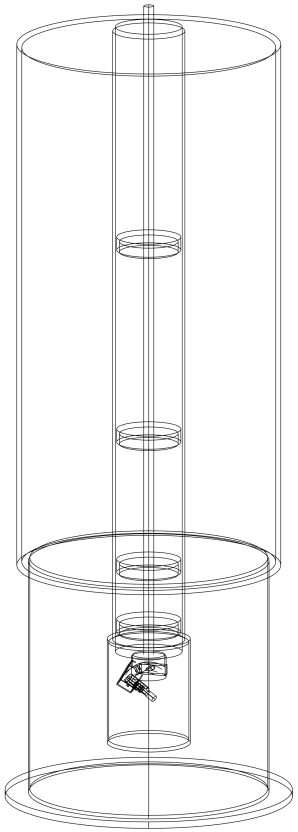


COMPONENT c = Container_2(**concentric=0**,…)
AT (0,0,0) RELATIVE Container_1

Union introduction

- Modular geometry and physics
- Aims to simulate complex systems
- All trajectories allowed



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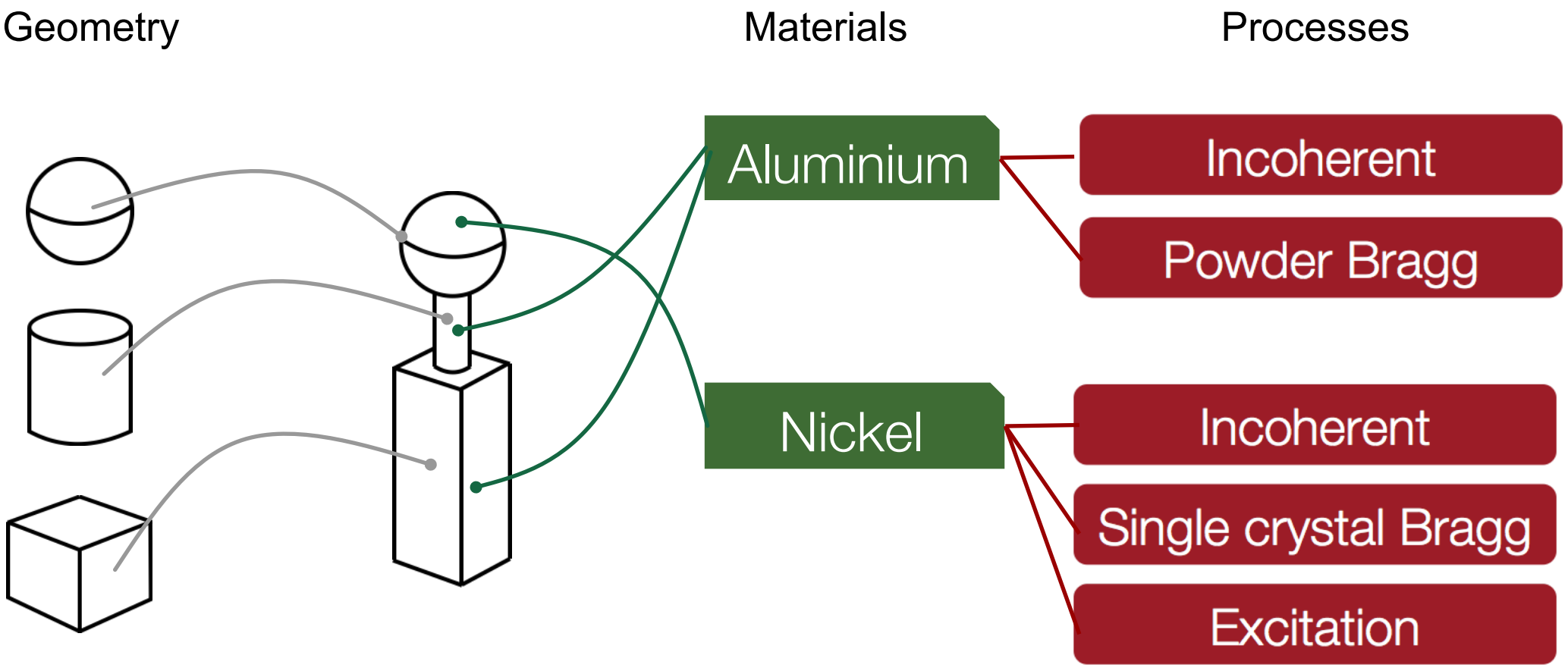
Union overview



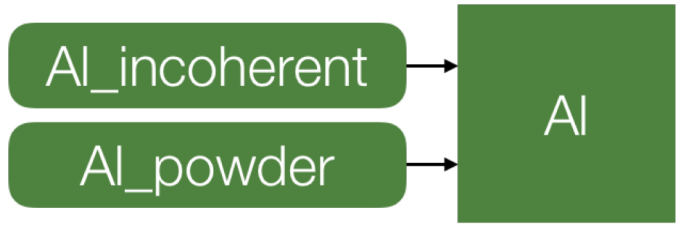
Union process syntax

```
COMPONENT Al_incoherent = Incoherent_process(
  sigma=4*0.0082,packing_factor=1,
  unit_cell_volume=66.4)
AT (0,0,0) ABSOLUTE

COMPONENT Al_powder = Powder_process(
  reflections="Al.laz")
AT (0,0,0) ABSOLUTE

COMPONENT Al = Union_make_material(
  my_absorption=100*4*0.231/66.4,
  process_string="Al_incoherent,Al_powder")
AT (0,0,0) ABSOLUTE
```

sigma in [barns]
unit_cell_volume in [Å^3]



my [1/m] = cross section per unit cell / unit cell volume

Union concepts: Priority

- Priority to handle overlapping geometries
- The highest priority is simulated in regions where more are overlapping

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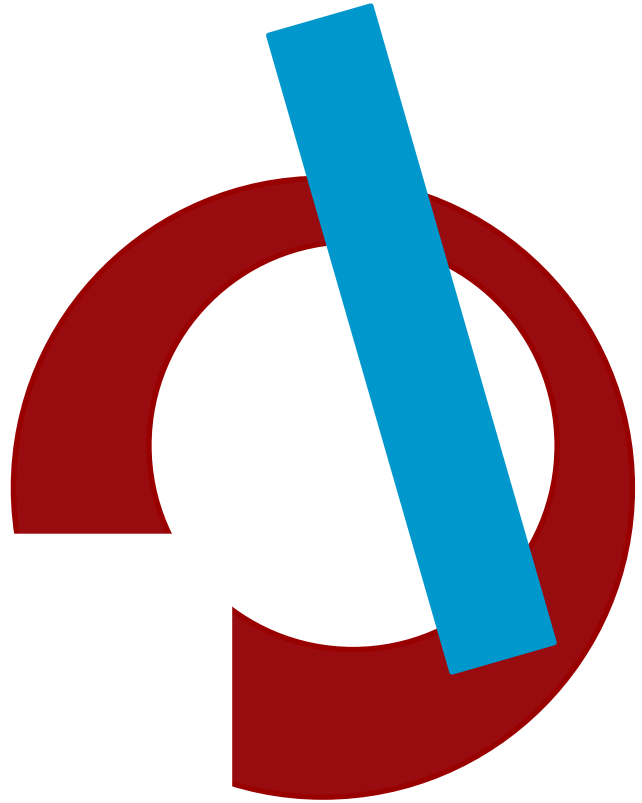

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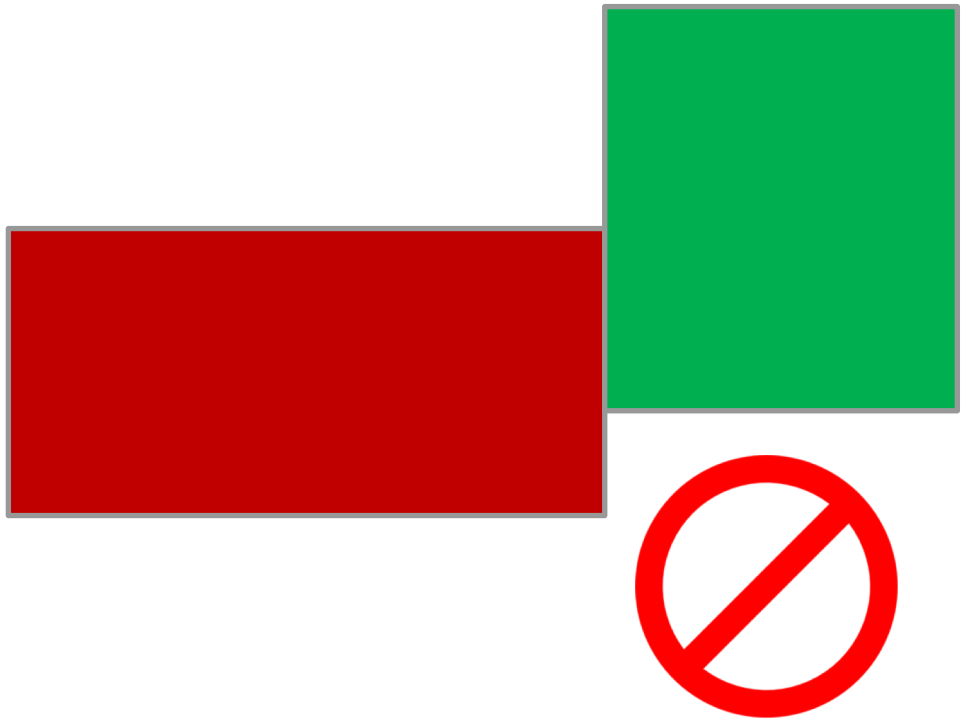
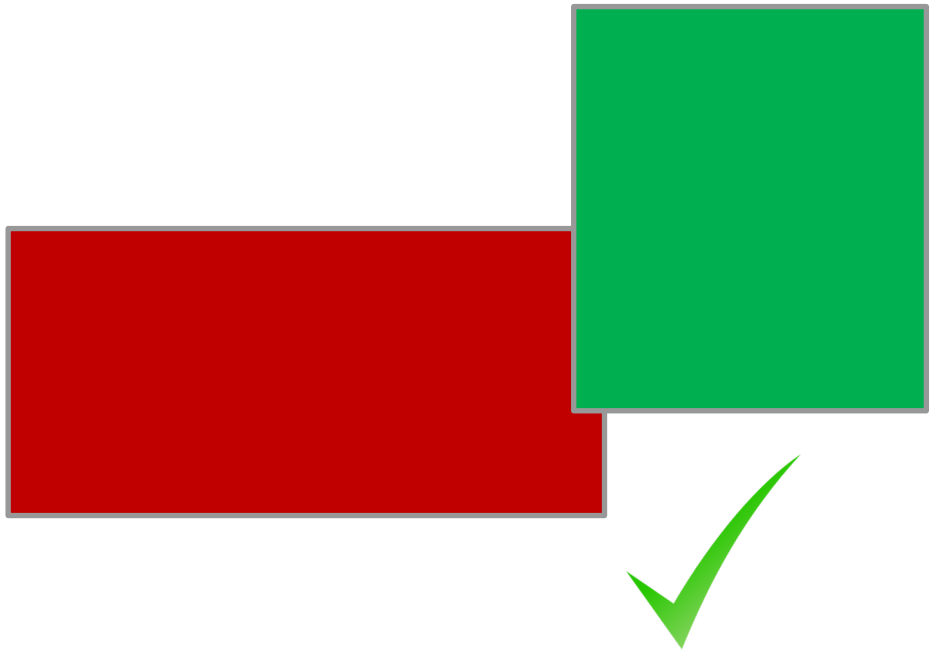
- Problem: Sides can not be tangennts



Union concepts: Priority

- Priority to handle overlapping geometries
- The highest priority is simulated in regions where more are overlapping
- Problem: Sides can not be tangennts
- Solution: A few micrometers is plenty



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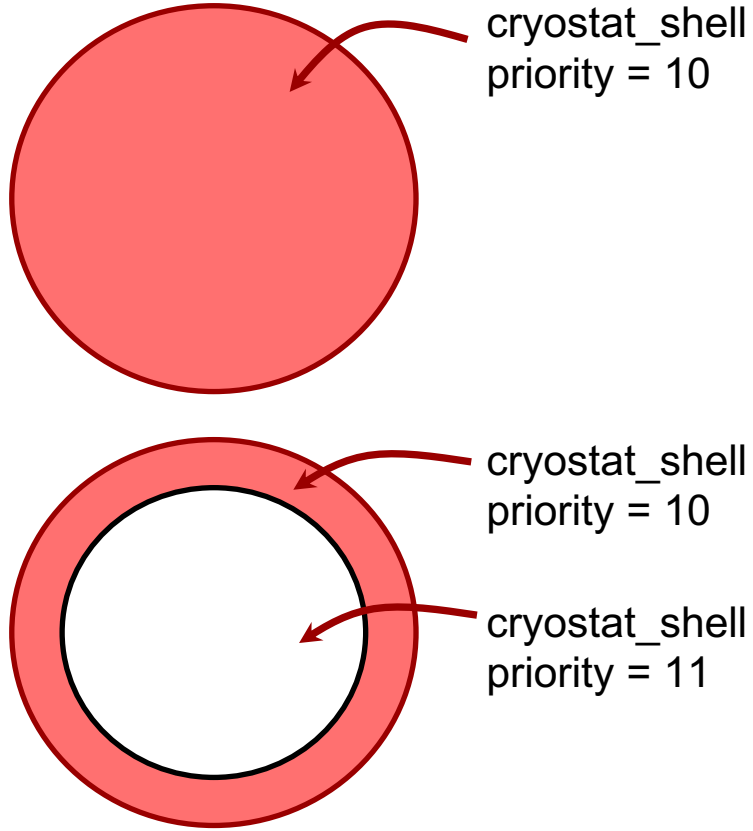
Union geometry syntax

```
COMPONENT cryostat_shell = Union_cylinder(
  radius=0.15,height=0.4,
  priority=10,material_string="Al")
AT (0,0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target

COMPONENT cryostat_vacuum = Union_cylinder(
  radius=0.147,height=0.39,
  priority=11,material_string="Vacuum")
AT (0,0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target
```



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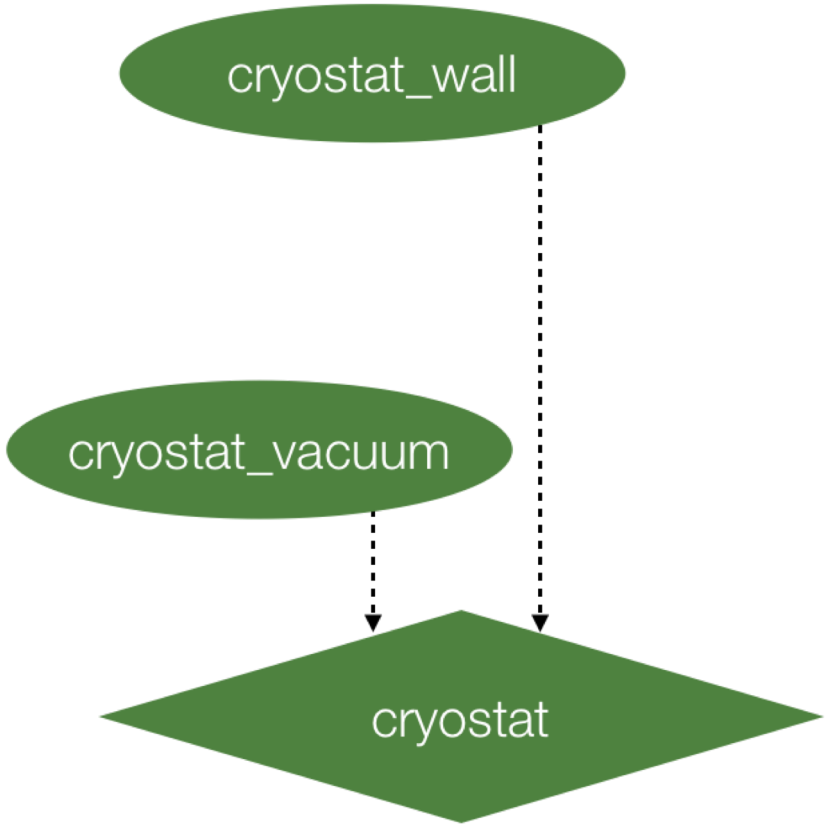
COMPONENT cryostat = Union_master()
AT (0,0,0) RELATIVE target
ROTATED (0,0,0) RELATIVE target
```



Union components working together

Processes

Al_incoherent

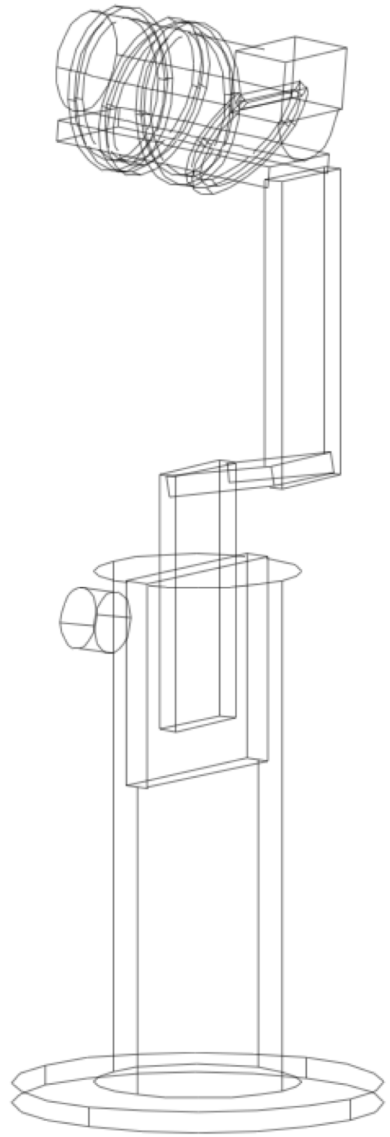
Al_powder

Cu_incoherent

Cu_powder

What can you make?

- Easy assembly of complex geometries
- Rich materials for each geometry



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Exercise

- open_exercise.instr contains material definitions, source, Union sample and monitors
- Expand to include some sample environment!
- Exercise text on github with further help

- This exercise will continue after the next lecture

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