Bridging Monte-Carlo worlds: A new framework for accelerator simulations

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École Polytechnique Fédérale de Lausanne (EPFL)

Organisation européenne pour la recherche nucléaire (CERN)

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Director: Prof. Mike Seidel

Co-Director: Dr. Vasilis Vlachoudis

Outlines

Introduction

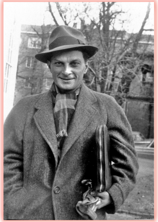
Introduction

A Bit of History

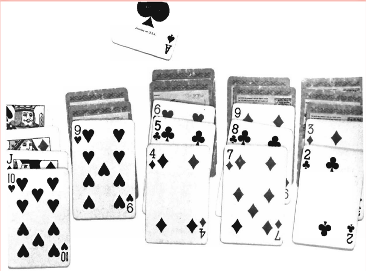
A Bit of History

Project Manhattan - 1940s

"What is the probability of winning a solitaire game?"



S. Ulam



A Bit of History

Project Manhattan - 1940s

"A statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences"

S. Ulam

N. Metropolis

J. Von Neumann

A Bit of History

Monte Carlo Particle Transport Codes

Introduction

SY-STI-BMI

SY-STI-BMI Section

SY-STI- **Accelerator Systems - Source Target Interactions**

- **Among others:** . . . The group is responsible for the design, construction, operation of all interception devices across the CERN complex.

-BMI **Beam-Machine Interactions**

- It is responsible of the development, dissemination and support of the **FLUKA** code
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Beam Loss Monitoring (BLM) system

- Series of ionization chambers utilized for accelerator machine protection
- In the LHC, there are approximately 3600 of these chambers at critical loss locations
- The losses measured by the BLMs are integrated and compared to defined thresholds. It defines if the beam should be abort or not.

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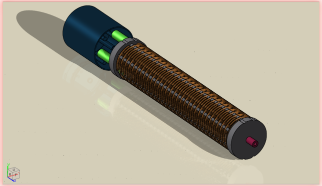

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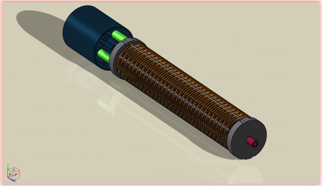

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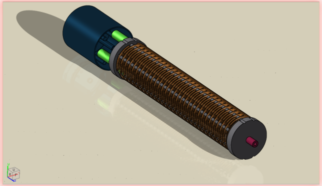

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- In a particle accelerator, **beam losses affect** in several ways the collider **equipment and operation**
- **Studies** are crucial to assess the losses effects and develop **mitigation strategies**
- **BLM benchmarking** is one of the **studies performed** by BMI. (FLUKA simulations)
- **BLM calculation:** Estimate results that would be obtained in a real run [a]. Results used to compare with experimental data, or to predict the radiation layout in a future run (e.g. HL-LHC, FCC)

[a] dose per unit of time in BLMs active region

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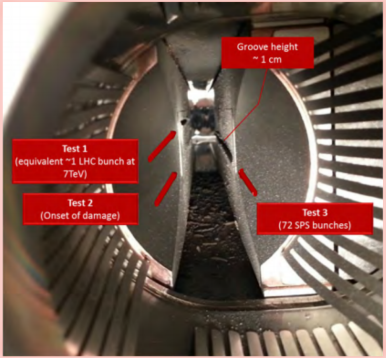

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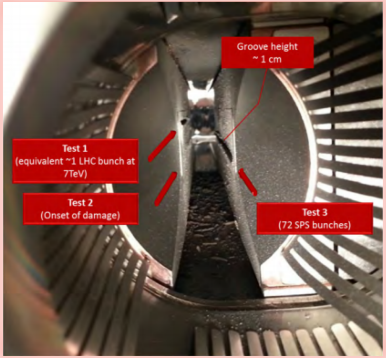

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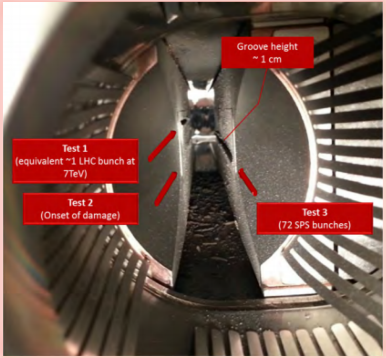

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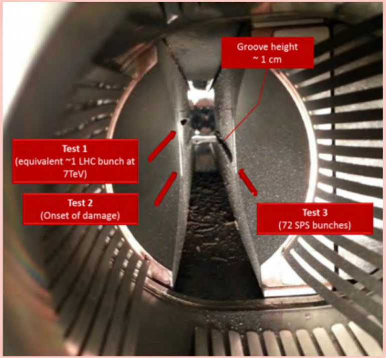

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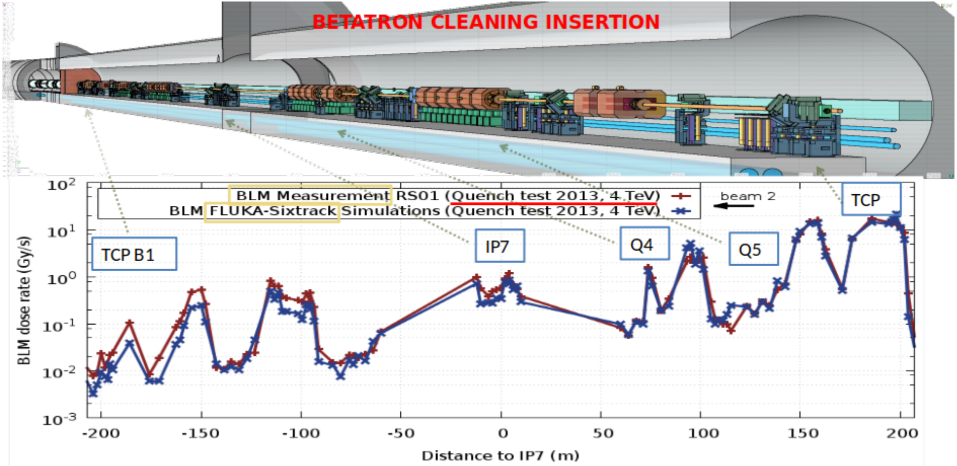

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Previous Results

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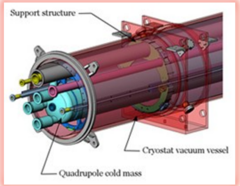
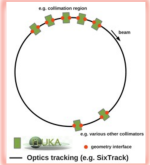
+15 years invested in BMI section in developing all the necessary infrastructure for the CERN studies (Always based on FLUKA)

Fluka Element DataBase	Line Builder	FLUKA-SixTrack coupling
		

These features help in creating and simulating assembly of actual beam lines, in an easy, flexible and consistent way

Motivation

- **Develop a new framework for particle transport simulations:**
  - Having the possibility to run both codes (FLUKA and G4) in an "easy way"
  - Allowing the employ of developed tools (Line Builder, FEDB, SixTrack)
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Monte Carlo limitations

- There are many sources of systematic uncertainties in Monte Carlo simulations
  - Incomplete knowledge:
    - Material composition not always well known
    - Presence of additional material, not well defined
  - Simplification:
    - Geometries that cannot be reproduced exactly
    - Air contains humidity and pollutants, has a density variable with pressure
  - Code mistakes("bugs")
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Monte Carlo limitations

- **Adopted physics model**: Different codes are based on different physics models. Some models are better than others. Some models are better in a certain energy range. Model quality is best shown by benchmarks at the microscopic level.
- **Transport algorithm**: Due to imperfect algorithms, e.g., energy deposited in the middle of a step, inaccurate path length correction for multiple scattering, missing correction for cross section and dE/dx change over a step, etc. Algorithm quality is best shown by benchmarks at the macroscopic level.
- **Cross-section data uncertainty**: An error of 10% in the absorption cross section can lead to an error of a factor 2.8 in the effectiveness of a thick shielding wall (10 attenuation lengths).

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The main method to evaluate the uncertainties is against measured data, but in the case it is not available, a second code with different physics model, transport algorithm and/or cross-section data uncertainty is the best approach in order to quantify them

PhD Structure

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- **1st Part - Development**:
  Create a new simulation framework, called preliminarily "Moira", to bridge FLUKA and Geant4. The goal is to provide to the user a FLUKA experience using the Geant4 toolkit.
- **2nd Part - BLM Benchmarking**:
  Utilize the developed tool for the simulation of BLM benchmarking calculations.

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  /primary/select/ gps
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- Textgeom: Geometry definition based on a plain text description. E.g.:
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FLUKA

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Position and rotation of 3D finite macro objects, e.g. box, sphere, cone.. twisted solid, are defined *wrt* the local coordinate system of another volume. Due to this, these volumes are denominated daughter and mother volume respectively.

FLUKA (Combinatorial)

This description is based on the definition of the regions in the simulation geometry through boolean operations (intersection, subtraction and union) of basic second order objects and/or infinite planes and cylinders.

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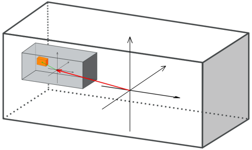

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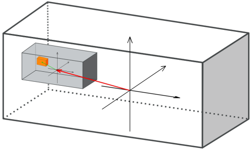

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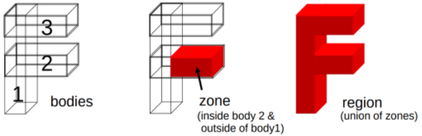

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Physics, Scoring, Primary sources, Biasing, Fields, postprocessing, etc

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Various, but mainly on visualization

FLUKA

Flair

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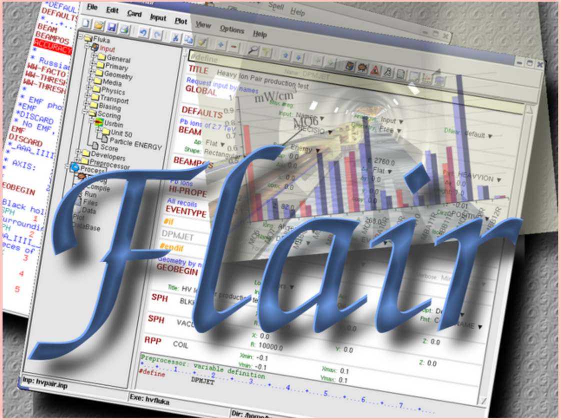

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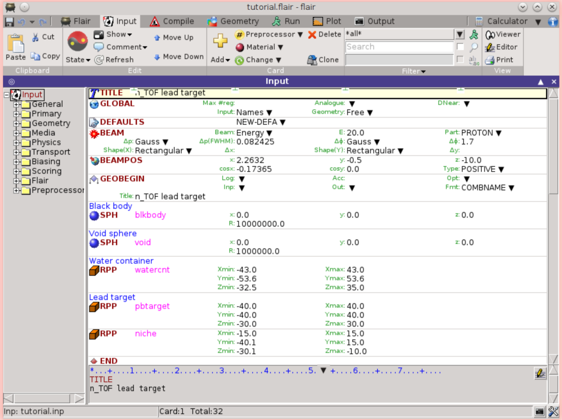

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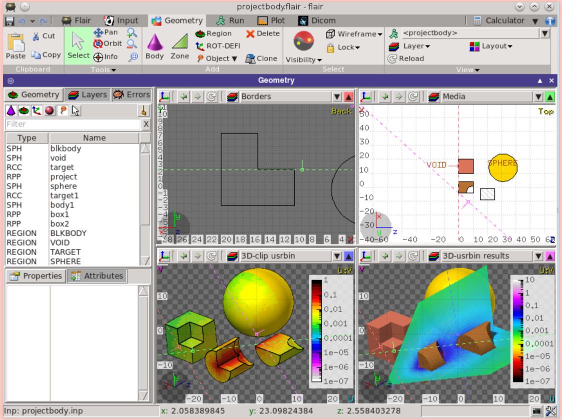

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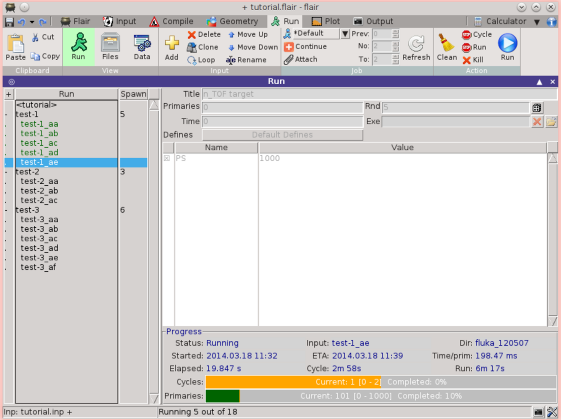

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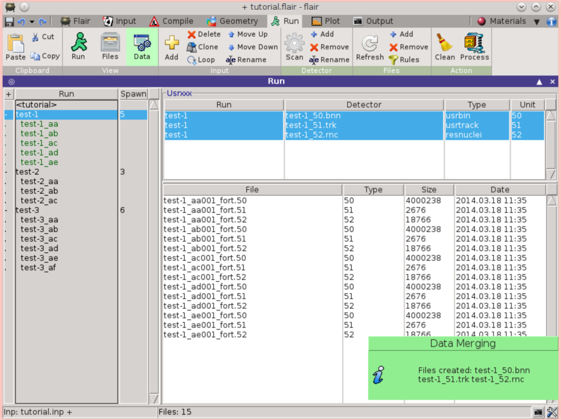

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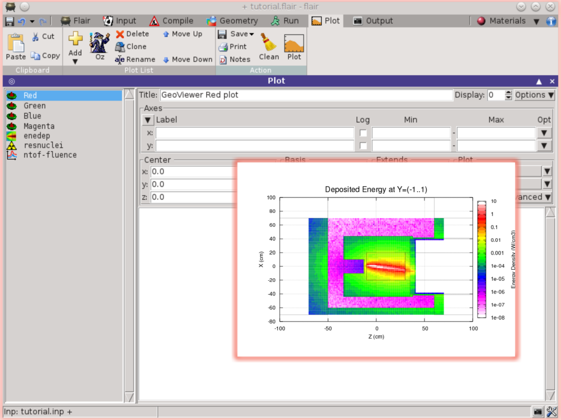

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Development: Moira - The New Framework

- Hybrid G4 "application" that provides a FLUKA experience using the Geant4 toolkit:
  - **Geometry description** equivalent to FLUKA (Combinatorial Geometry)
  - Two ASCII files as **input files**:
    - For Geometry: Textgeom (+ extension)
    - For the rest of components[1]: UI commands via macro file (built in + own commands)
  - Fully integrated with **Flair**

- For this thesis: Application that allows to perform BLM benchmarking studies
- Beyond: Application equivalent to FLUKA in Geant4
- Even Beyond: Expand it in the future with the best from each code

[1] Physics, Scoring, Primary sources, Biasing, etc

PhD Structure

Development: Moira - The New Framework

- Hybrid G4 "application" that provides a FLUKA experience using the Geant4 toolkit:
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PhD Structure

BLM Benchmarking

PhD Structure

BLM benchmarking

- Utilize Moira to simulate BLM benchmarking calculations for many points and sections of the LHC
- Make quantitative assessments of the differences and systematic uncertainties of both codes for these studies
- BMI executes simulations of sections highly radiated, e.g. IR6 and IR7. Initially the simulations performed will be based on these geometries, where numerous FLUKA simulations have a good agreement with experimental data

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State of the Art

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Moira Status

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Moira Status: +Geometry

- **Analog FLUKA geometry using Textgeom & extending it:**
  BODIES ⇔ FLUKA BODIES — CELL ⇔ FLUKA REGION
  G4Zone ⇔ FLUKA ZONE — LATTICE ⇔ FLUKA LATTICE
- A Moira External Navigator performs the tracking in G4Zone (Analog to FLUKA)
- .moira file as an input

```
// Default identity rotation matrix
:ROTM __IDENT__ 0 0 0

//
// Cylindrical target
:BODY target RCC 0.0 0.0 0.0 0.0 0.0 100.0 50.0
// Void sphere
:VOLU void ORB 1000.0 G4_Galactic
// Void around
:CELL VOID void G4_Galactic +void -target
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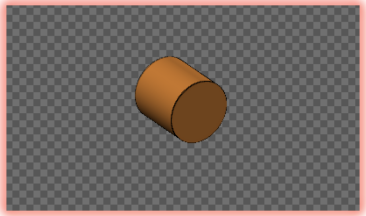

State of the art

Moira Status: +Everything -Geometry

Macro file (ASCII file contains UI commands)

- **Physics:**
  - Physics lists: Set of many physics constructors
  - Physics constructors: Initializes particles and their processes
  - Enable/disable processes for each particle type
- **Scoring:**
  - Mesh scoring, Track length and boundary crossing
  - Particle track visualization
- **Biasing:**
  - Importance, Weight Window
  - Leading particle (electromagnetic, hadronic)
  - Interaction Biasing
- **Fields:**
  - Magnetic: Multipoles, 2D/3D interpolated fields, userdefined

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State of the art

Moira Status: Flair

- **Operational**:
  - Input Editor
  - Inspecting the files and progress of a run
  - Merging all output data files to combine the statistics
  - Some basic plotting (geometry, mesh, 1D and 2D distributions)
  - **Partial conversion of a FLUKA input file to Moira**

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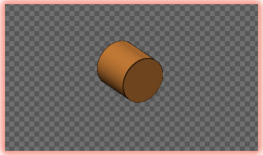
State of the art

Moira Status: Flair

```
/moira/title
#
# Select physics list
/physics_lists/select FTFP_BERT_HP EMY
#
# Cylindrical scoring
/score/create/cylinderMesh cylindrical
/score/mesh/cylinderSize 5 10 cm
/score/mesh/nBin 50 10 8
/score/mesh/translate/xyz 0 0 5 cm
/score/quantity/energyDeposit energy MeV
/score/quantity/cellFlux neutron percm2
/score/filter/particle neutron neutron
#
# Tally scoring
/tally/file fluence.hist
/tally/track/add neutron_track
/tally/track/volume TARGET
/tally/track/particle neutron
/tally/track/histogram log 300 1e-9 1000 MeV
/tally/track/norm 1.0 cm3
/tally/boundary/add neutron_boundary fluence
/tally/boundary/volume TARGET VOID
/tally/boundary/particle neutron
/tally/boundary/histogram log 300 1e-9 1000 MeV
/tally/boundary/norm 1. cm2
#
# Initialize run
/run/initialize
#
# Particle generator selection
/primary/select gps
# Define the beam characteristics
/gps/particle neutron
/gps/energy 100 MeV
# Define the beam position
/gps/pos/centre 0.0 0.0 0.0 cm
/gps/direction 0.0 0.0 1.0
/tracking/verbose 1
/score/close
/run/beamOn 1
/score/dumpAllQuantitiesToFile cylindrical cylindrical.bnn
```

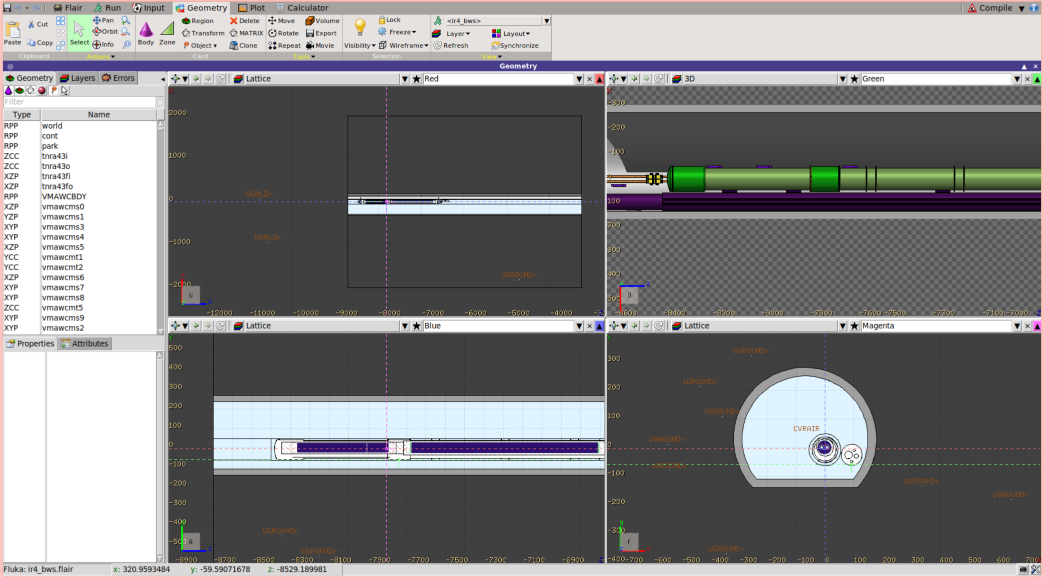


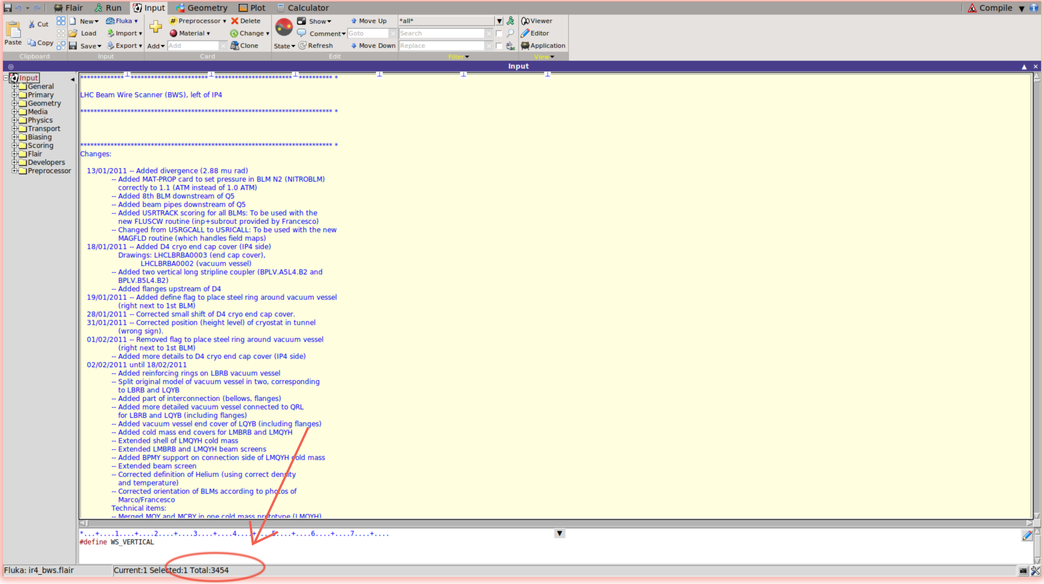
```
// Default identity rotation matrix
:ROTM __IDENT__ 0 0 0

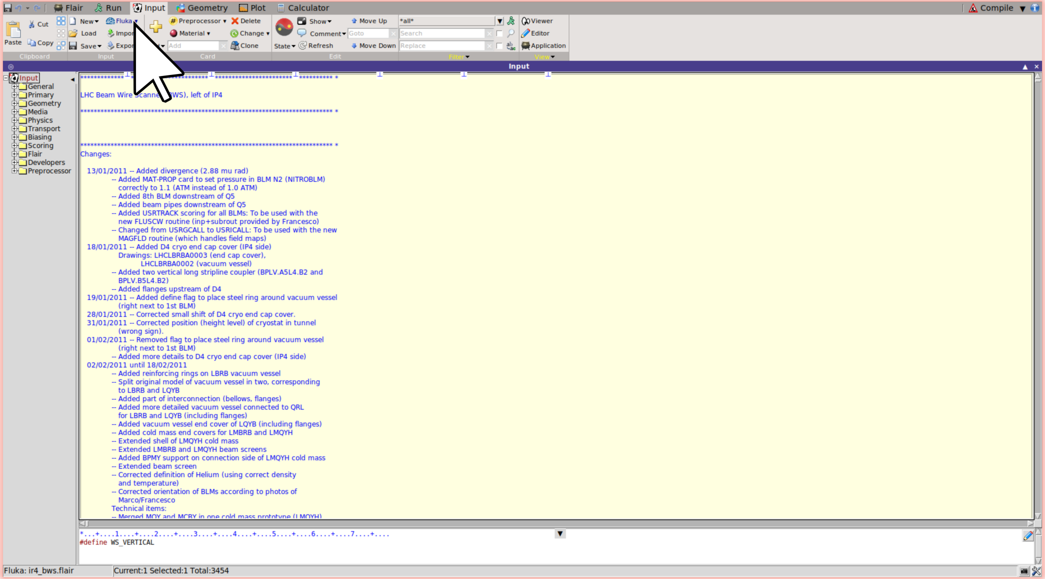
//
// Cylindrical target
:BODY target RCC 0.0 0.0 0.0 0.0 0.0 100.0 50.0
// Void sphere
:VOLU void ORB 1000.0 G4_Galactic
// Void around
:CELL VOID void G4_Galactic +void -target
// Target volume
:CELL TARGET void G4_Cu +target
```

```
TITLE

* Set the defaults for precision simulations
DEFAULTS                                                              PRECISIO
* Define the beam characteristics
BEAM           -0.1        0.        0.        0.        0.        NEUTRON
* Define the beam position
BEAMPOS           0.        0.        0.        0.        0.
GEOBEGIN                                                              COMBNAME
    0    0
* Black body
SPH blkbody    0.0 0.0 0.0 100000.0
* Void sphere
SPH void       0.0 0.0 0.0 10000.0
* Cylindrical target
RCC target     0.0 0.0 0.0 0.0 0.0 10.0 5.0
END
* Black hole
BLKBODY        5 +blkbody -void
* Void around
VOID           5 +void -target
* Target
TARGET         5 +target
END
GEOEND
USRBIN           11.   NEUTRON      -21.       50.                 10.cylinder
USRBIN            0.                  0.       50.        8.       10. &
USRTRACK               NEUTRON      -22.    TARGET                    track
USRTRACK       1000.      1E-9                                        &
USRBDX          109.   NEUTRON      -23.    TARGET      VOID       boundary
USRBDX         1000.      1E-9      300.                              &
* ..+....1....+....2....+....3....+....4....+....5....+....6....+....7..
ASSIGNMA     BLCKHOLE   BLKBODY
ASSIGNMA       VACUUM      VOID
ASSIGNMA       COPPER    TARGET
* Set the random number seed
RANDOMIZ         1.0
* Set the number of primary histories to be simulated in the run
START             1.
STOP
```




Flair
Run
Input
Geometry
Plot
Calculator
Compile
Input
General
Primary
Geometry
Media
Physics
Transport
Biasing
Scoring
Flair
Developers
Preprocessor
LHC Beam Wire Scanner (BWS), left of IP4
Changes:
13/01/2011 -- Added divergence (2.88 mu rad)
-- Added MAT-PROP card to set pressure in BLM N2 (NITROBLM) correctly to 1.1 (ATM instead of 1.0 ATM)
-- Added 8th BLM downstream of Q5
-- Added beam pipes downstream of Q5
-- Added USRTRACK scoring for all BLMs: To be used with the new FLUSCW routine (inp+subrout provided by Francesco)
-- Changed from USRGCALL to USRICALL: To be used with the new MAGFLD routine (which handles field maps)
18/01/2011 -- Added D4 cryo end cap cover (IP4 side)
Drawings: LHCLBRBA0003 (end cap cover), LHCLBRBA0002 (vacuum vessel)
-- Added two vertical long stripline coupler (BPLV.A5L4.B2 and BPLV.B5L4.B2)
-- Added flanges upstream of D4
19/01/2011 -- Added define flag to place steel ring around vacuum vessel (right next to 1st BLM)
28/01/2011 -- Corrected small shift of D4 cryo end cap cover.
31/01/2011 -- Corrected position (height level) of cryostat in tunnel (wrong sign).
01/02/2011 -- Removed flag to place steel ring around vacuum vessel (right next to 1st BLM)
-- Added more details to D4 cryo end cap cover (IP4 side)
02/02/2011 until 18/02/2011
-- Added reinforcing rings on LBRB vacuum vessel
-- Split original model of vacuum vessel in two, corresponding to LBRB and LQYB
-- Added part of interconnection (bellows, flanges)
-- Added more detailed vacuum vessel connected to QRL for LBRB and LQYB (including flanges)
-- Added vacuum vessel end cover of LQYB (including flanges)
-- Added cold mass end covers for LMBRB and LMQYH
-- Extended shell of LMQYH cold mass
-- Extended LMBRB and LMQYH beam screens
-- Added BPMY support on connection side of LMQYH cold mass
-- Extended beam screen
-- Corrected definition of Helium (using correct density and temperature)
-- Corrected orientation of BLMs according to photos of Marco/Francesco
Technical items:
#define WS_VERTICAL
Fluka: ir4_bws.flair
Current:1 Selected:1 Total:3454


Flair
Run
Input
Geometry
Plot
Calculator
Compile
Paste
Cut
Copy
Clipboard
New
Load
Save
Fluka
Preprocessor
Delete
Material
Change
Clone
Card
Show
Comment
State
Refresh
Move Up
Move Down
Edit
all
Search
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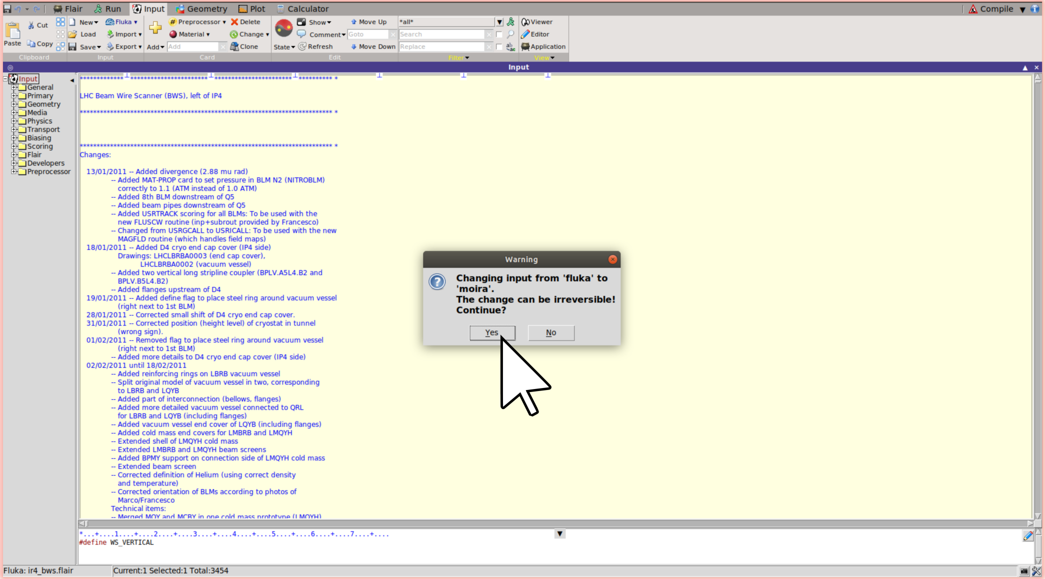
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Marco/Francesco
Technical items:
Warning
Changing input from 'fluka' to 'moira'.
The change can be irreversible!
Continue?
Yes
No
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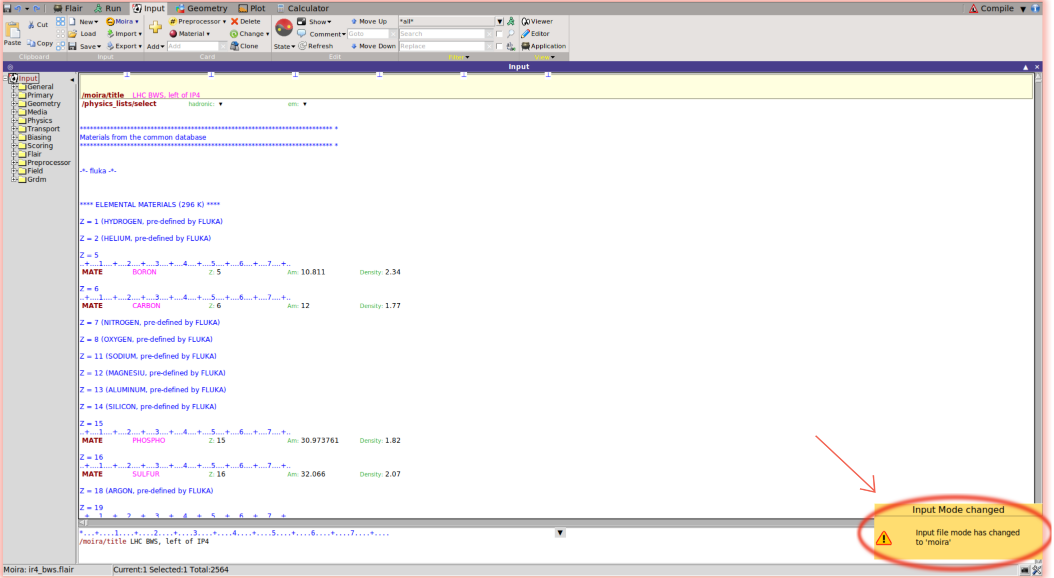
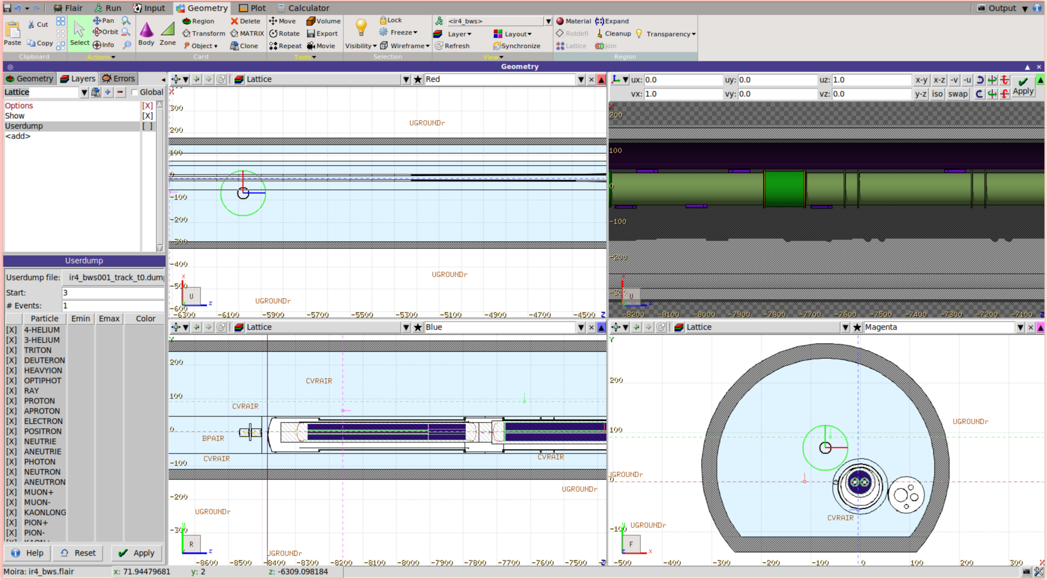
Fluka: ir4_bws.flair
Current:1 Selected:1 Total:3454

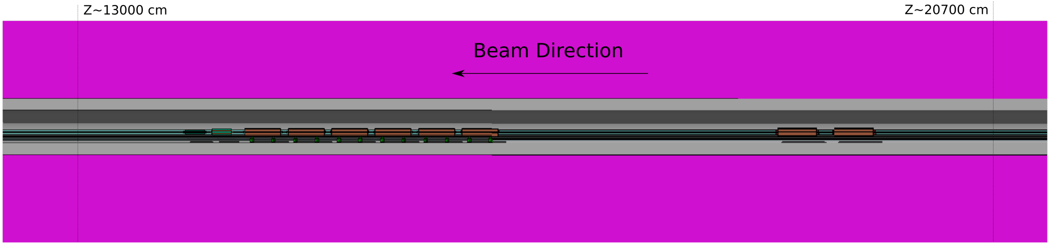

Flair
Run
Input
Geometry
Plot
Calculator
Compile
Input
/moira/title LHC BWS, left of IP4
/physics_lists/select
Materials from the common database
-*- fluka -*-
**** ELEMENTAL MATERIALS (296 K) ****
Z = 1 (HYDROGEN, pre-defined by FLUKA)
Z = 2 (HELIUM, pre-defined by FLUKA)
Z = 5
MATE BORON Z: 5 Am: 10.811 Density: 2.34
Z = 6
MATE CARBON Z: 6 Am: 12 Density: 1.77
Z = 7 (NITROGEN, pre-defined by FLUKA)
Z = 8 (OXYGEN, pre-defined by FLUKA)
Z = 11 (SODIUM, pre-defined by FLUKA)
Z = 12 (MAGNESIU, pre-defined by FLUKA)
Z = 13 (ALUMINUM, pre-defined by FLUKA)
Z = 14 (SILICON, pre-defined by FLUKA)
Z = 15
MATE PHOSPHO Z: 15 Am: 30.973761 Density: 1.82
Z = 16
MATE SULFUR Z: 16 Am: 32.066 Density: 2.07
Z = 18 (ARGON, pre-defined by FLUKA)
Z = 19
/moira/title LHC BWS, left of IP4
Input Mode changed
Input file mode has changed to 'moira'
Moira: ir4_bws.flair
Current:1 Selected:1 Total:2564


Flair
Run
Input
Geometry
Plot
Calculator
Output
Lattice
Options [X]
Show [X]
Userdump [ ]
<add>
Userdump
Userdump file: ir4_bws001_track_t0.dum
Start: 3
Events: 1
Particle
Emin
Emax
Color
4-HELIUM
3-HELIUM
TRITON
DEUTERON
HEAVYION
OPTIPHOT
RAY
PROTON
APROTON
ELECTRON
POSITRON
NEUTRIE
ANEUTRIE
PHOTON
NEUTRON
ANEUTRON
MUON+
MUON-
KAONLONG
PION+
PION-
Help
Reset
Apply
UGROUNDr
CVRAIR
BPAIR
Moira: ir4_bws.flair
x: 71.94479681
y: 2
z: -6309.098184

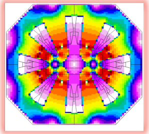
State of the Art
A Few Results

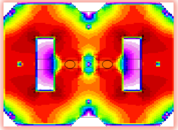
State of the Art

A Few Results: IR7 - Particles Transport Test



- Approx. 80 meters line
- 2 dipole magnets
- 6 quadrupole magnets
- 2 correctors magnets





State of the Art

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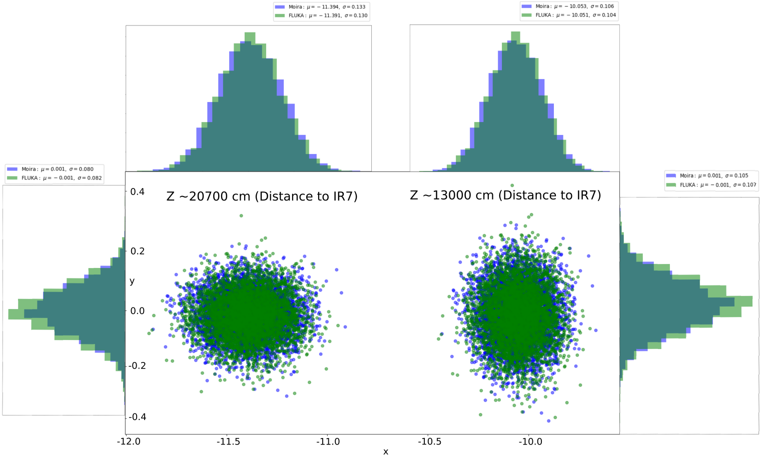
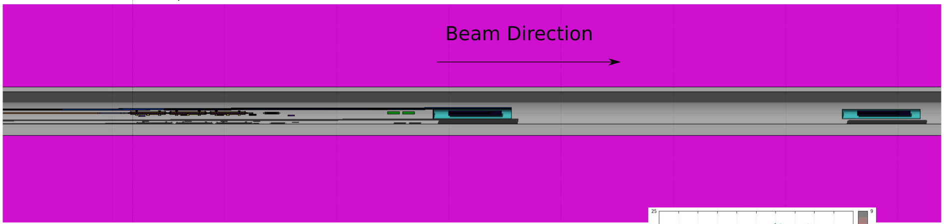


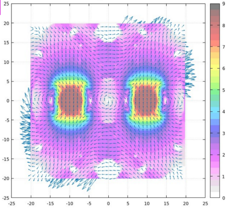
State of the Art

A Few Results: IR6 - Preliminary BLM Benchmark

Initial point



- Collimators: 3 TCDQ, 1 TCSP, 2 TCDQM.
- Magnets: MQY4 and MQY5
- 5 BLMs



State of the Art

A Few Results: IR6 - Preliminary BLM Benchmark

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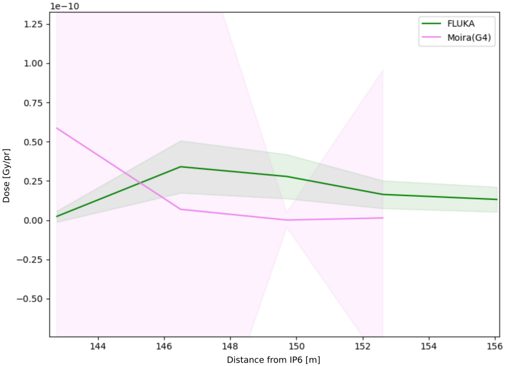

Future Plans

Future Plans

Development

Future Plans

Development

Develop a code capable of simulating BLM benchmarking studies.
Main implementations needed:

- A functional scoring to obtain fluence and energy deposited in a volumetric mesh
- Threshold and production cuts per particle
- A complete integration of the most important functionalities to Flair
- Extend the automatic converter FLUKA-Moira in Flair to contain all the components

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Future Plans
BLM Benchmarking

Future Plans

BLM benchmarking

Road Map:

- Tracking calculations to verify the field implementations
- Replication of simple cases (e.g. a simple cylindrical target with materials as for LHC collimators)
- Test in simple cases, with different beams, the scoring, physics models, biasing, thresholds, etc
- Advance with more and more complicated cases like sections of the tunnel
- Complete tunnel and realistic beam losses, obtaining BLM outputs
- Compare results with FLUKA and experimental measurements
- Improve convergence with the use of biasing techniques

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Thanks for your attention

Questions?

Backup Slides

Statistical Uncertainty

Statistical Uncertainty in MC simulations

The Central Limit Theorem provides the mathematical foundation of the Monte Carlo method:

Given any physical observable Z, that can be expressed as the result of a convolution of random processes, and the average value of Z can be obtained by sampling many values of Z according to the probability distribution of the random processes

$$Z = \frac{1}{n}\sum_{i=1}^{n} f(X_i)$$

Z is a random variable following a Gaussian distribution with mean $\langle Z\rangle = \langle f(x)\rangle$ and standatd deviation $\sigma \approx \frac{1}{\sqrt{n}}$

Thus, the precision of a MC estimator depends on the number of samples:

$$\sigma \propto \frac{1}{\sqrt{N}}$$

Statistical Uncertainty in MC simulations

The variance of the mean of an estimated quantity x calculated in N batches, is:

$$\sigma^2_{\langle x \rangle} = \frac{1}{N-1}\left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n}\right)^2\right]$$

where,

n_i = number of histories in the ith batch

n = $\sum n_i$ = total number of histories in the N batches

x_i = average of x in the ith batch: $x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$

Geometry Description

Geometry Description

Geant4

Geometry description	G4 Hierarchical	FLUKA Boolean flat in space - Combinatorial Geometry (CG) -

"**Solid**": a 3D finite macro object e.g. box, sphere, cone…twisted solid (high order). Shape and size.

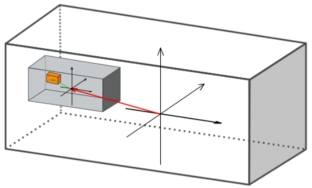
"**Logical Volume**": Give physical properties to a solid, material, B/E field, sensitive detector etc.

"Physical Volume": Place it (once or multiple times) in the 3D space wrt the mother volume coordinate system

- hierarchical geometry
- Boolean solids (union+multiunion, intersection, subtraction) are available, but not recommended by G4 for performance issues

"**World**": the top most logical volume which is placed at the origin

"**Region**": a group of logical volumes to apply physical properties e.g. magnetic field, emf range cuts etc..



Geometry Description

FLUKA

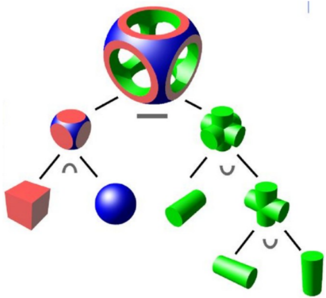
Geometry description	Hierarchical	Boolean flat in space - Combinatorial Geometry (CG) -

"**Bodies**": Basic convex objects (up to 2nd order) + infinite planes & infinite cylinders

"**Zones**": Sub-region defined only with intersection and subtraction of bodies (used internally)

"**Regions**": Defined as Boolean operations of bodies (union of zones)

"**Lattices**" - duplication of existing objects (translated & rotated)



Cross section error calculus

We have that the attenuation of the beam intensity in matter is given by:

$$I(L) \approx I_0 e^{-L/\lambda}$$

The mean free path (λ_c) is defined as:

$$\lambda_c = \frac{1}{\mathcal{N}\sigma_c}$$

Where $\mathcal{N}$ is the number of atoms/volume and σ_c is the "correct" absorption cross section. Thus, we get:

$$I(L) = I_0 e^{-L\mathcal{N}\sigma_c}$$

So, considering 10 attenuation lengths ($L = 10\lambda_c$):

$$I(10\lambda_c) = I_0 e^{-\frac{10}{\mathcal{N}\sigma_c}\mathcal{N}\sigma_c} = I_0 e^{10}$$

If the absorption cross section is wrong by a factor $1+\Delta$, evaluating at the same L, we have:

$$I' = I_0 e^{-\frac{10}{\mathcal{N}\sigma_c}(1+\Delta)} = I_0 e^{-10(1+\Delta)}$$

Which would be off by a factor:

$$\frac{I}{I'} = \frac{I_0 e^{-10}}{I_0 e^{-10(1+\Delta)}} = e^{10\Delta}$$

Taking $\Delta = 0.1$

$$\frac{I}{I_1} = e \approx 2.7$$