ISAPP School 2024 · KIT / Bad Liebenzell

Geant4 Simulations for Rare Event Searches

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1/3: Theory of MC Simulations, Programming Environment, Basics of Geant4

Scope

- Q: What will you gain from this lecture?
- A: You will get a basic understanding how to implement and run a Monte Carlo (MC) simulation with the Geant4 code. You should get an understanding what MC background models of rare event searches can do and what their limitations are.

Schedule

- Today:
  Theory of MC simulations, **programming** environment,
  and basics of **Geant4**
- Friday (20 Sep., 14:00 – 15:45):
  Implement experimental **geometries**, generate **primary particles**, store **data** and analyse it with ROOT
- Wednesday (25 Sep., 16:15 – 18:00):
  Simulation of
  - **intrinsic** backgrounds for **deep underground** experiments searching for Dark Matter
  - **atmospheric** backgrounds for reactor based neutrino experiments at **shallow experimental sites**

Mode of the lecture

- The lecture will alternate between theory parts (~15min, me talking) and hands-on examples (~20min, you simulating)
- During the hands-on you can also discuss the problem at hand with your fellow student
- If you have questions – don't hesitate to ask them at any time!

What is your previous knowledge?

Theory* of MC simulations

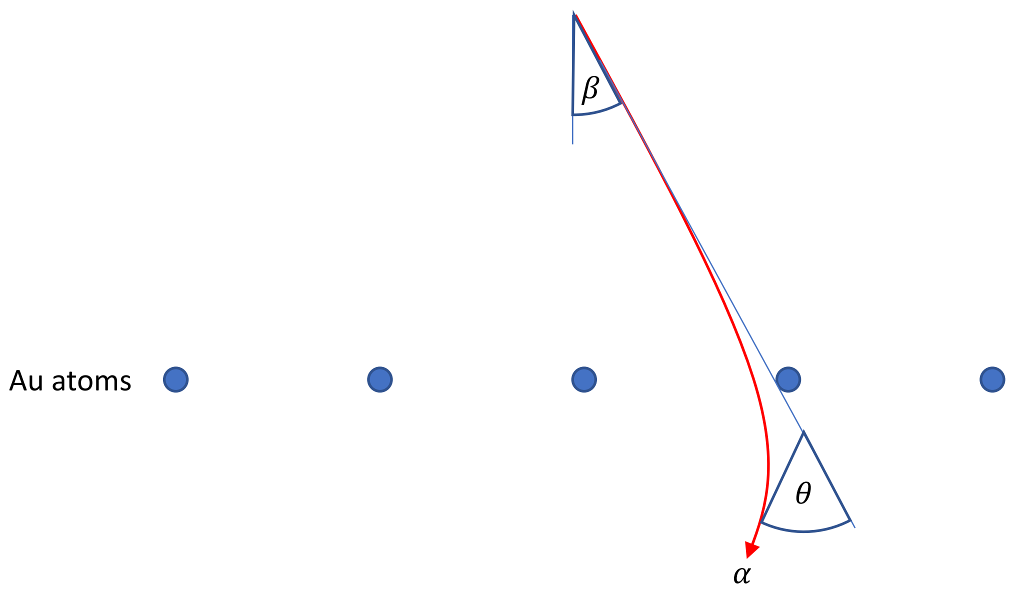
*To the extend needed to understand an actual simulation and its terminology
 - not more

Research Objectives

- Treat a MC simulation as a **virtual experiment** and decided before starting it*:
  - What is the **research objective**? What question should the experiment answer?
  - What is the **observable**? What should be (virtually) measured?
  - What is known about the **boundary conditions** of the experiment? Are positions constrained by the geometry of the apparatus that should be simulated?

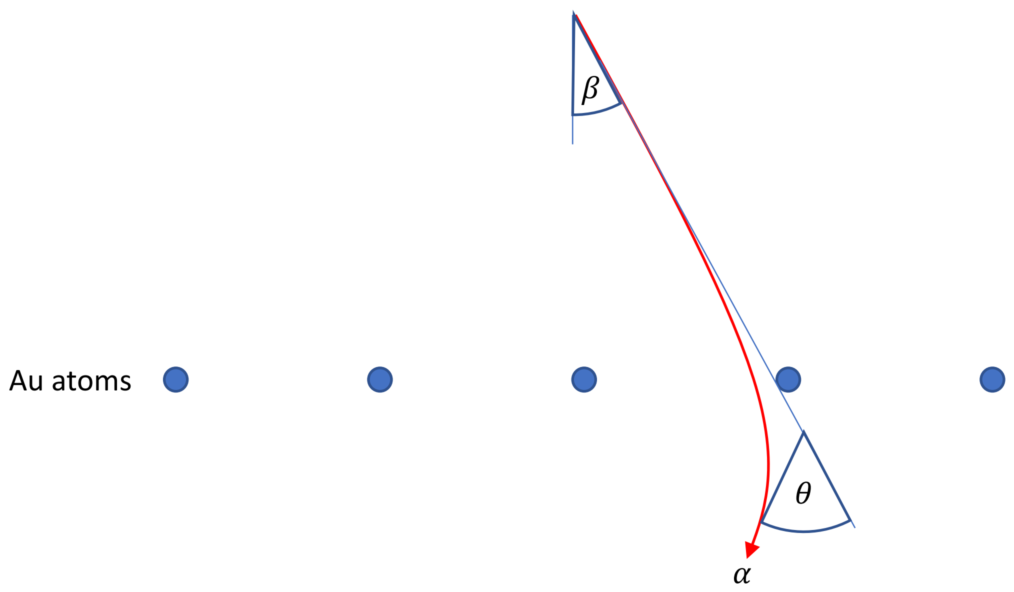
*At least in a first approximation; as with real experiments, first results may cause refinements or extension of the initial objectives

Research Objectives



- ***Objective:*** What is the deflection angle θ of an alpha particle of energy E emitted in direction β at position r_0 after passing through a monoatomic gold layer with atoms at $r_{\mathrm{Au},i}$?

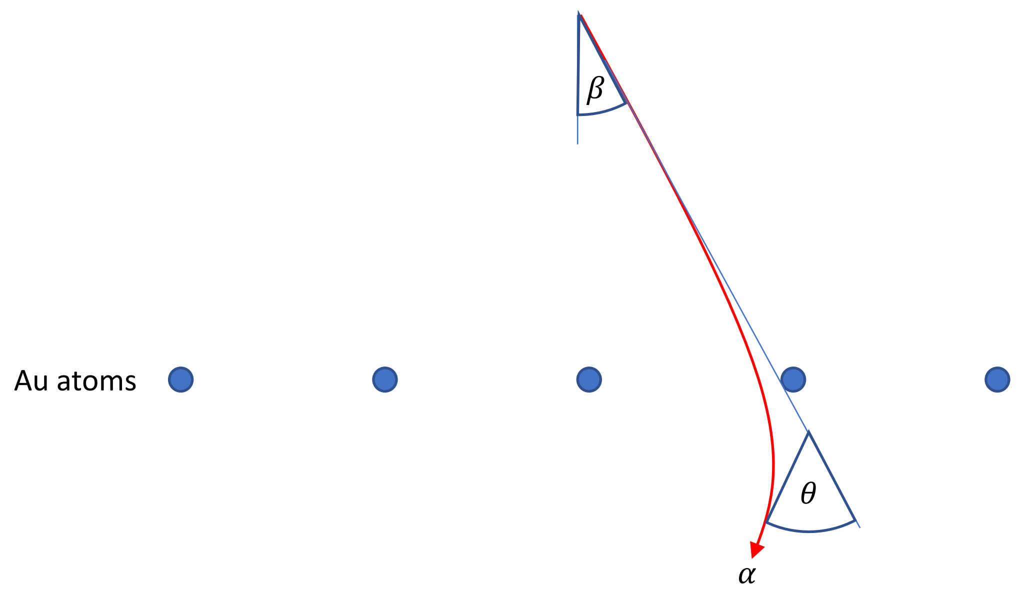
Input And Output



- ***Input:***
  - Incident particle: alpha
  - Initial energy E
  - Initial direction β
  - Initial position r_0
  - Scatterer particle: Au
  - Scatterer positions $r_{\mathrm{Au},i}$

- ***Output:***
  - Deflection angle θ

Primary Particle, Geometry, Observable



- ***Input:***
  - Incident particle: alpha
  - Initial energy E
  - Initial direction β
  - Initial position r_0
  - Scatterer particle: Au
  - Scatterer positions $r_{\mathrm{Au},i}$

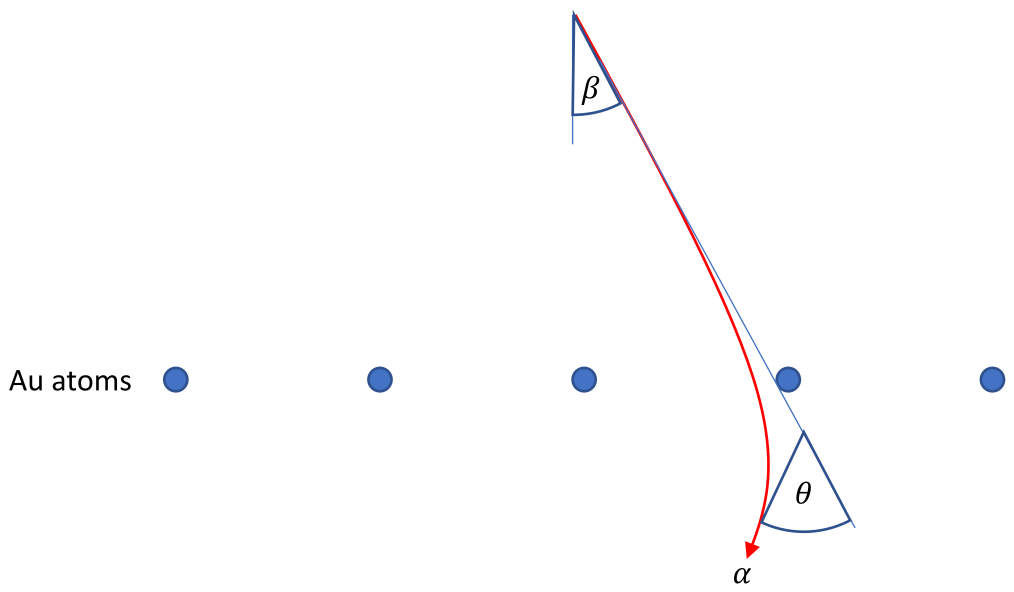
Defines the **primary particle**

Defines the **geometry** of the experiment

- ***Output:***
  - Deflection angle θ

The **observable** that should be measured

Physics Model



- ***Input:***
  - Incident particle: alpha
  - Initial energy E
  - Initial direction β
  - Initial position r_0
  - Scatterer particle: Au
  - Scatterer positions $r_{\mathrm{Au},i}$
- **Process: ?**
  (input → output)
- ***Output***:
  - Deflection angle θ

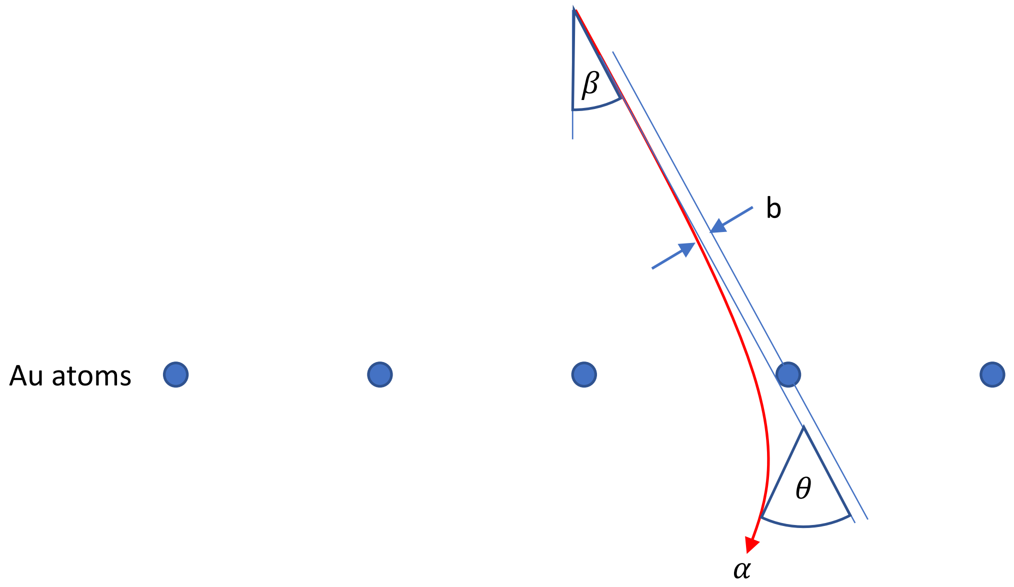
Defines the primary particle

Defines the geometry of the experiment

A **model** of the **physic**al interactions

The observable that should be measured

Ideal Rutherford Scattering



- ***Process*** (input → output): Rutherford scattering

$$\cot\left(\frac{\theta}{2}\right) = \frac{4\pi\epsilon_0\mu v^2}{Q_{\mathrm{Au}} \cdot Q_{\alpha}} \cdot b$$

with impact parameter

$$b = b(\beta, r_0, r_{\mathrm{Au}}),$$

projectile velocity

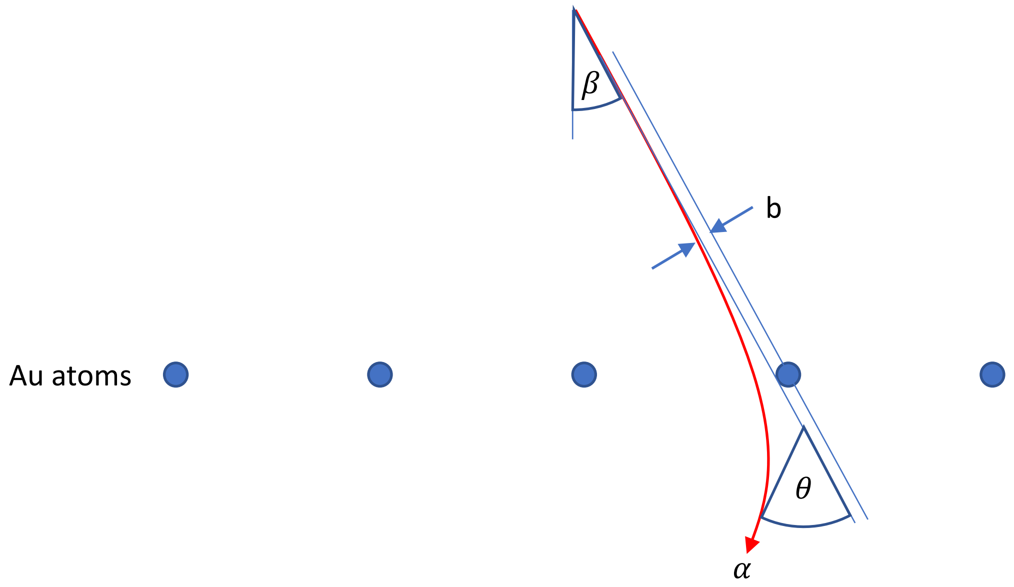
$$v = v(E),$$

and reduced mass

$$\mu = \mu(m_{\mathrm{Au}}, m_{\alpha})$$

computable from inputs

Ideal Rutherford Scattering

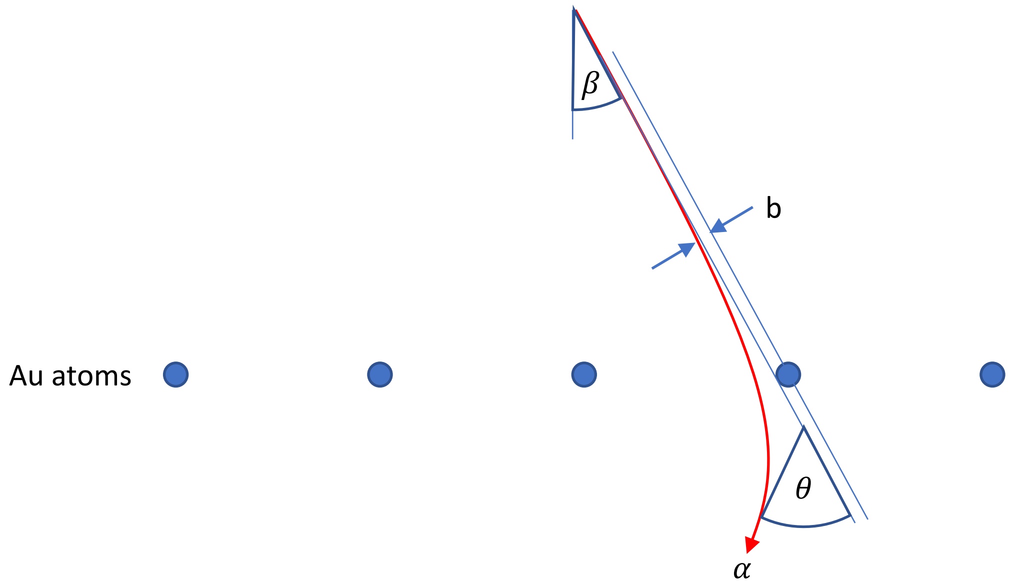


- ***Process*** (input → output):

$$\theta = \theta(E, \beta, r_0, r_{\mathrm{Au}}),$$

- Rutherford scattering is a classic theory – no randomness is involved
- In an ideal world (perfect preparation of incident particle, perfect knowledge of scatterer), repetitions of the experiment will yield same results

~~Ideal~~ Real Rutherford Scattering



- ***Process*** (input → output):

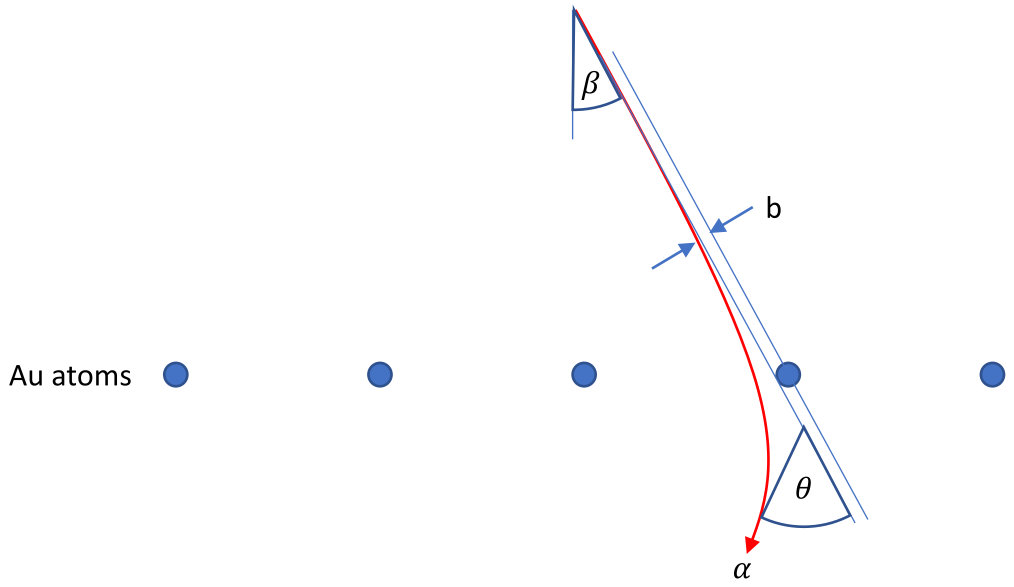
$$\theta = \theta(E, \beta, r_0, r_{\text{Au}}),$$

- In reality, there are uncertainties:
  - No particle can be perfectly prepared (E, β, r_0)
  - No perfect knowledge about scatterer ($b(r_{\text{Au}})$)

→Repetition of the experiment will yield different results

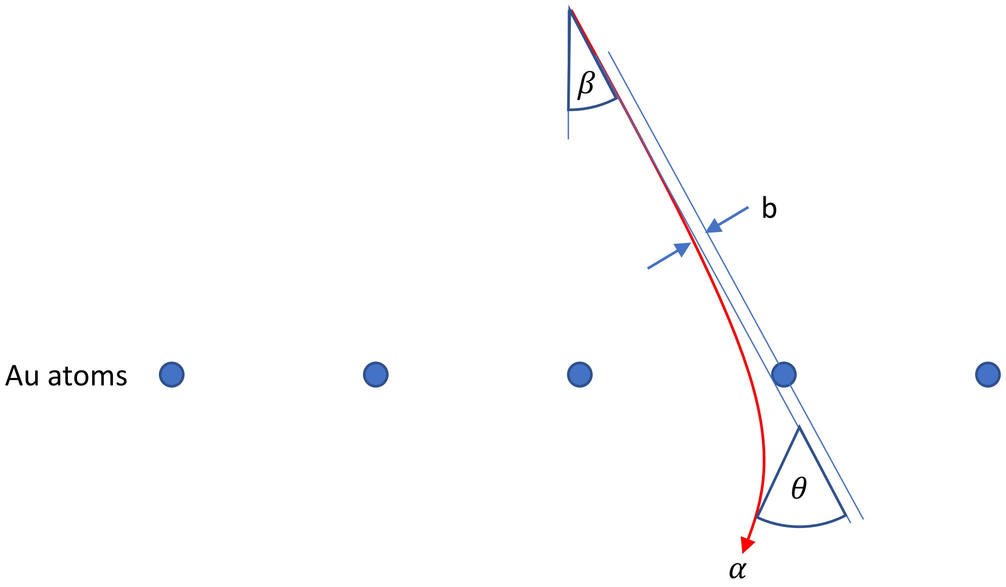
→Randomness!

Randomness



- Assume that the input variables are the components of a **random vector**
  $$\vec{X} = (E, \beta, r_0, r_{\text{Au}})$$
  with dimension $n = 4$, …
- With all possible realisations $\vec{x}$ that $\vec{X}$ can take are given by the **sample space** Ω: $\vec{x} \in \Omega$, …
- And the **probability** density function (pdf) to realize an actual $\vec{x}$ is $P(\vec{x})$, …
  - In physics, with cross section σ: $P(\vec{x}) \propto \sigma(\vec{x})$

Expectation Value

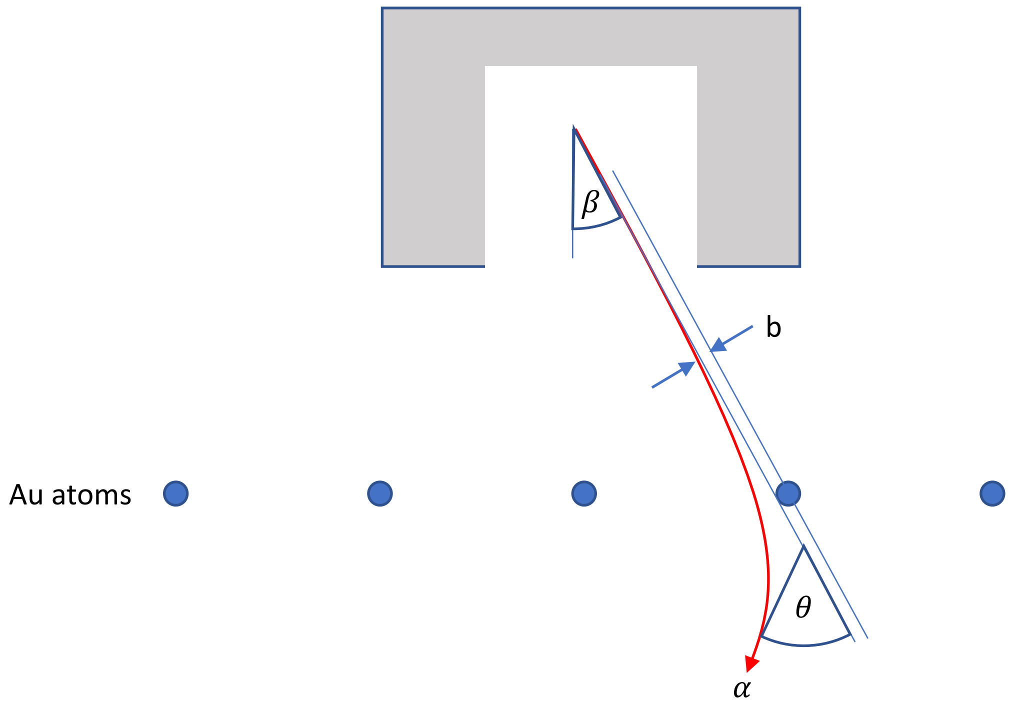


- Then also the output $\Theta(\vec{X})$ is a random variable with realisation θ
- And we can use the **expectation value**

$$E[\Theta] = \int_{\vec{x}\in\Omega} P(\vec{x}) \cdot \theta(\vec{x}) \mathrm{d}^n x$$

to consider the randomness of the searched for output

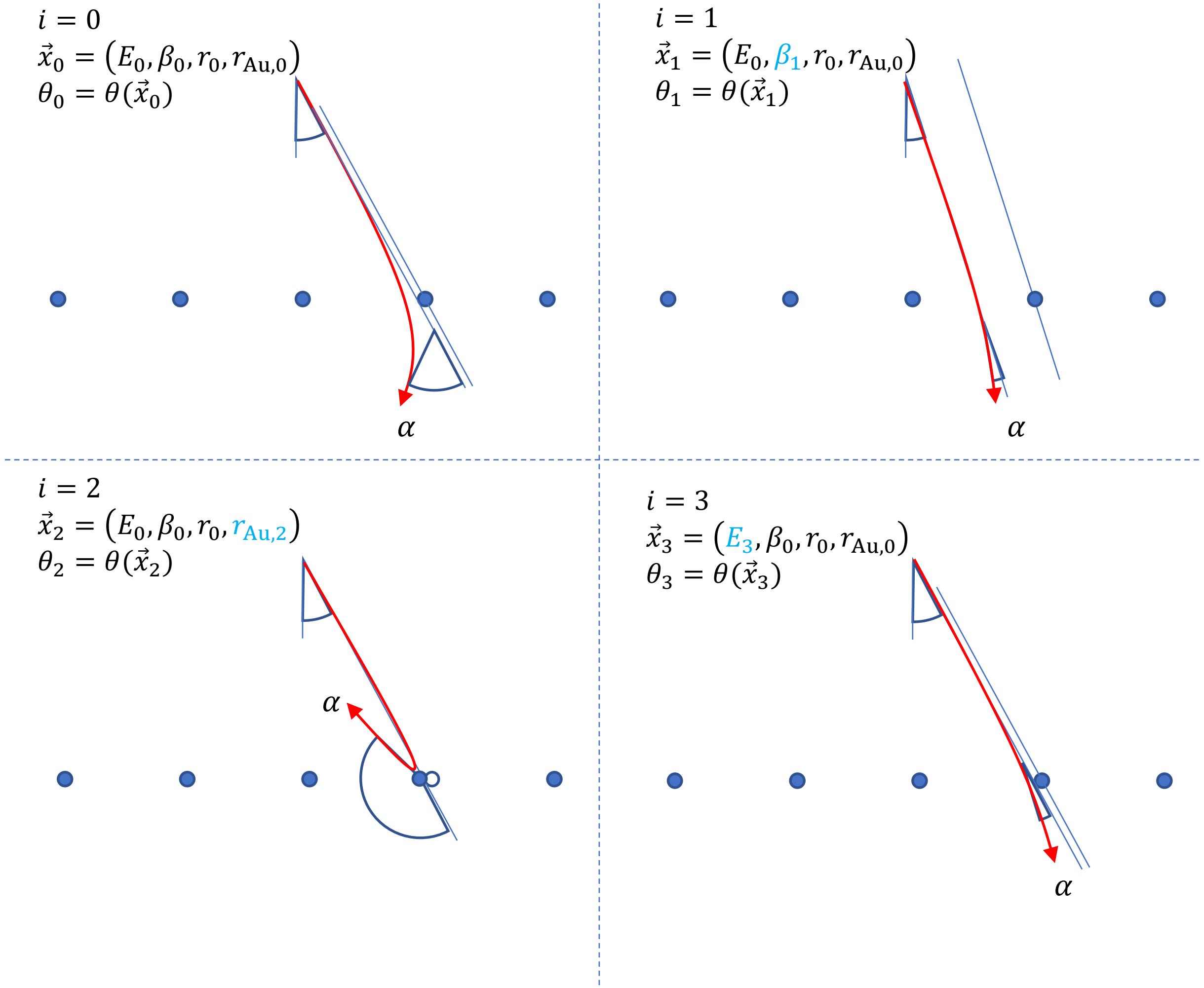
Disadvantages



$$E[\Theta] = \int_{\vec{x}\in\Omega} P(\vec{x}) \cdot \theta(\vec{x})\mathrm{d}^n x$$

- But it has some potential disadvantages:
  - Already this simple experiment requires a 4-dimensional integration
  - Dimensionality increase rapidly with more realistic modelling of the experiment
  - Ω (and $P(\vec{x})$) can be very complex, e.g. if r_0 is constrained by some complex source geometry

Monte Carlo Simulation



Monte Carlo Simulation: draw N samples $(\vec{x}_i)_{i=0}^{N}$ from Ω and approximate

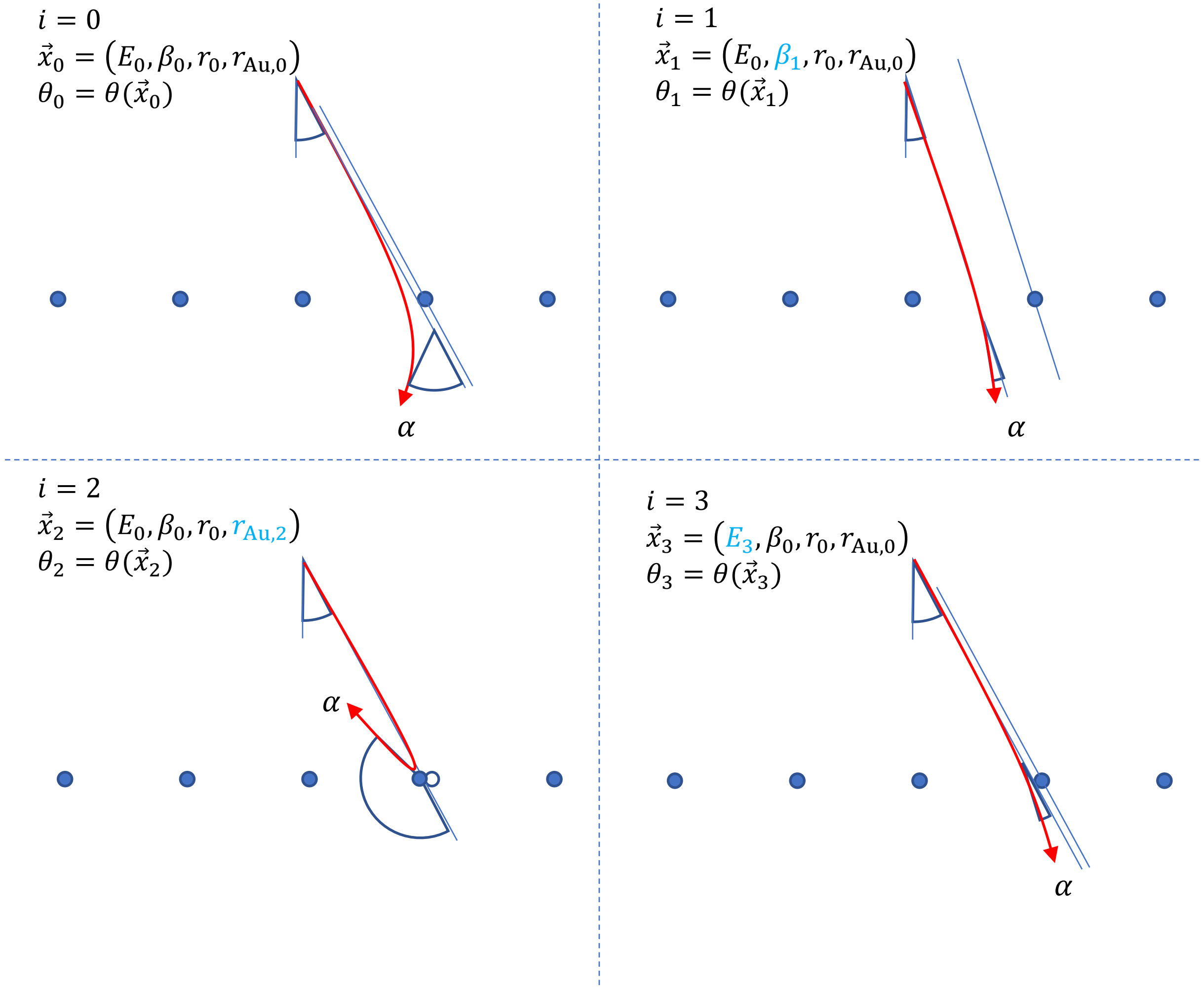
$$E[\Theta] = \int_{\vec{x}\in\Omega} P(\vec{x}) \cdot \theta(\vec{x})\mathrm{d}^n x$$

with the estimator of the expectation value

$$\hat{E}[\Theta] = \frac{1}{N}\sum_{i=0}^{N} \theta(\vec{x}_i)$$

→ Solve the integral via **Monte Carlo integration**

Advantanges



- Due to the **Law of Large Numbers**

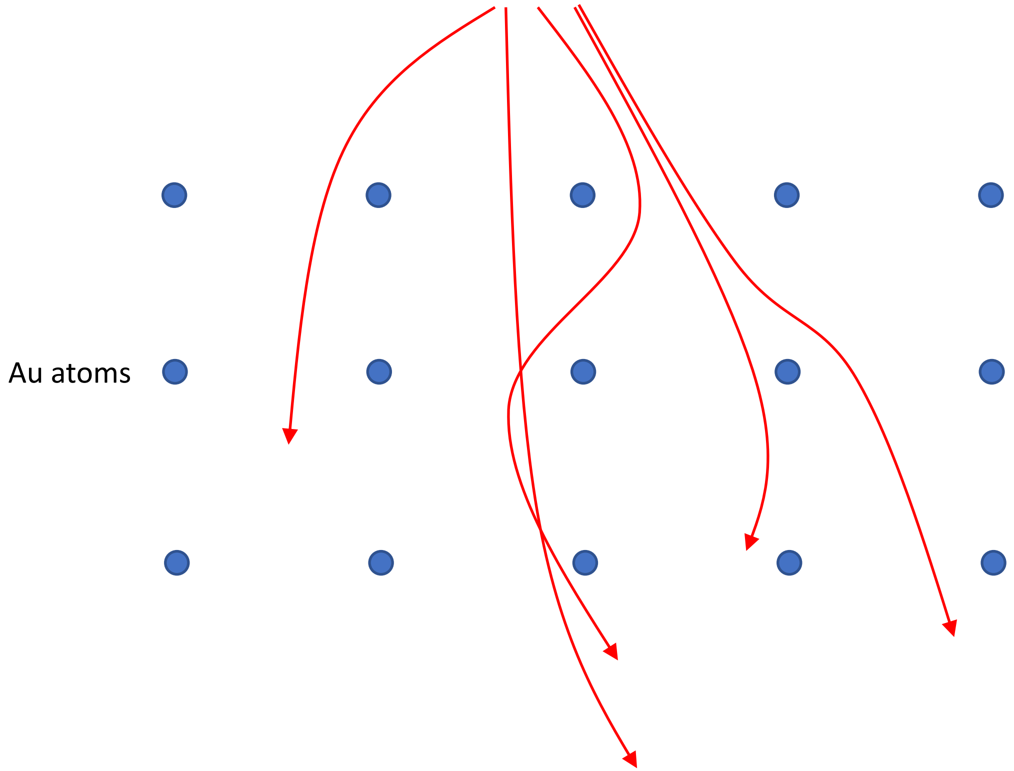
$$\lim_{N\to\infty} \hat{E}[\Theta] = E[\Theta]$$

accuracy can get arbitrary good

- Compared to numerical integration, e.g. trapezoidal rule, MC integration is **fast**: Improve accuracy for *d*-dimensional integral like
  - $1/n^{2/d}$ for trapezoidal rule with *n* points
  - $1/n^{1/2}$ for MC integration with *n* samples:

  → for *d>4*, MC integration is faster

Samples as Particle Trajectories



As particle physics simulation can be considered virtual experiments, the samples have a clear interpretation:

→They describe the **trajectory (=track)** a particle using the sampled values as input variables would follow within the given physics model

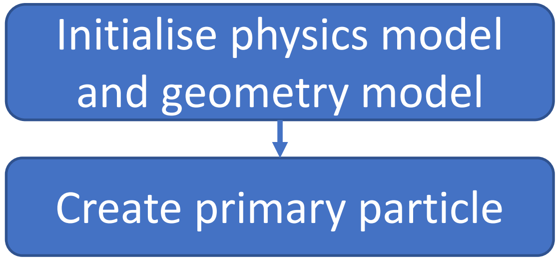
→Like in real experiments, one can "measure" more than one observable, e.g. also energy loss ΔE:
the output is then a tuple $\theta \rightarrow \vec{\theta} = (\theta, \Delta E)$

Workflow of a Simulation

Initialise physics model and geometry model

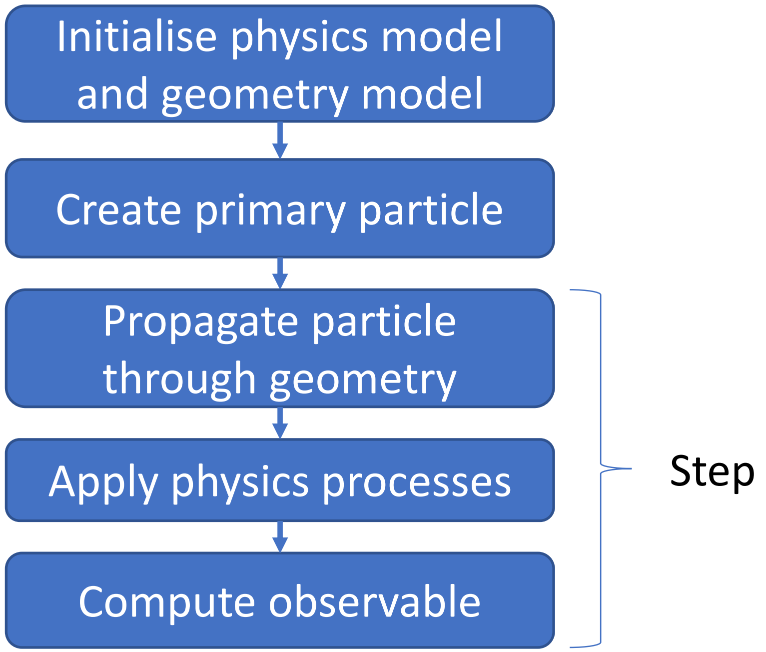
- Setup the virtual experiment:
  - Initialize the geometry model: which materials are placed at which regions or positions?
  - Initialize the physics model: compute material dependent model parameters (based on the geometry model)
  - Decide how many samples N should be drawn

Workflow of a Simulation



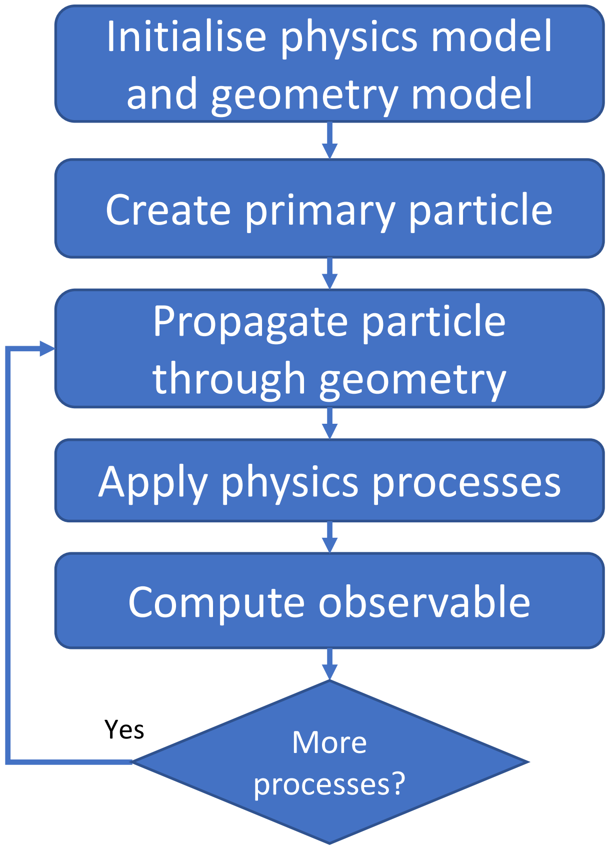
- Use a **primary particle generator** to sample the random variables that define the primary particle
  - Initial direction
  - Initial position (considering constrains from the geometry model, e.g. if primary particles can only be created within a **source** region)
  - Kinetic energy
  - Particle type

Workflow of a Simulation



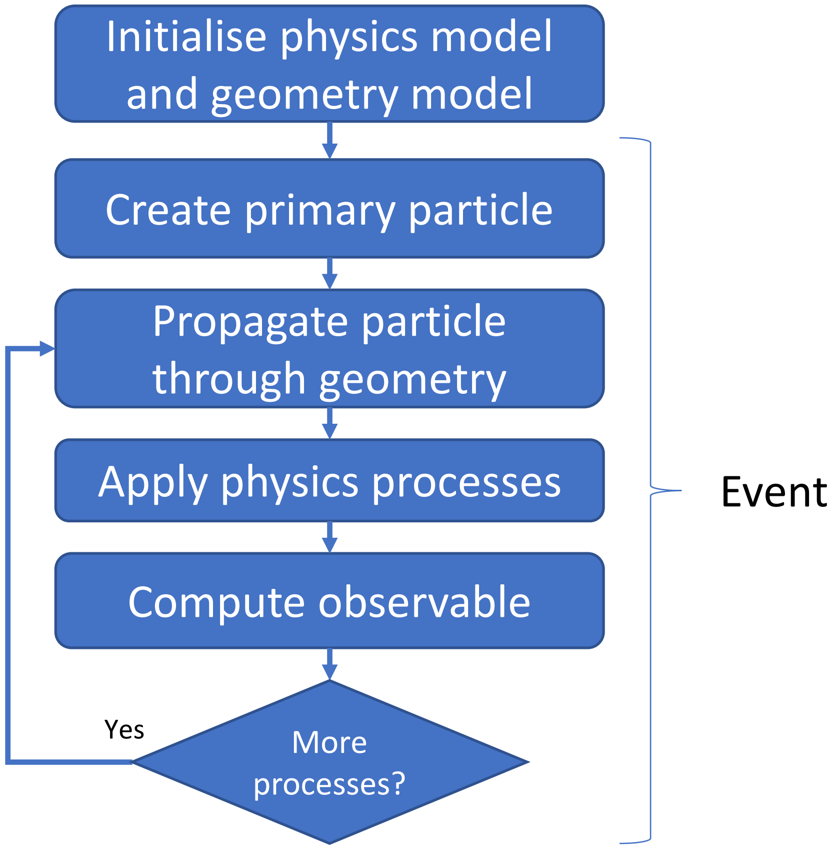
- Start the track of the primary particle
- Based on the physics model, compute the mean free path λ, i.e. average distant between two interactions
- Move the particle along the track by λ, make one **step**
- Compute the interaction, if needed sample input parameters, apply resulting changes on the track, e.g. changing direction due to deflection, reduce kinetic energy due to energy loss
- Update the observable**(s)** (e.g. deflection angle, energy loss) accordingly

Workflow of a Simulation



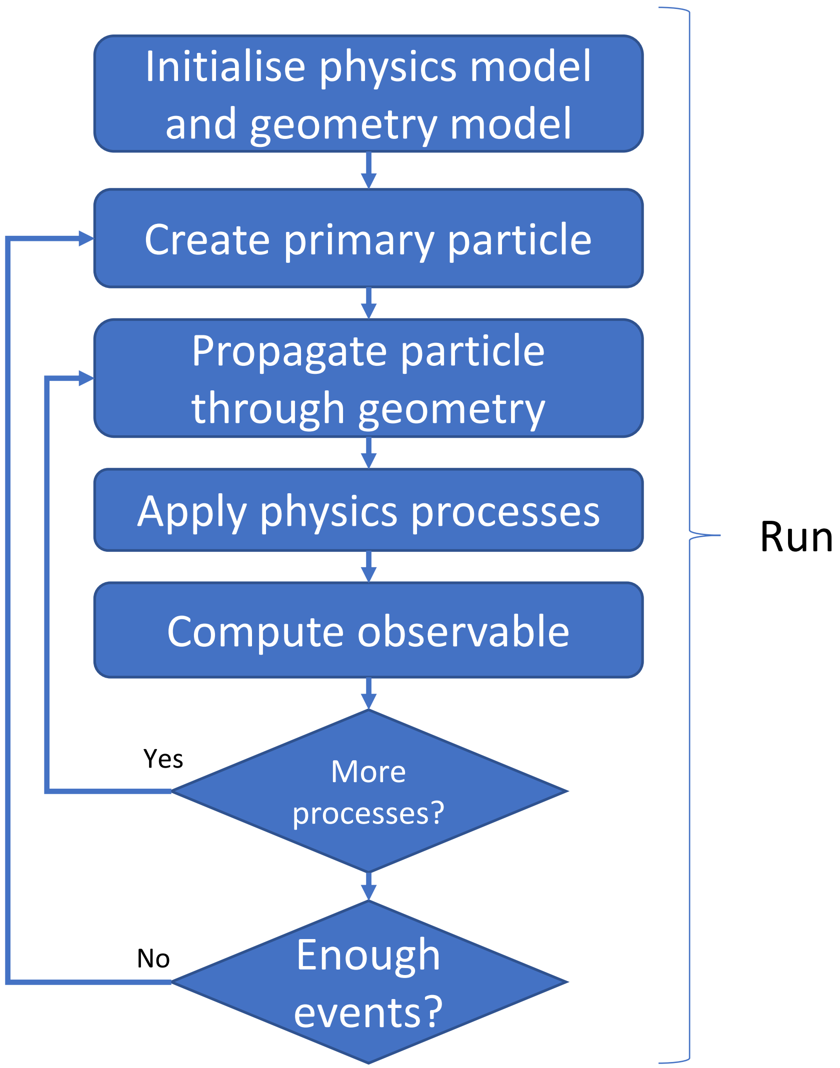
- Are there more processes that can apply to the particle?
- If yes (e.g. multiple scattering in a finite volume), repeat the previous step
- "No" could mean
  - The particle is unstable, and ceased to exist
  - The particle moved out of the finite geometrical model
  - The user deliberately limited the amount of iterations due to time or computing costs
- If no, then the track is finished
  → one sample $\vec{x}$ from the total sample space Ω was drawn
  → observable $\vec{\theta}(\vec{x})$ was computed

Workflow of a Simulation



- All steps from creating the primary particle until ending the track are some times referred to as an **event**
- Within one event, one sample from the *total* sample space Ω was drawn

Workflow of a Simulation



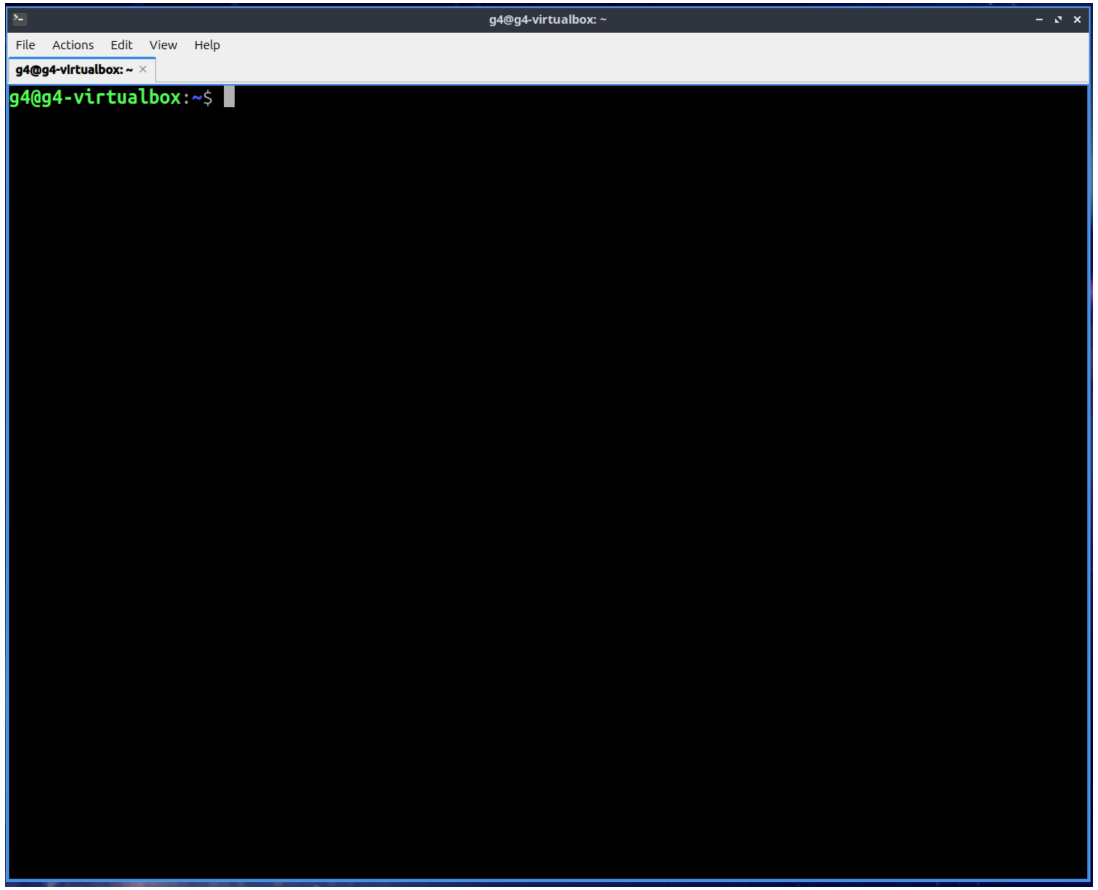
- Draw more samples (=compute more events) until N is reached
- Sometimes, all steps needed to obtain N samples is referred to as one **run**

Questions?

Programming Environment

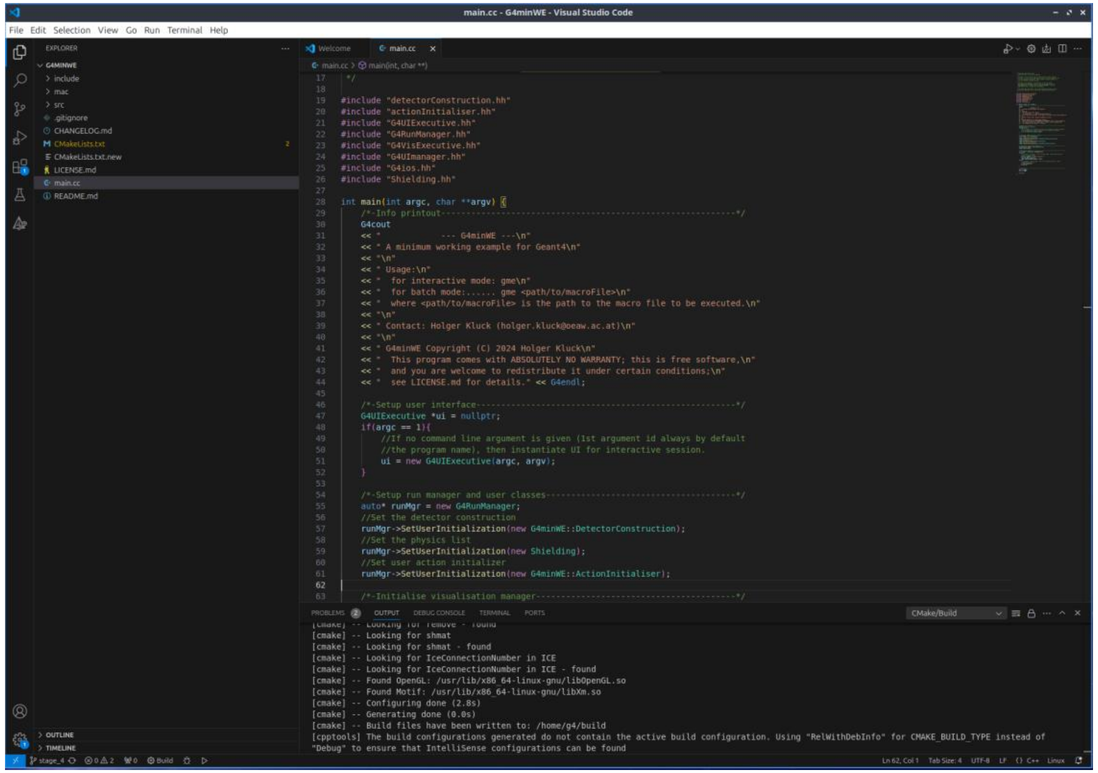
Linux; Terminal; Visual Studio Code; Git; CMake; Geant4

Programming Environment



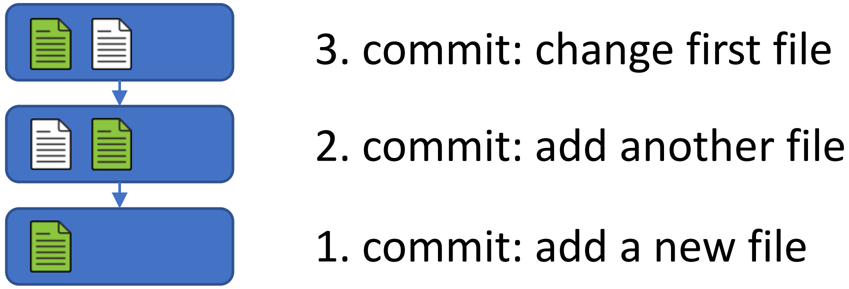
- For the hand-ons examples, we will use the MC simulation framework "Geant4"
- It is best to run it under Linux
- You will interact with Linux mostly via text commands, entered in a **terminal** window – it's a "Text User Interface" (TUI)

Linux



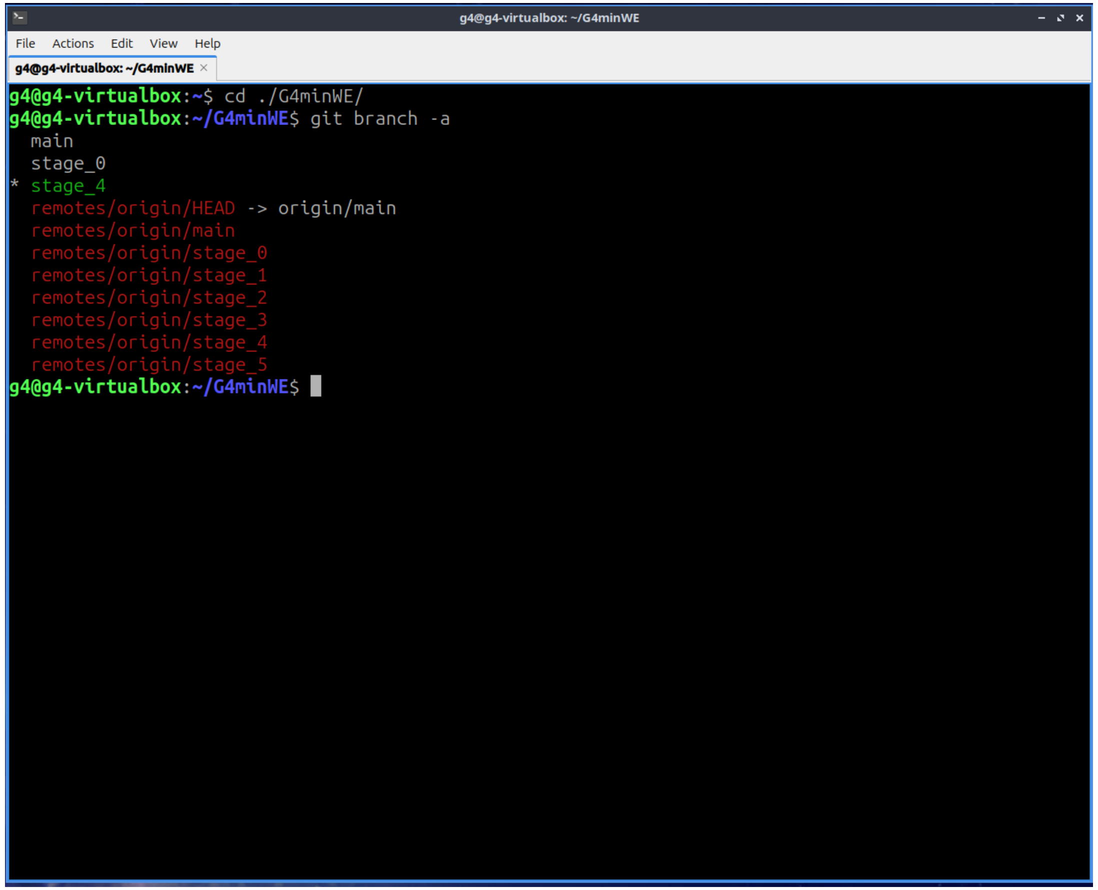
- For the actual programming, there are also **integrated development environments** (IDE) which provide many benefits:
  - syntax highlighting
  - code completion
  - etc.
- We will use **Microsoft Visual Studio Code (VSC)** https://code.visualstudio.com/
- Other common IDEs are, e.g.
  - eclipse https://projects.eclipse.org/projects/tools.cdt
  - CLion https://www.jetbrains.com/de-de/clion/

Git



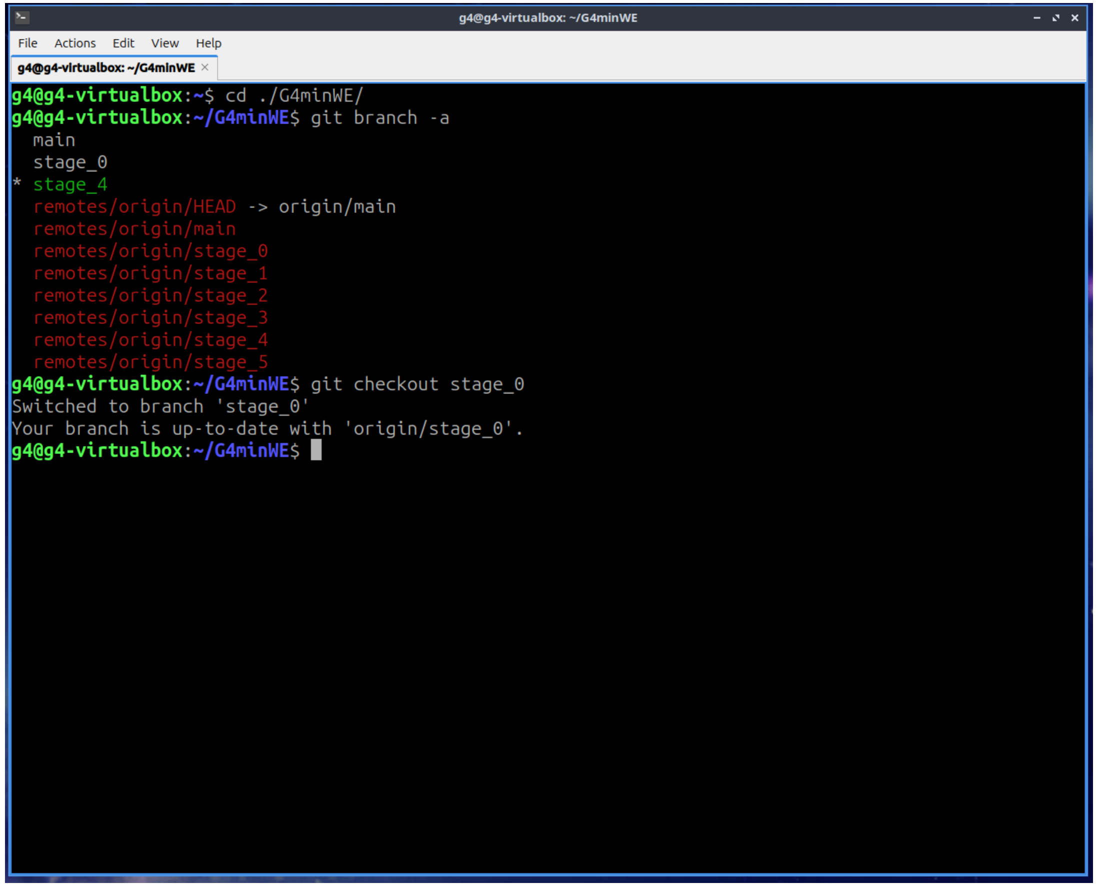
- Git is a code repository, it allows a user to track the changes made to a set of file over time
- We will use it for the files with the source code for the hands-on examples: **~/G4minWE**
- Via so-called **commits** the user can ask Git to make snapshots of the files within the repository
- Each commit is identified by its **hash**
- One can go to other commits (e.g. earlier ones) without losing the current state via the **checkout** command

Git



- The hands-on examples follow a bottom-up approach: each example is an extension of the previous one
- The examples-repository provides branches that contain the “extra code” needed to go from one examples to the next: stage_0, stage_1, etc.
- Branches with prefix “remotes” are not yet copied from remote repository

Git



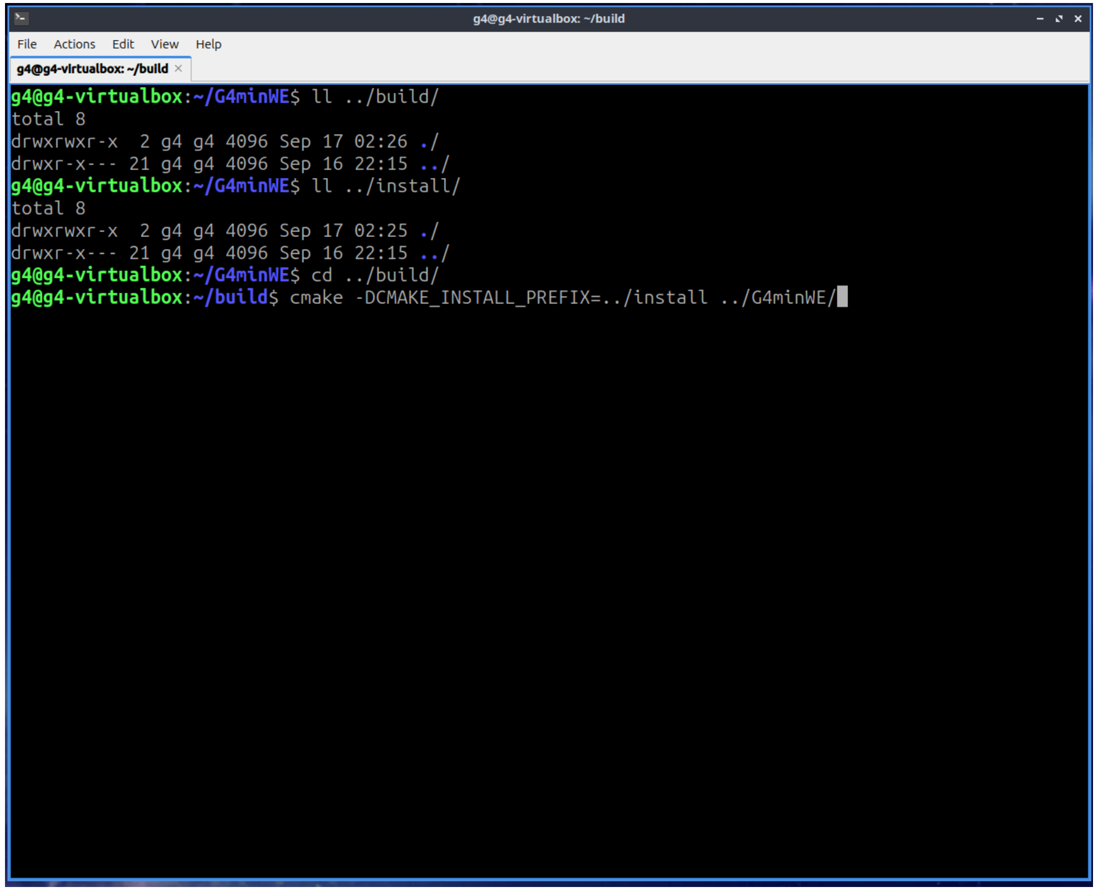
- Use **checkout** command to change to a branch

- We will use “stage_0” for the very first hands-on
- For latter hands-on we will use “stage_4”

CMake

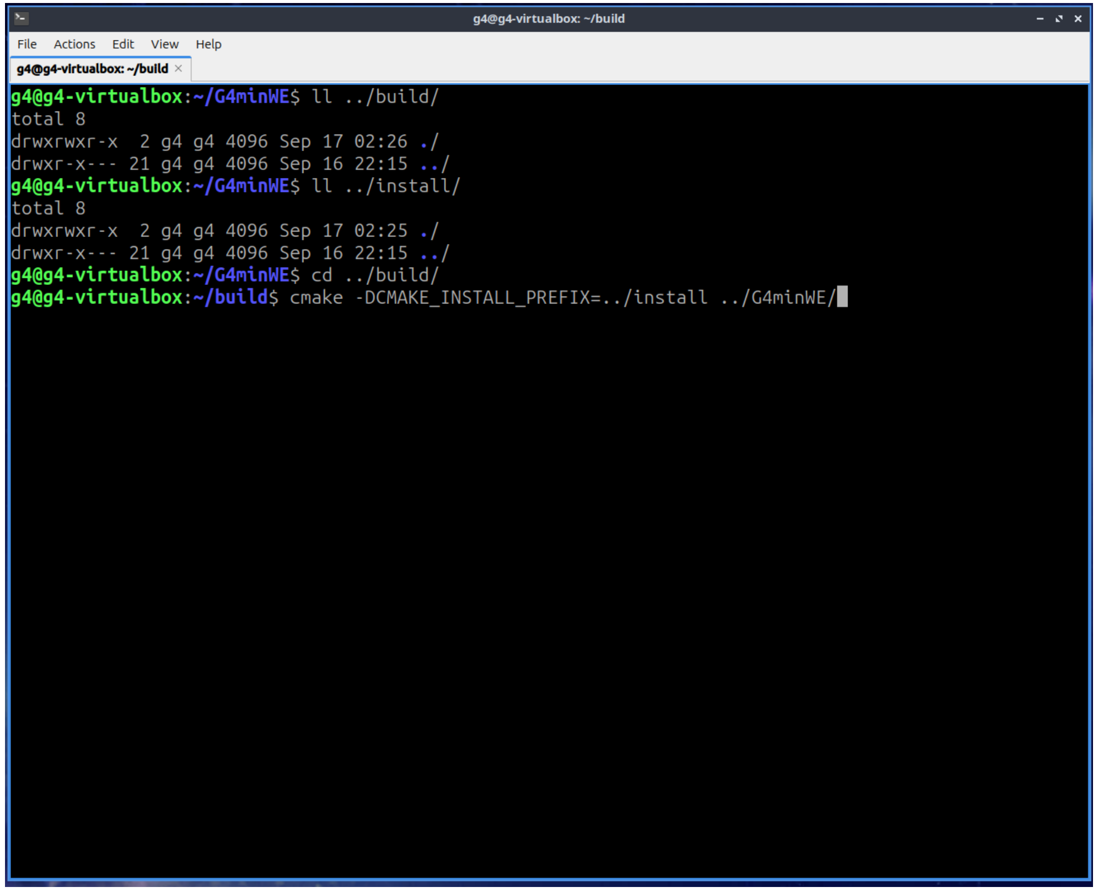
- To manage the compilation of the simulation code, we will use CMake: https://cmake.org/
  - Depending on the provide CMakeLists.txt file CMake will determine the dependencies between the different parts of the code and generate a **build script** – called **configuring** the project
  - Depending on this build script, it will then call the **compiler** to compile the source code to object files and call the **linker** to link the object files together to the executable – called **building** the project
  - As actual compiler we will use the GNU Compiler Collection – but thanks to CMake we do not interact directly with it

CMake



- CMake uses 3 directories:
  - One that contains the **source code** of the program to be build, e.g. the local copy of a repository
  - The **build directory** where Cmake creates the build script, runs the compiler, etc.
  - The **install directory** where the compiled executable will be copied to
- This way, build artefacts (=temporary files needed during building) will not “pollute” the source files and after installing one can simply delete the build directory with all its temporary files

CMake



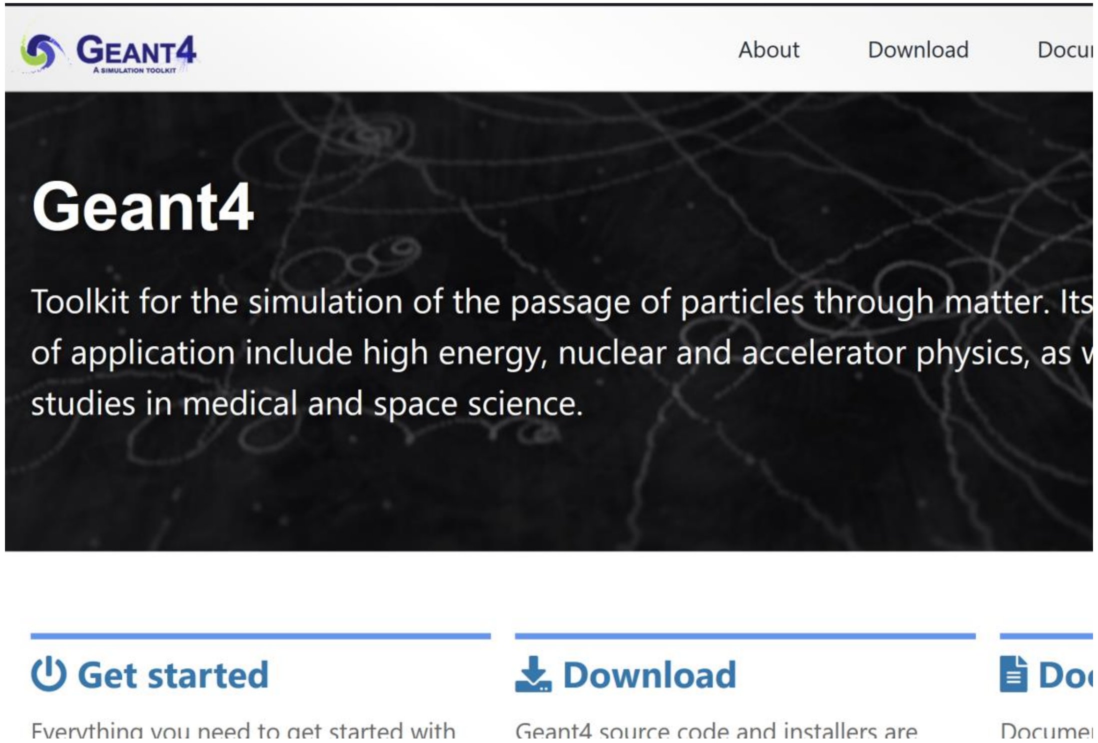
- The **cmake** command configure a project
  - One can specify the install directory via the option –DCMAKE_INSTALL_PREFIX
  - The argument to cmake is the source directory
  - It’s necessary if one adds or removes source code files from a project
  - In the pre-installed VSC, you can configure your project by pressing the [F8] key

CMake

```
g4@g4-virtualbox: ~/build
File  Actions  Edit  View  Help
g4@g4-virtualbox: ~/build
-- Found ZLIB: /usr/lib/x86_64-linux-gnu/libz.so (found suitable version "1.3", minimum required i
s "1.3")
-- Found XercesC: /usr/lib/x86_64-linux-gnu/libxerces-c.so (found suitable version "3.2.4", minimu
m required is "3.2.4")
-- Found Freetype: /usr/lib/x86_64-linux-gnu/libfreetype.so (found suitable version "2.13.2", mini
mum required is "2.13.2")
-- Found X11: /usr/include
-- Looking for XOpenDisplay in /usr/lib/x86_64-linux-gnu/libX11.so;/usr/lib/x86_64-linux-gnu/libXe
xt.so
-- Looking for XOpenDisplay in /usr/lib/x86_64-linux-gnu/libX11.so;/usr/lib/x86_64-linux-gnu/libXe
xt.so - found
-- Looking for gethostbyname
-- Looking for gethostbyname - found
-- Looking for connect
-- Looking for connect - found
-- Looking for remove
-- Looking for remove - found
-- Looking for shmat
-- Looking for shmat - found
-- Looking for IceConnectionNumber in ICE
-- Looking for IceConnectionNumber in ICE - found
-- Found OpenGL: /usr/lib/x86_64-linux-gnu/libOpenGL.so
-- Found Motif: /usr/lib/x86_64-linux-gnu/libXm.so
-- Configuring done (1.1s)
-- Generating done (0.0s)
-- Build files have been written to: /home/g4/build
g4@g4-virtualbox:~/build$ ll
total 76
drwxrwxr-x  3 g4 g4  4096 Sep 17 02:27 ./
drwxr-x--- 21 g4 g4  4096 Sep 16 22:15 ../
-rw-rw-r--  1 g4 g4 51034 Sep 17 02:27 CMakeCache.txt
drwxrwxr-x  6 g4 g4  4096 Sep 17 02:27 CMakeFiles/
-rw-rw-r--  1 g4 g4  3339 Sep 17 02:27 cmake_install.cmake
-rw-rw-r--  1 g4 g4  7032 Sep 17 02:27 Makefile
g4@g4-virtualbox:~/build$ cmake --build . --target install -j2
```

- Once the build script is generate, **cmake --build** start the actual building
  - The **–target install** option tells cmake to copy the built files to the install directory
  - If one has more CPU cores available, one can assign *n* of them to the build process via the **-j*n*** option
  - In the pre-installed VSC, you can compile your project by pressing the [F7] key
  - And install it by pressing the [F9] key

Geant4



- Geant4 is freely available from CERN: https://geant4.web.cern.ch/
- Most current version is 11.2.1, we will use 10.6.3
- Manuals: https://geant4.web.cern.ch/docs/ especially the Book For Application Developer (BAD)
- API documentation: https://geant4.kek.jp/Reference/ https://geant4.kek.jp/LXR/

Hands-on

- Change to the source directory under your home directory:
- Checkout the „stage_0“ branch:
- Change to the „build“ directory, configure and build the program via the command line:
- Change to the “install” directory and run G4minWE

Hands-on

- Change to the source directory under your home directory:
```
cd ~/G4minWE
```
- Checkout the „stage_0“ branch:
```
git checkout stage_0
```
- Change to the „build“ directory, configure and build the program via the command line:
```
cd ../build
cmake -DCMAKE_INSTALL_PREFIX=../install ../G4minWE
cmake --build . --target install -j2
```
- Change to the “install” directory and run G4minWE
```
cd ../install
./bin/G4minWE
```

Basics of Geant4

Basic Structure; Visualisation; Macro Files

Geant4

```
#include "detectorConstruction.hh"

#include "G4UIExecutive.hh"
#include "G4RunManager.hh"
#include "G4VisExecutive.hh"
#include "G4UImanager.hh"
#include "G4ios.hh"
#include "Shielding.hh"

int main(int argc, char **argv) {
    /*-Info printout-------------------------------------------------
    G4cout
    << "            --- G4minWE ---\n"
    << " A minimum working example for Geant4\n"
    << "\n"
    << " Usage:\n"
    << "  for interactive mode: gme\n"
    << "  for batch mode:...... gme <path/to/macroFile>\n"
```

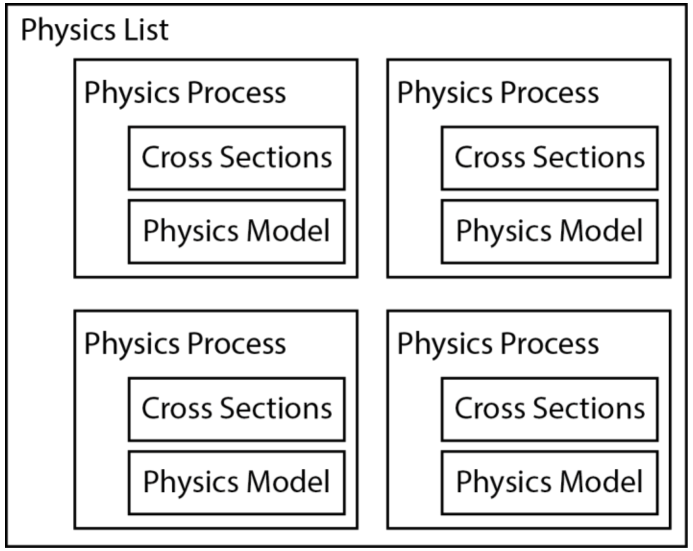
- The user interacts with the Geant4 framework via the `main()` function
  - Geometry model, physics list, primary particle generation are specified in **classes the user derived from Geant4 base classes**
  - Some features are provided as ready-to-use, e.g. **visualisation**
  - In the main function, instances of these user defined classes are passed to the **manager classes** provided by Geant4

Physics List

```
//Set the physics list
runMgr->SetUserInitialization(new Shielding);
```

- The physics list has to be
  - Instantiated in the `main()` function
  - Registered to the `G4RunManger`
  - And must not be deleted
- Geant4 provides several pre-defined physics lists tuned for several use cases, see Guide for Physics Lists
- In our examples, we use `Shielding`

Physics List



- Geant4 offers the users flexibility which kind of physics to apply in the simulation via **physics lists** [BAD §6.2.2]
  - List of **physics processes** that are applicable for a **particle**
  - A physics process is a combination of **physics model** and **cross sections**
  - Physics models give the **final state** of the reaction products, including any **secondary particles**

Visualisation

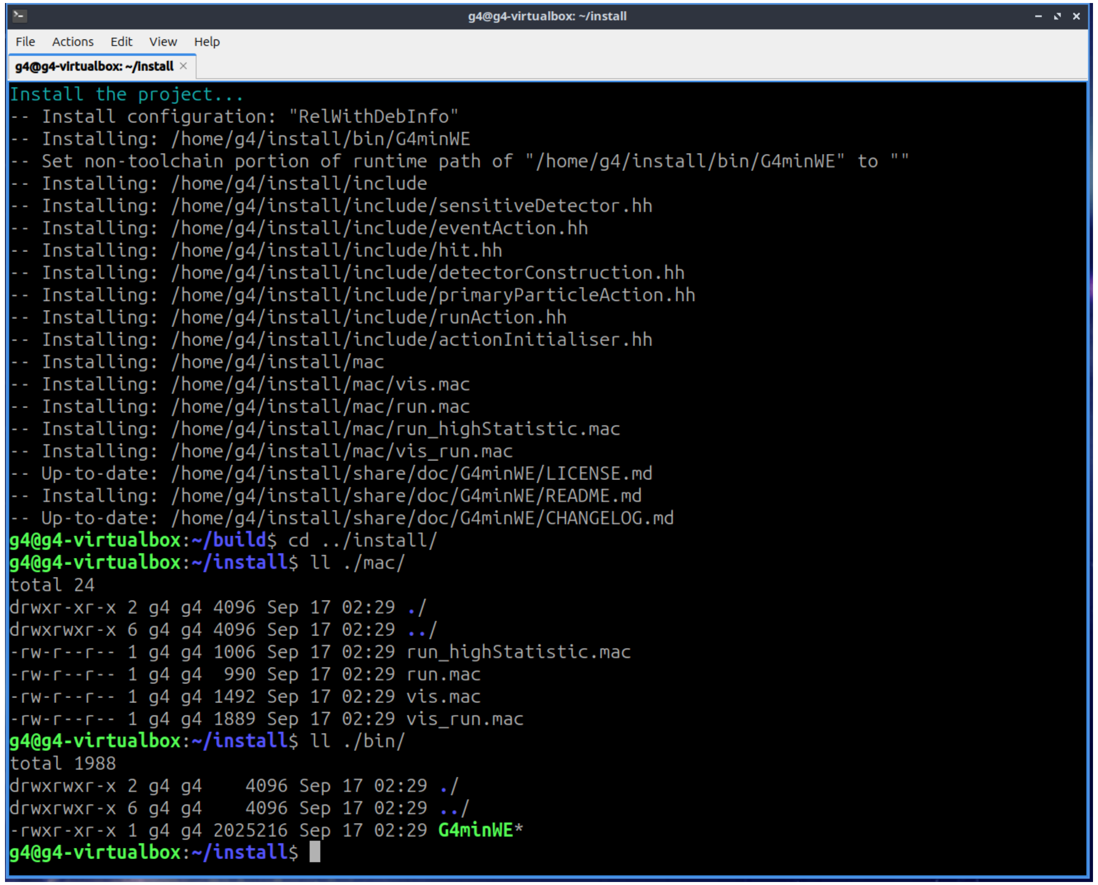
```cpp
/*-Initialise visualisation manager---------
G4VisManager* visMgr = new G4VisExecutive;
visMgr->Initialize();

```

- Geant4 can **visualize** the implemented geometry (and the particle interaction happening within)
- To enable visualisation, the **visualisation manager** has to be instantiated in the main function
- Depending on the way Geant4 as installed, several **visualisation drivers** are available [BAD, §8.1.2]
- User can configure it via **macro files**

Macro Files

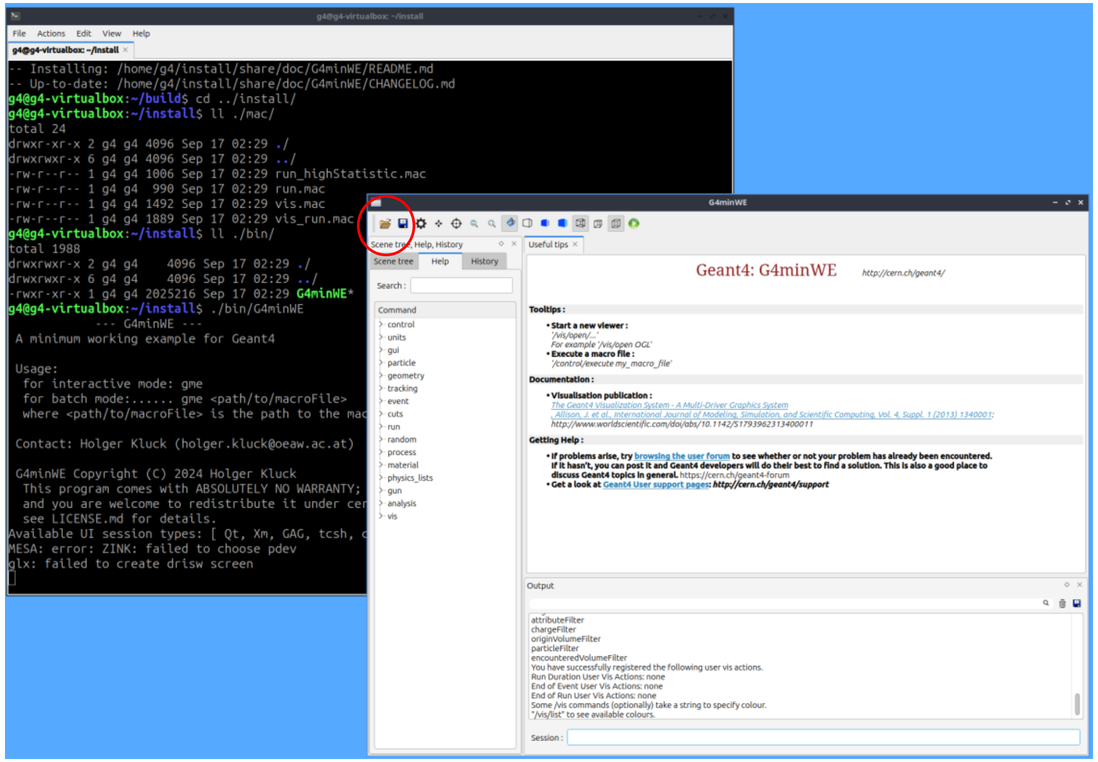
- Geant4 can be controlled via **macro files** (file extension: mac)

Macro Files



- Geant4 can be controlled via **macro files**
- Pass a macro file either on the command line for **batch mode**

Macro Files



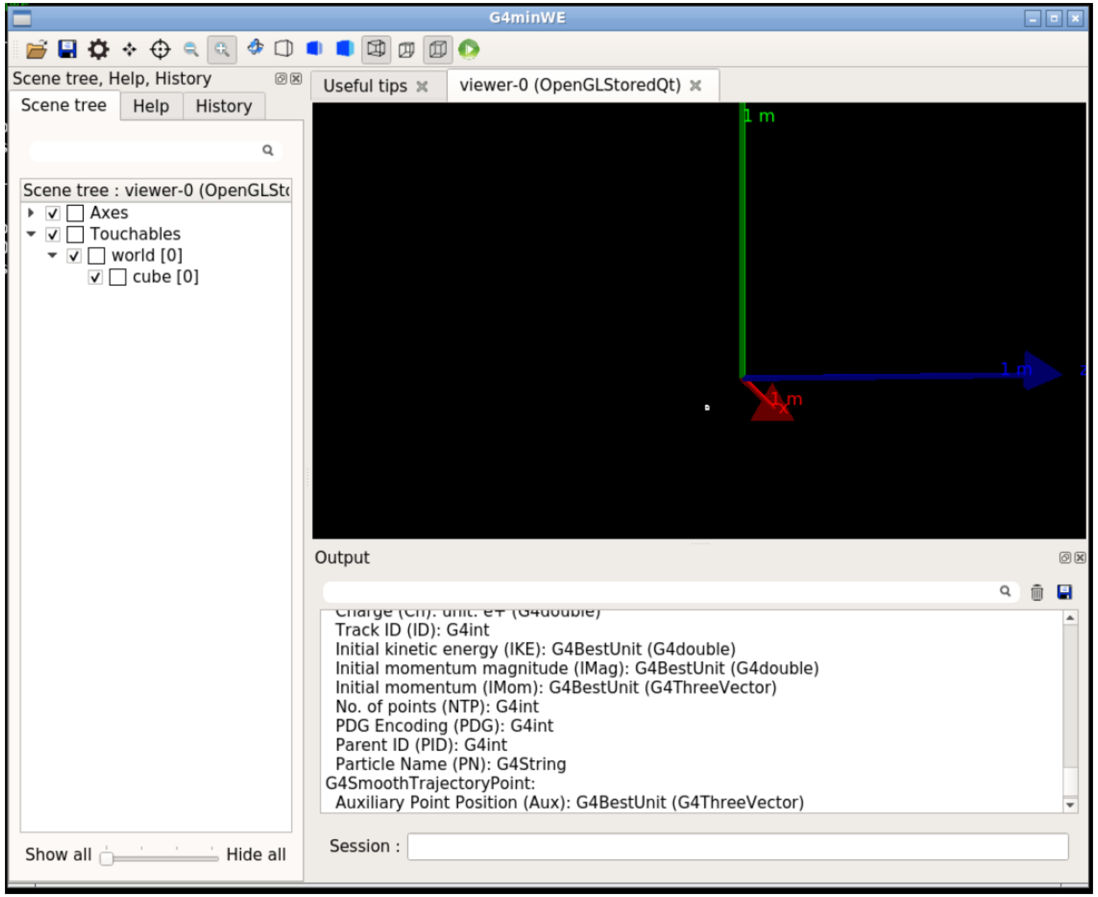
- Geant4 can be controlled via **macro files**
- Pass a macro file either on the command line for **batch mode**
- Or select it in an **interactive GUI** (via the „open file“ icon)
- If you want to simulate large numbers of events, use batch mode; use GUI only for test or debugging purposes

Visualisation

```
#Initialse Geant4
/run/initialize

#Use OpenGL visualiser with 600 pixel x 600 pixel window size
/vis/open OGL 600x600-0+0

#Or create a HepRepXML file containing the visualisation
#view it with JAS3
#/vis/open HepRepXML

#Visualiser should report errors
/vis/verbose errors

#Draw the geometry
/vis/drawVolume

#View on the scene from top
/vis/viewer/set/viewpointVector -1 0 0

#Draw the scene as wireframe
/vis/viewer/set/style wireframe
/vis/viewer/set/auxiliaryEdge true
#Increase number of sampling points for circles
/vis/viewer/set/lineSegmentsPerCircle 100

#Add a axes cross which length of each axes of 1 m
/vis/scene/add/axes 0 0 0 1 m

#For file-based drivers, use this to create an empty detector view:
#/vis/viewer/flush
```

- Control the visualisation settings via macro file commands
  - Before the geometry can be visualised, Geant4 need to be initialised
  - Select the visualization driver
    - OGL for interactive visualisation
    - HepRepXML / **JAS3** for offline use
  - Draw the geometry
  - Configure the visualisation style, add axes cross, orient the point of view, etc.
    see list of all commands

Interactive Visualisation



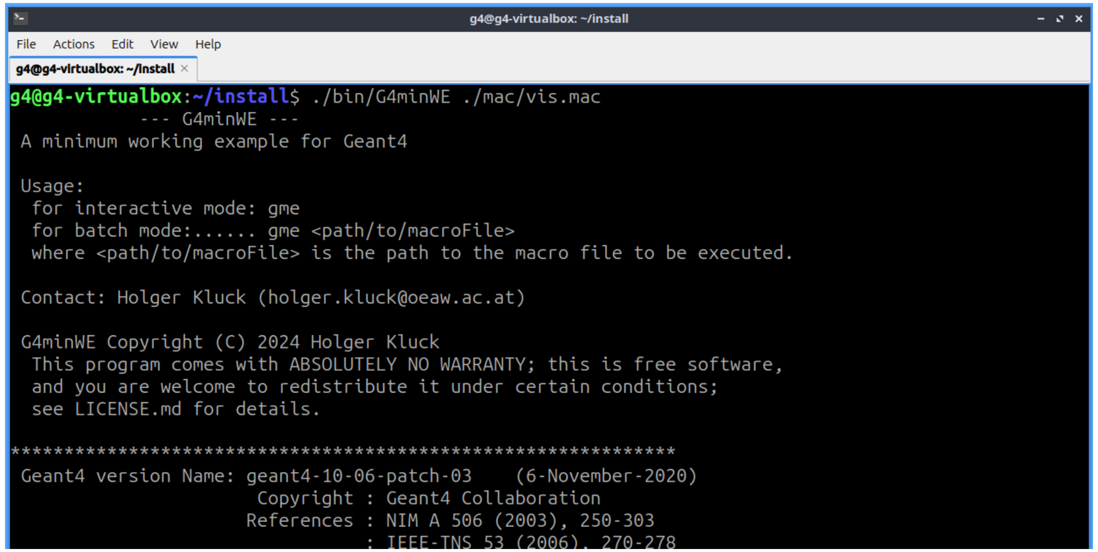
- In G4minWE, by default **OpenGL** is used a visualisation driver
  - It is interactive: one can pan and rotate the scene via mouse
  - Zoom in and out
  - Switch on/off individual volumes via the scene tree
  - Macro file vis.mac from stage_1 of G4minWE onwards adds an axes cross to the small PMMA (=Acrylic glass) cube defined in `DetectorConstruction`

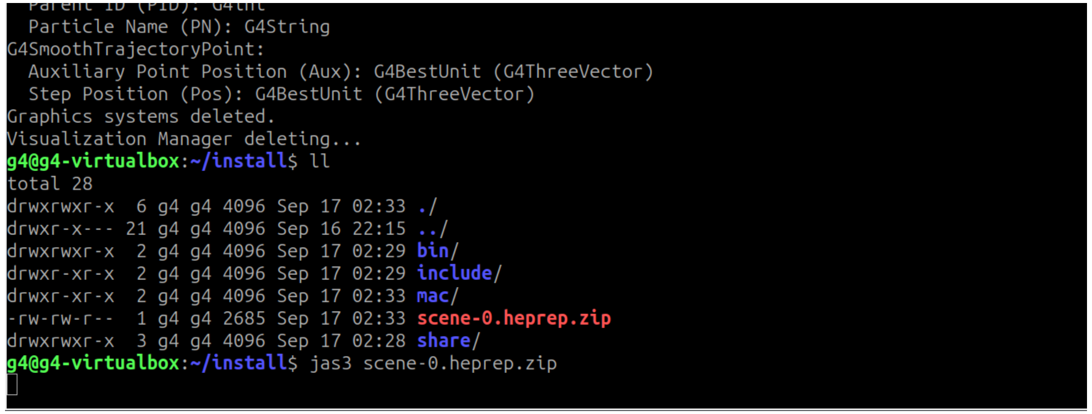
Offline Visualisation

```
#Initialse Geant4
/run/initialize

#Use OpenGL visualiser with 600 pixel x 600 pixel window size
#/vis/open OGL 600x600-0+0

#Or create a HepRepXML file containing the visualisation
#view it with JAS3
/vis/open HepRepXML

#Visualiser should report errors
/vis/verbose errors

#Draw the geometry
/vis/drawVolume

#View on the scene from top
/vis/viewer/set/viewpointVector -1 0 0

#Draw the scene as wireframe
/vis/viewer/set/style wireframe
/vis/viewer/set/auxiliaryEdge true
#Increase number of sampling points for circles
/vis/viewer/set/lineSegmentsPerCircle 100

#Add a axes cross which length of each axes of 1 m
/vis/scene/add/axes 0 0 0 1 m

#For file-based drivers, use this to create an empty detector view:
/vis/viewer/flush
```

- One can also create an **HepRepXML** file that contains a description of the geometry → adapt vis.mac as shown on the screen shot

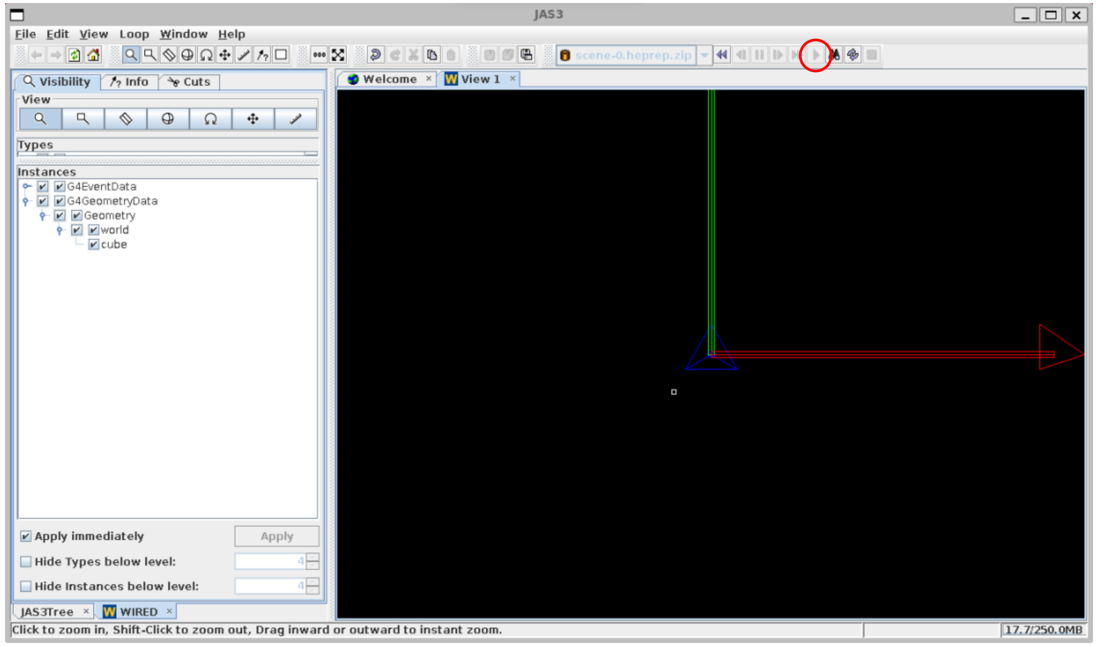
Offline Visualisation





- The **JAS3** tool can visualise the geometry described in a HepRepXML file
- The default name of the HepRepXML file is **scene-0.heprep.zip**

Offline Visualisation



- `jas3 ./scene-0.heprep.zip`
- Open a Wire4 view via:
  “File > New > Wired4 View”
- If there is no „Wired4 View“ go to “View > Plugin Manager > Available > common”
  select „WIRE4“ and click „Install selected plugins“
- Click the „play“ button to start visualisation

Hands-on

- Change to the source directory and checkout the „stage_4“ branch:

- Configure, build and install the code via VSC:
- Change to the install directory and run ./mac/vis.mac via the GUI

- Use VSC to activate the JAS3 visualisation in ./mac/vis.mac, install it
- Run ./mac/vis.mac in batch mode and open the output file in JAS3

Hands-on

- Change to the source directory and checkout the „stage_4“ branch:
  ```
  cd ~/G4minWE
  git checkout stage_4
  ```
- Configure, build and install the code via VSC:
  ```
  In VSC, press the [F8], [F7], [F9] keys
  ```
- Change to the install directory and run ./mac/vis.mac via the GUI
  ```
  cd ../install
  ./bin/G4minWE
  In the GUI click "File open" icon, select ./mac/vis.mac
  ```
- Use VSC to activate the JAS3 visualisation in ./mac/vis.mac, install it
  ```
  Comment line 21, uncomment lines 25,46, press [F9]
  ```
- Run ./mac/vis.mac in batch mode and open the output file in JAS3
  ```
  ./bin/G4minWE ./mac/vis.mac
  jas3 scene-0.heprep.zip
  ```

Take Home Messages

- Simulations can be regarded as virtual experiments
- A background simulation depends crucially on its model assumptions
- Each simulated event is one drawn sample from the sample space – more samples results in a more precise result
- Geant4 is a free and widely used software framework to implement a MC simulation – the scope of the simulation is the responsibility of its developers
- Unfortunately, some tools are needed (e.g. Linux, IDEs, C++, etc.) to create a MC simulation – like real experiments depends on tools