Geant4 Technical Forum

Geant4.jl - New Interface to Simulation Applications

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https://github.com/JuliaHEP/Geant4.jl

Motivation

- **Julia is a priori a good programming language candidate for HEP**
  - It combines **high-level expressibility** for scientific computational problems together with **high-performance** execution, avoiding the **two language problem**
- One essential aspect is to **evaluate its interoperability with existing C++ libraries** in HEP
- An excellent case for this evaluation is to use Geant4
  - It is large, complex, and not easy to re-write
  - The result of this evaluation is a 'nice-to-have' new functionality for Geant4

Julia wrappers to Geant4

- Similarly to Python, to call C++ from Julia you need to write (better generate) wrappers for each method you want to offer to Julia
- Using the **CxxWrap.jl** package
  - The user needs to write small code (in C++) to wrap each class and method (similar to pybind11 or Boost.Python)
  - The package **WrapIt** developed by Ph. Gras makes use of LLVM libraries to generate the wrappers automatically 😀

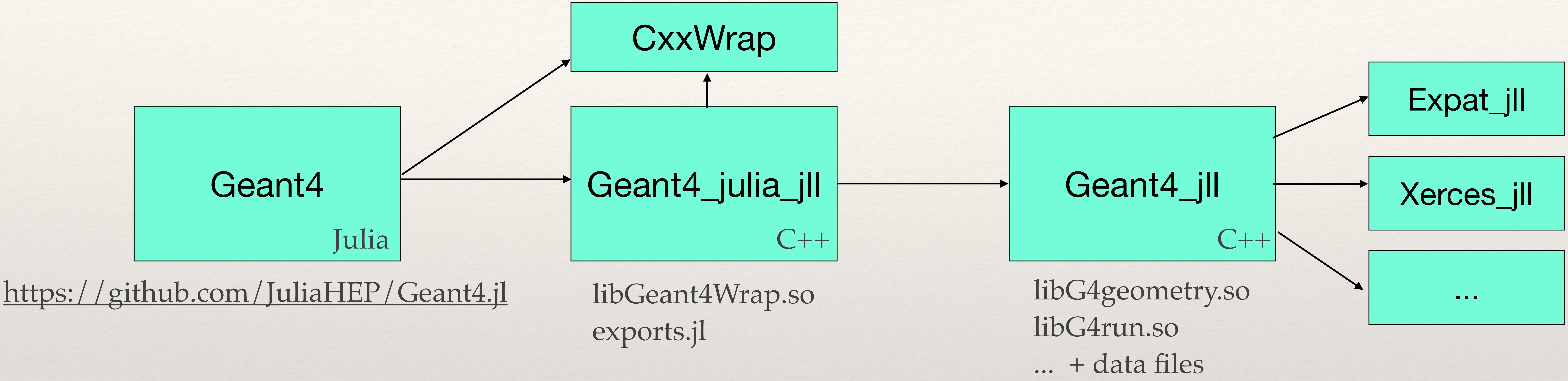
```
Generated wrapper statistics
 enums:               28
 classes/structs:     209
   templates:         0
   others:            209
 class methods:       2846
 field accessors:     19 getters and 19 setters
 global variable accessors: 10 getters and 0 setters
 global functions: 53
```

Basic Interface

- The interaction to Geant4 from Julia needs to be adapted to the native Julia language
  - E.g., only structs, no real inheritance, no class methods
- Since all classes start with ‘G4’ we can `export` all types when issuing `using Geant4`
  - This is very good, no clashes
- Sometimes native Julia types are not obtained directly and require some extra step
  - e.g. G4String

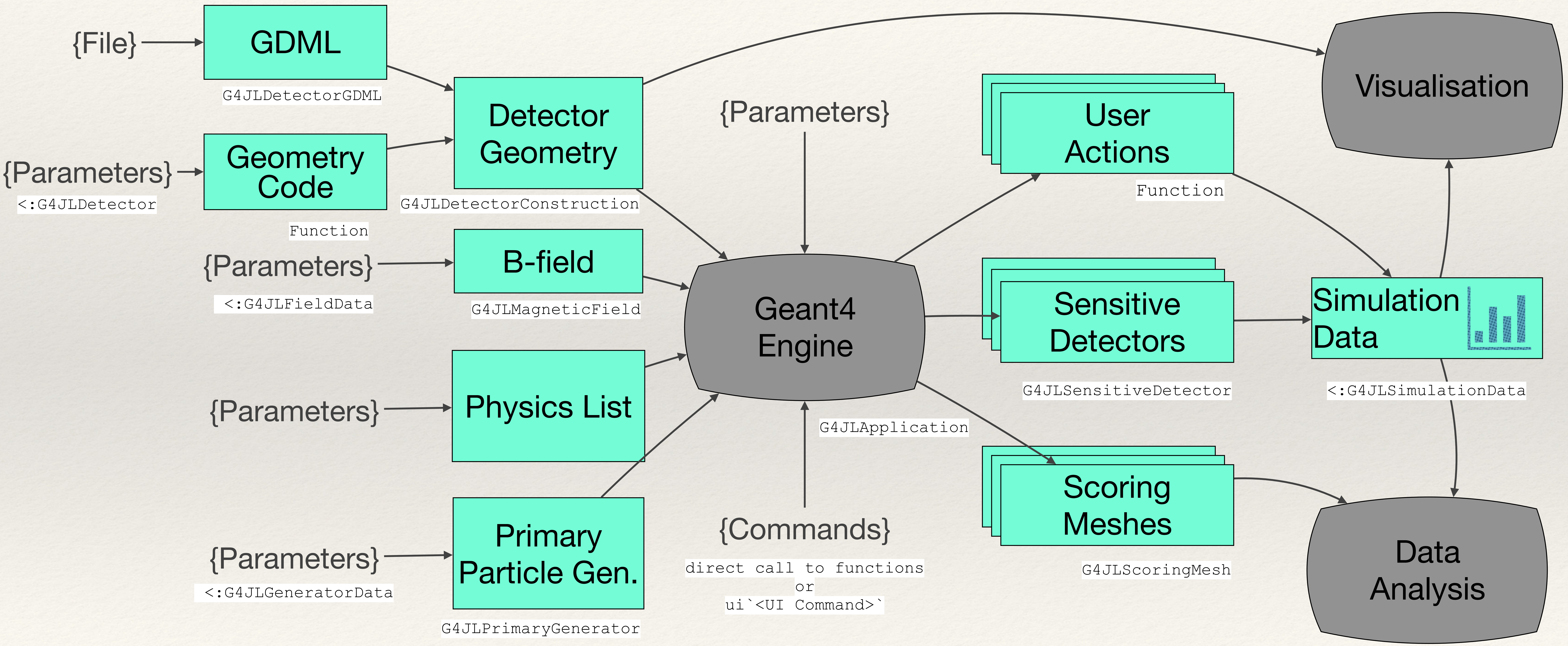
```
julia> using Geant4
julia> runManager = G4RunManager()
**************************************************************
 Geant4 version Name: geant4-11-01-patch-01 [MT]   (10-February-2023)
                      Copyright : Geant4 Collaboration
                     References : NIM A 506 (2003), 250-303
                                : IEEE-TNS 53 (2006), 270-278
                                : NIM A 835 (2016), 186-225
                            WWW : http://geant4.org/
**************************************************************

Geant4.G4RunManagerAllocated(Ptr{Nothing} @0x00007f9fcb6f9c50)

julia> methodswith(G4RunManager, supertypes=true)
[1] convert(t::Type{G4RunManager}, x::T) where T<:G4RunManager in Geant4 at ...
[2] AbortEvent(arg1::Union{CxxWrap.CxxWrapCore.CxxRef{<:G4RunManager},
...
[94] rndmSaveThisRun(arg1::Union{CxxWrap.CxxWrapCore.CxxRef{<:G4RunManager}, ...

julia> v = GetVersionString(runManager)
ConstCxxRef{G4String}(Ptr{G4String} @0x00007ffed34df2d8)

julia> String(v)
" Geant4 version Name: geant4-11-01-patch-01 [MT]   (10-February-2023)"
```

Package Structure



- The package **Geant4.jl is a pure Julia package** (platform independent)
- The binary libraries (platform dependent) for Geant4 and the wrapper library are downloadable artifacts of Julia **_jll packages** produced by the **BinaryBuilder** package, and stored at the Julia infrastructure (GitHub)

Rethinking the Application Interface



Application Interface: Wish List

- The idea is to exploit the Julia language to provide a simple and ergonomic user interface
  - **Minimalistic**. Define only what you really need for the simulation application. Avoid any boilerplate code.
  - **Do the necessary at the right time**. Hide the application state and calling sequence
  - **Interactive**. Using the Julia REPL, as well as support for Jupyter and Pluto notebooks
  - **Transparent MT**. As much as possible hide behind the scenes, the handling of Multi-Threading (e.g. per-thread calls and thread-local instances)
  - **Integrated simulation and analysis**. In the same application the simulation data can be analyzed and presented

Detector Geometry

- Main detector parameters encapsulated in a user `struct` inheriting from `G4JLDetector`
- A user defined Julia function will be called at the right moment to construct the geometry, receiving the detector parameters
  - For the time being the same API
  - Object ownership is delicate and in most cases hidden

{Parameters}

```
mutable struct TestEm3Detector <: G4JLDetector
    # main input parameters
    const fNbOfAbsor::Int64
    const fNbOfLayers::Int64
    const fCalorSizeYZ::Float64
    const fAbsorThickness::Vector{Float64}

    # mutable (computed) detector data
    fLayerThickness::Float64
    fCalorThickness::Float64
    fWorldSizeYZ::Float64
    fWorldSizeX::Float64
    ...
    function TestEm3Detector(;nbOfLayers = 50,
                              calorSizeYZ = 40cm,
                              absorThickness = [2.3mm, 5.7mm],
                              absorMaterial = ["G4_Pb", "G4_lAr"])
        self = new(length(absorThickness), nbOfLayers, calorSizeYZ, absorThickness)
        ...
    end
end
```

{Construct Function}

```
function TestEm3Construct(det::TestEm3Detector)

    (; fNbOfAbsor, fNbOfLayers, fCalorSizeYZ, fAbsorThickness, fLayerThickness,
       fCalorThickness, fWorldSizeYZ, fWorldSizeX, fWorldMaterial) = det

    println("Building Geometry now!!!")

    #---World-----------------------------------------------------------------
    det.fSolidWorld = G4Box("World", fWorldSizeX/2,fWorldSizeYZ/2,fWorldSizeYZ/2)
    det.fLogicWorld = G4LogicalVolume(det.fSolidWorld, fWorldMaterial, "World")
    det.fPhysiWorld = G4PVPlacement(nothing,              # no rotation
                                    G4ThreeVector(),      # at (0,0,0)
                                    det.fLogicWorld,      # its fLogical volume
                                    "World",              # its name
                                    nothing,              # its mother  volume
                                    false,                # no boolean operation
                                    0)                    #copy number
    ...
end

Geant4.getConstructor(::TestEm3Detector)::Function = TestEm3Construct
```

Magnetic Field

- The user provides a data struct inheriting from `G4JLFieldData` and the function `getfield(...)`
- Also can use pre-defined fields such as `G4JLUniformMagField`

{Parameters}

```
mutable struct CustomFieldData <: G4JLFieldData
    field::G4ThreeVector
end
```

{Function}

```
function CustomField{CustomFieldData}(field::G4ThreeVector)

    data = CustomFieldData(field)

    function getfield!(field::G4ThreeVector, pos::G4ThreeVector,
                       data::CustomFieldData)::Nothing
        assign(field, data.field)
        return
    end

    G4JLMagneticField("Uniform", data; getfield_method=getfield!)
end
```

Primary Particle Generator

- The user can use the predefined `G4JLGunGenerator` generator, or define his/her own generator by defining a `struct` for the parameters and two functions: `init` and `generate` that will be called at the adequate moment
- Implicit multiple instances will be created in case on MT

```
# Predefined Particle Gun-----------------------------------------------------------
particlegun = G4JLGunGenerator(particle = "e-",
                               energy = 1GeV,
                               direction = G4ThreeVector(1,0,0),
                               position = G4ThreeVector(0,0,0))
```

{Parameters}

```
mutable struct MedicalBeamData <: G4JLGeneratorData
  particleName::String
  particlePtr::CxxPtr{G4ParticleDefinition}
  energy::Float64
  ssd::Float64
  fieldXY::Float64
  surfaceZ::Float64
end
```

{Functions}

```
function MedicalBeam(;particle="e-", energy=10MeV, ssd=100cm, fieldXY=10cm)
  data = MedicalBeamData(particle, CxxPtr{G4ParticleDefinition}(C_NULL),
                         energy, ssd, fieldXY, 0.)

  function init(data::MedicalBeamData, app::G4JLApplication)
    data.particlePtr = FindParticle(data.particleName)
    data.surfaceZ = -app.detector.phantomZ/2
  end

  function generate( evt::CxxPtr{G4Event}, data::MedicalBeamData)::Nothing
    mass = data.particlePtr |> GetPDGMass
    momemtum = √((mass + data.energy)^2 - mass^2)
    pvec = momemtum * generateBeamDir(data.ssd, data.fieldXY);
    primary = G4PrimaryParticle(data.particlePtr, pvec |> x, pvec |> y, pvec |> z )
    vertex = G4PrimaryVertex(G4ThreeVector(0, 0, data.surfaceZ - data.ssd), 0ns)
    SetPrimary(vertex, move!(primary))
    AddPrimaryVertex(evt, move!(vertex))
  end

  G4JLPrimaryGenerator("MedicalBeam", data; init_method=init,
                                            generate_method=generate)
end
```

Simulation Data

- With the ‘user actions’ and ‘sensitive detectors’ the user will collect all simulation data in a user defined struct inheriting from `G4JLSimulationData`
  - Typically it will consists of counters, histograms, temporary structs to be written event-by-event, etc.
- In case of MT, a function (`add!`) to reduce the contents of the data struct for each worker thread needs to be provided by the user

```
#---Simulation Data struct------------------------------------------------------
mutable struct TestEm3SimData <: G4JLSimulationData
    #---Run data----------------------------------------------------------------
    fParticle::CxxPtr{G4ParticleDefinition}
    fEkin::Float64

    fChargedStep::Int32
    fNeutralStep::Int32

    fN_gamma::Int32
    fN_elec::Int32
    fN_pos::Int32

    fEnergyDeposit::Vector{Float64}     # Energy deposit per event
    fTrackLengthCh::Vector{Float64}     # Track length per event

    fEdepEventHistos::Vector{Hist1D}
    fTrackLengthChHistos::Vector{Hist1D}
    fEdepHistos::Vector{Hist1D}
    fAbsorLabel::Vector{String}

    TestEm3SimData() = new()
end

#---add function---------------------------------------------------------------
function add!(x::TestEm3SimData, y::TestEm3SimData)
    x.fChargedStep += y.fChargedStep
    x.fNeutralStep += y.fNeutralStep
    x.fN_gamma += y.fN_gamma
    x.fN_elec += y.fN_elec
    x.fN_pos += y.fN_pos
    x.fEdepEventHistos += y.fEdepEventHistos
    x.fTrackLengthChHistos += y.fTrackLengthChHistos
    x.fEdepHistos += y.fEdepHistos
end
```

counters

array of histograms

User Actions

- **User actions** are native Julia functions (called by C++)
- In addition to the G4 standard arguments they get a reference to the `G4JLApplication` to get all simulation context (no globals!)
- All worker threads are calling the same user action functions (user needs to prevent data racing)

```
#---Begin Event Action-----------------------------------------------------------
function beginevent(evt::G4Event, app::G4JLApplication)::Nothing
    data = getSIMdata(app)
    fill!(data.fEnergyDeposit, 0.0)
    fill!(data.fTrackLengthCh, 0.0)
    return
end
```

its own thread local copy of the simulation data

```
#---Stepping action--------------------------------------------------------------
function stepaction(step::G4Step, app::G4JLApplication)::Nothing
    detector = app.detector
    data = getSIMdata(app)
    prepoint = GetPreStepPoint(step)
    track = GetTrack(step)

    # Return if step in not in the world volume
    prepoint |> GetPhysicalVolume |> GetLogicalVolume |> GetMaterial
             == detector.fWorldMaterial && return nothing

    particle = GetDefinition(track)
    charge  = GetPDGCharge(particle)
    stepl = 0.
    if charge != 0.
        stepl = GetStepLength(step)
        data.fChargedStep += 1
    else
        data.fNeutralStep += 1
    end
    edep = GetTotalEnergyDeposit(step) * GetWeight(track)
    absorNum  = GetCopyNumber(GetTouchable(prepoint), 0)
    layerNum  = GetCopyNumber(GetTouchable(prepoint), 1) + 1

    data.fEnergyDeposit[absorNum] += edep
    data.fTrackLengthCh[absorNum] += stepl

    push!(data.fEdepHistos[absorNum], layerNum, edep)
    return
end
```

its own thread local copy of the simulation data

Sensitive Detectors

- A **sensitive detector** is defined with a custom user `struct` to collect hit information and three user functions (`initialize`, `endOfEvent` and `processHits`)
- Functions receive its own worker thread copy of the data
- Associations to the corresponding G4LogicalVolume are declared at instantiation of `G4JLApplication`

```
#---Define Tracker Hit-----
struct TrackerHit
  trackID::Int32
  chamberNb::Int32
  edep::Float64
  pos::Point3{Float64}
end
```

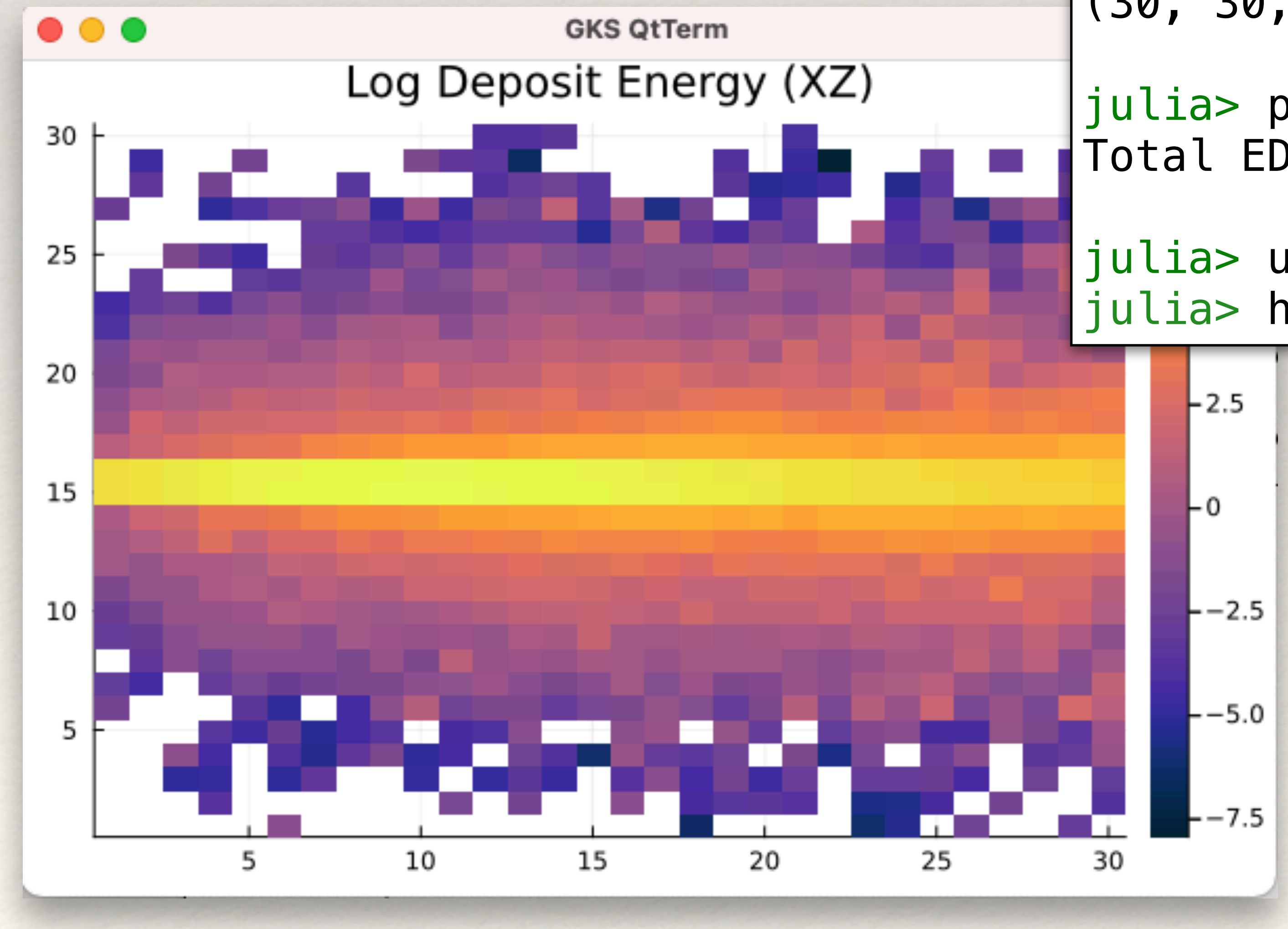
```
#--------------------------------------------------------------------------------
#---Define Sensitive Detector----------------------------------------------------
#--------------------------------------------------------------------------------
#---SD collected data------------------------------------------------------------
struct B2aSDData <: G4JLSDData
  trackerHits::Vector{TrackerHit}
  B2aSDData() = new([])
end

#---Initialize method------------------------------------------------------------
function _initialize(data::B2aSDData, ::G4HCofThisEvent)::Nothing
  empty!(data.trackerHits)
  return
end

#---End of Event method----------------------------------------------------------
function _endOfEvent(data::B2aSDData, ::G4HCofThisEvent)::Nothing
  # write the event hits to permanent storage
  return
end

#---Process Hit method-----------------------------------------------------------
function _processHits(data::B2aSDData, step::G4Step, ::G4TouchableHistory)::Bool
  edep = step |> GetTotalEnergyDeposit
  edep <  0. && return false
  pos = step |> GetPostStepPoint |> GetPosition
  push!(data.trackerHits,
       TrackerHit(step |> GetTrack |> GetTrackID,
                  step |> GetPreStepPoint |> GetTouchable |> GetCopyNumber,
                  edep,
                  Point3{Float64}(x(pos),y(pos),z(pos))))
  return true
end

#---Create SD instance-----------------------------------------------------------
chamber_SD = G4JLSensitiveDetector("Chamber_SD", B2aSDData();
                                   processhits_method=_processHits,
                                   initialize_method=_initialize,
                                   endofevent_method=_endOfEvent)
```

Scoring Meshes

- Geant4 provides natively UI-based scoring functionality
  - After the run a CSV file can be generated
- Provided a callable interface with functionality to retrieve the results in an ergonomic manner (Julia-friendly)

```
#---Scoring Setup-------------------------------------------------------------------------
sc1 = G4JLScoringMesh(
    "boxMesh_1",
    BoxMesh(1m,1m,1m),
    bins = (30, 30, 30),
    quantities = [energyDeposit("eDep")
                  nOfStep("nOfStepGamma", filters=[ParticleFilter("gammafilter", "gamma")])
                  nOfStep("nOfStepEMinus", filters=[ParticleFilter("eMinusFilter", "e-")])
                  nOfStep("nOfStepEPlus", filters=[ParticleFilter("ePlusFilter", "e+")])
                 ])
```

```
julia> totalE, totalE2, nEvents = sc1.eDep

julia> typeof(totalE)
Array{Float64, 3}

julia> size(totalE)
(30, 30, 30)

julia> println("Total EDep = $(sum(totalE))")
Total EDep = 859664.8367498876

julia> using Plots
julia> heatmap(log.(totalE[16,:,:]), title="Log Deposit Energy (XZ)", color=:thermal)
```



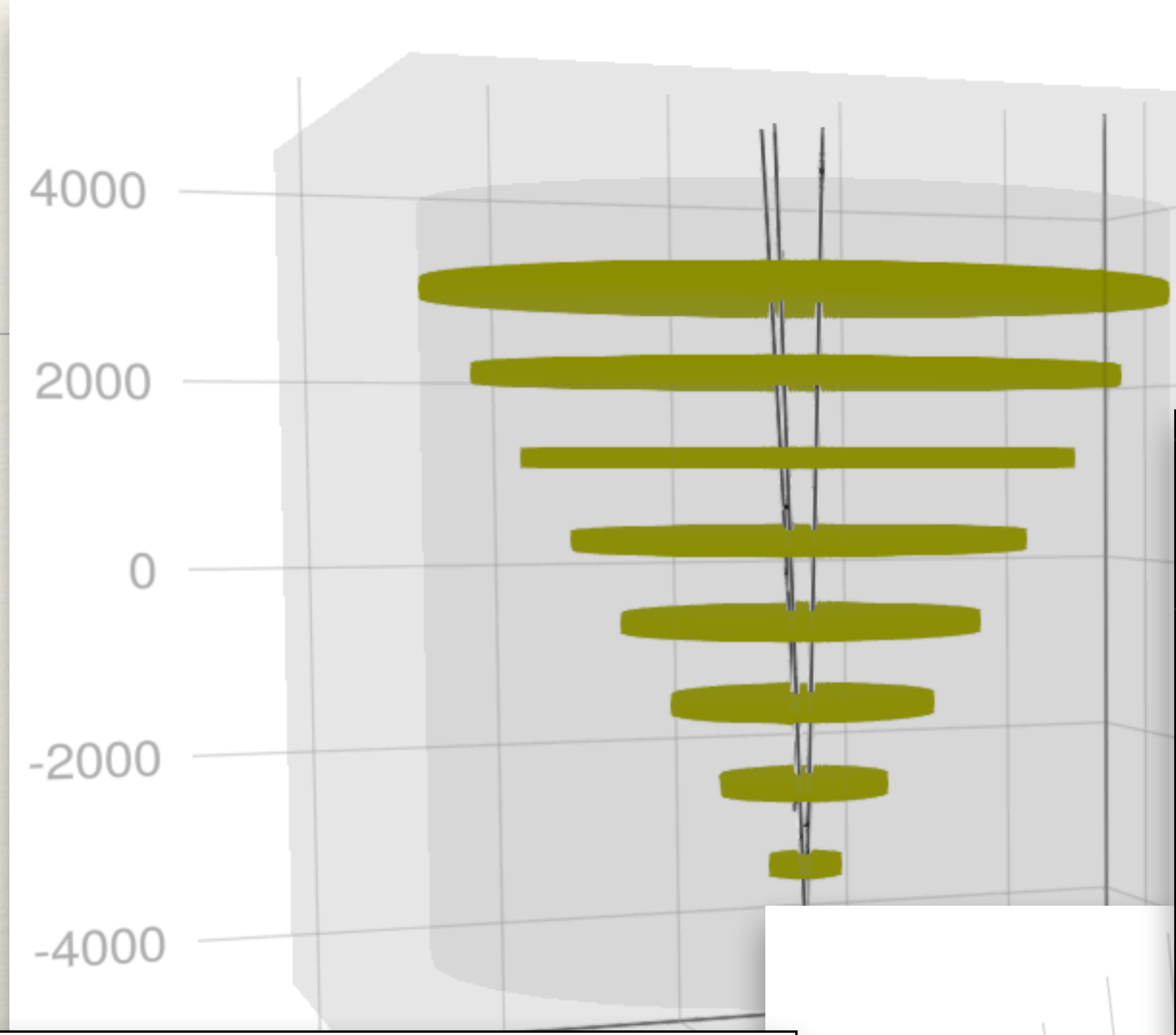
Simulation Application

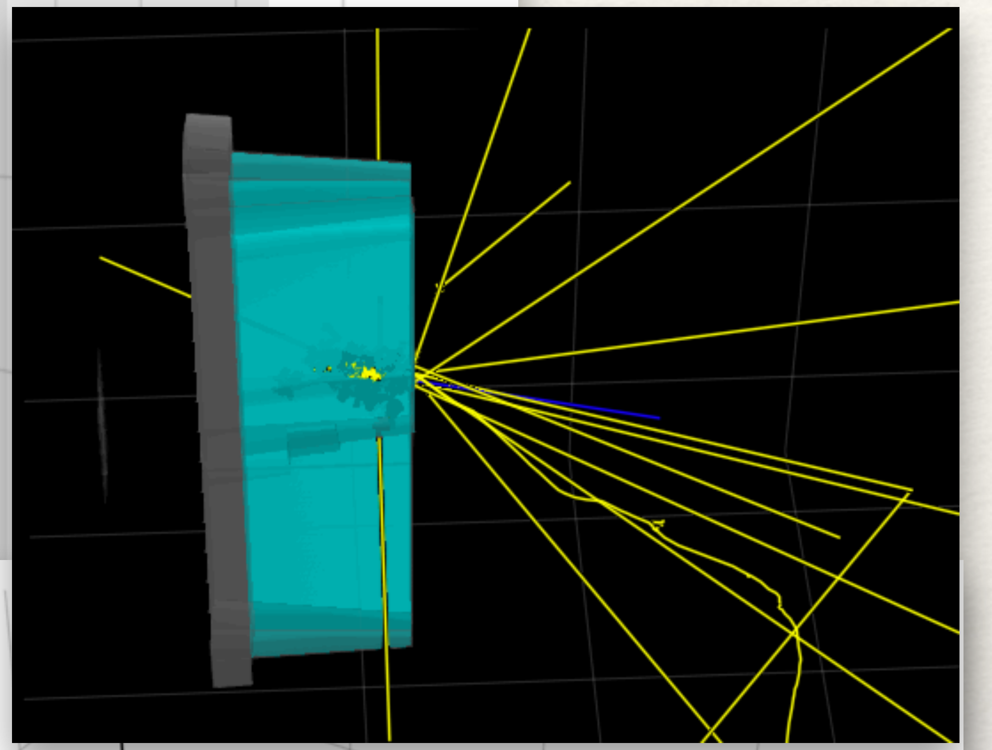
- Finally, the user can create a `G4JLApplication` with all the elements of the simulation application (detector geometry, primary generator, physics list, user actions, etc.)
- Geant4 requires a strict order of instantiation/configuration/initialization and this is guaranteed by Geant4.jl interface
- In case `nthreads` > 0 (default) the `G4MTRunManager` is instantiated and simulation data as well as sensitive detector data is replicated N times

```
#---Create the Application-------------------------------------------------------------------------------------
app = G4JLApplication(;detector = B2aDetector(nChambers=5),         # detector with parameters
                       physics_type = FTFP_BERT,                     # what physics list to instantiate
                       generator = G4JLParticleGun(...),             # primary particles generator
                       nthreads = 8,                                 # number of worker threads (>0 == MT)
                       endeventaction_method = endeventaction,       # end event action
                       sdetectors = ["Chamber_LV+" => chamber_SD]    # mapping of LVs to SDs (+ means multiple LVs)
                      )

#---Configure, Initialize and Run------------------------------------------------------------------------------
configure(app)
initialize(app)
beamOn(app, 1000)
```

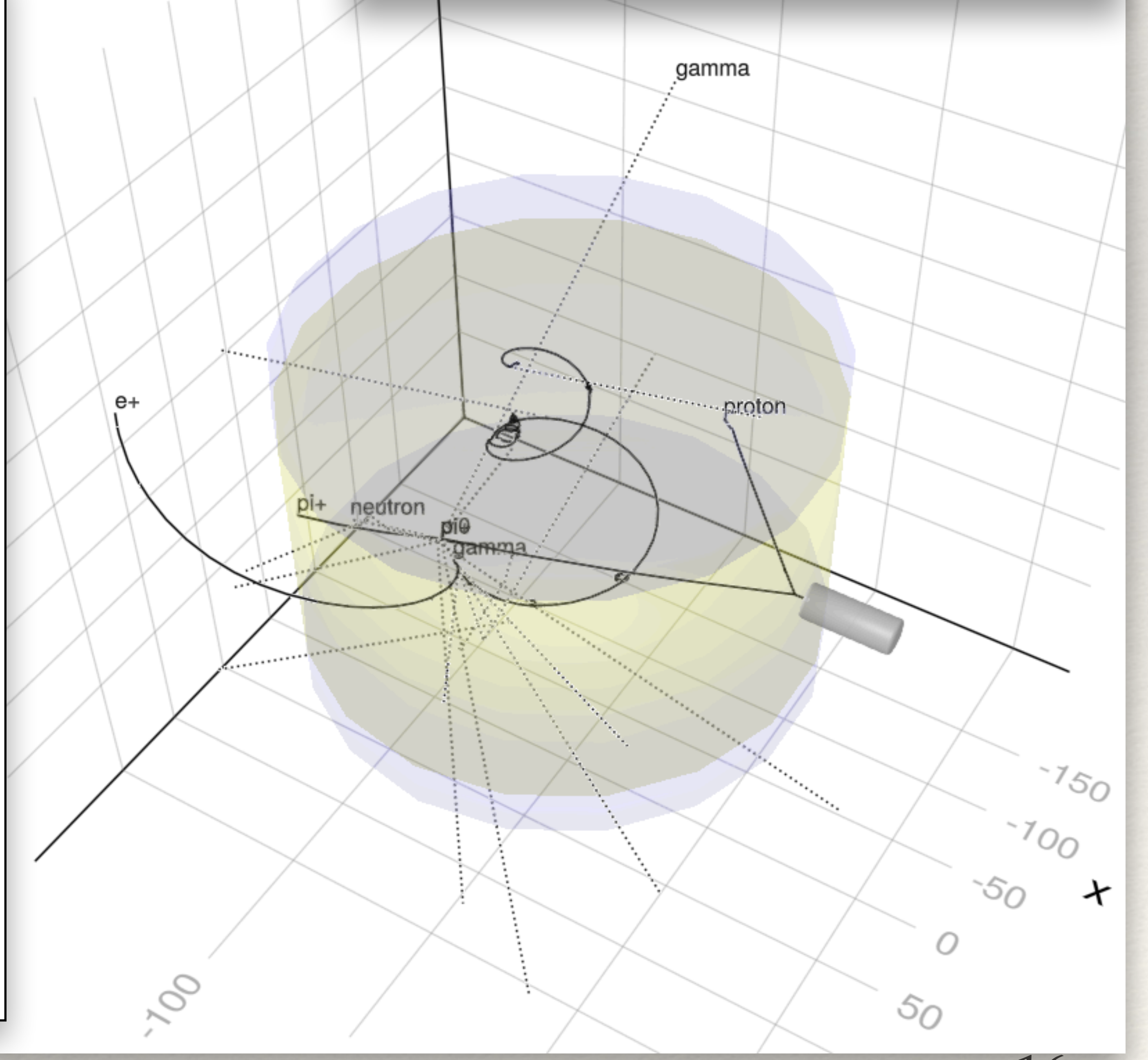
G4Visualization

- Implemented basic visualisation of the geometry using Makie.jl package
  - including boolean solids
- Also tested some trivial tracking visualisation
  - collected points (vector of points) in the stepping action





```julia
using Geant4
using G4Visualization
using GLMakie

include("../../examples/basic/B2/B2a.jl")
world = GetWorldVolume()
draw(world)

tracks = app.simdata.tracks
empty!(tracks)

beamOn(app, 1)

for t in tracks
    lines!(t)
end
```



Using GDML geometries

- Implemented special detector type, G4JLDetectorGDML, to define the detector geometry getting the GDML file name in the constructor
- The rest of the application is identical

```
#---Create the Application------------------------------------------------------------------------
app = G4JLApplication(detector = G4JLDetectorGDML("$(@__DIR__)/TestEm3.gdml"),  # detector defined with a GDML file
                      simdata = TestEm3SimData(),                      # simulation data structure
                      physics_type = FTFP_BERT,                        # what physics list to instantiate
                      generator = G4JLParticleGun(...),                # what primary generator to instantiate
                      #----Actions--------------------------------
                      stepaction_method = stepaction,                  # step action method
                      pretrackaction_method = pretrackaction,          # pre-tracking action
                      posttrackaction_method = posttrackaction,        # post-tracking action
                      beginrunaction_method=beginrun,                  # begin-run action (initialize counters and histograms)
                      endrunaction_method=endrun,                      # end-run action (print summary)
                      begineventaction_method=beginevent,              # begin-event action (initialize per-event data)
                      endeventaction_method=endevent                   # end-event action (fill histogram per event data)
                      )
```

TestEm3 example

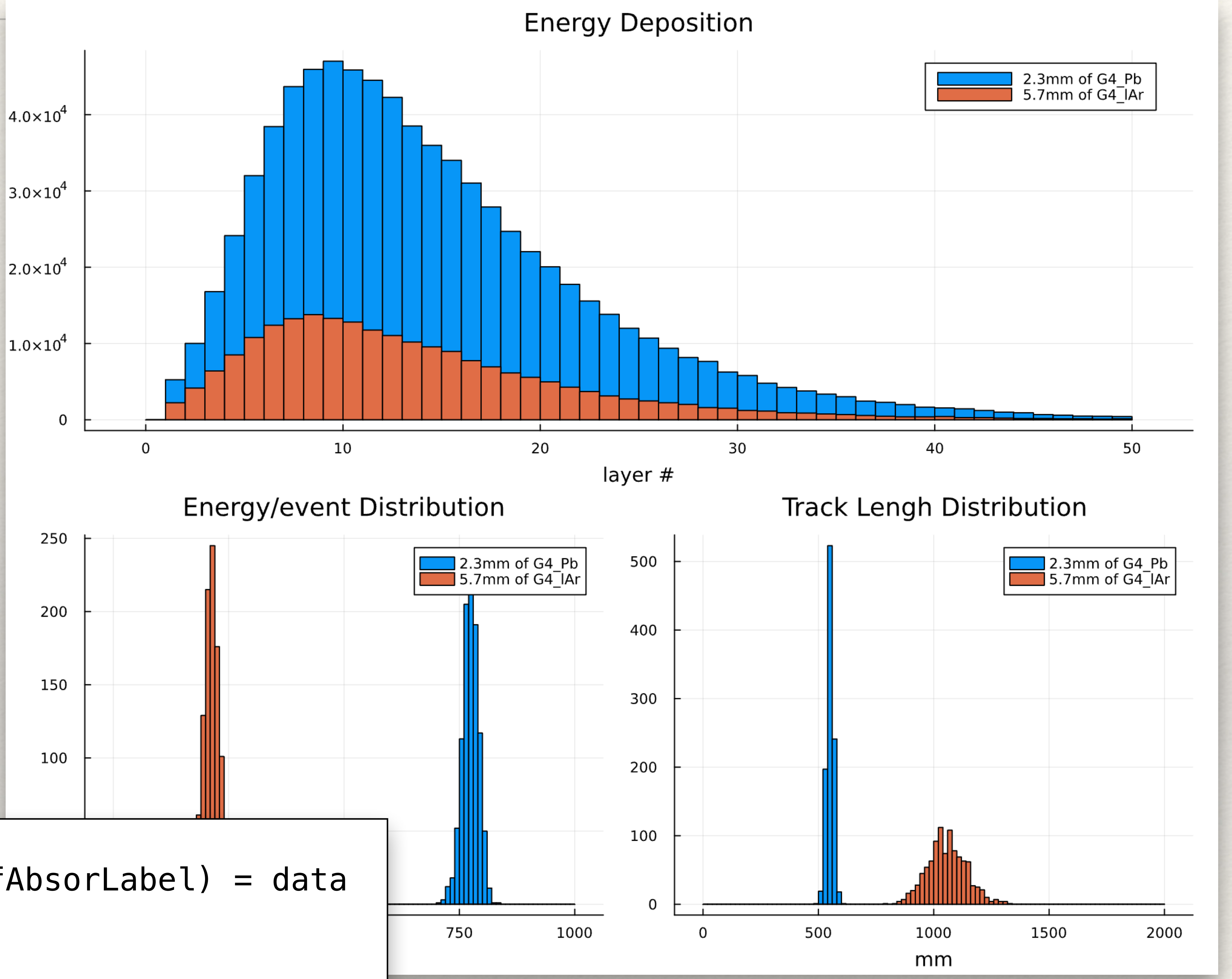
- This example works with user actions only (step, event, run, track)
  - simplified from the original
- Using histograms from FHist.jl

```
mutable struct TestEm3SimData <: G4JLSimulationData
  fParticle::CxxPtr{G4ParticleDefinition}
  fEkin::Float64

  fChargedStep::Int32
  fNeutralStep::Int32
  fN_gamma::Int32

  fN_elec::Int32
  fN_pos::Int32

  fEnergyDeposit::Vector{Float64}  # Energy deposit per evt
  fTrackLengthCh::Vector{Float64}  # Track length per evt

  fEdepEventHistos::Vector{Hist1D64}
  fTrackLengthChHistos::Vector{Hist1D64}
  fEdepHistos::Vector{Hist1D64}

  fAbsorLabel::Vector{String}
end
```

```
#---Create the Application-------------------------------------------------------------------
app = G4JLApplication(detector = TestEm3Detector(),             # detector with parameters
                      simdata = TestEm3SimData(),               # simulation data structure
                      nthreads = 8,                             # number of threads
                      physics_type = FTFP_BERT,                 # what physics list to instantiate
                      generator = G4JLGunGenerator(...),        # primary generator instance
                      #----Actions--------------------------------
                      stepaction_method = stepaction,           # step action method
                      pretrackaction_method = pretrackaction,   # pre-tracking action
                      posttrackaction_method = posttrackaction, # post-tracking action
                      beginrunaction_method = beginrun,         # begin-run action (initialise counters and histos)
                      endrunaction_method = endrun,             # end-run action (print summary)
                      begineventaction_method = beginevent,     # begin-event action (initialise per-event data)
                      endeventaction_method = endevent)         # end-event action (fill histogram per event data)
```

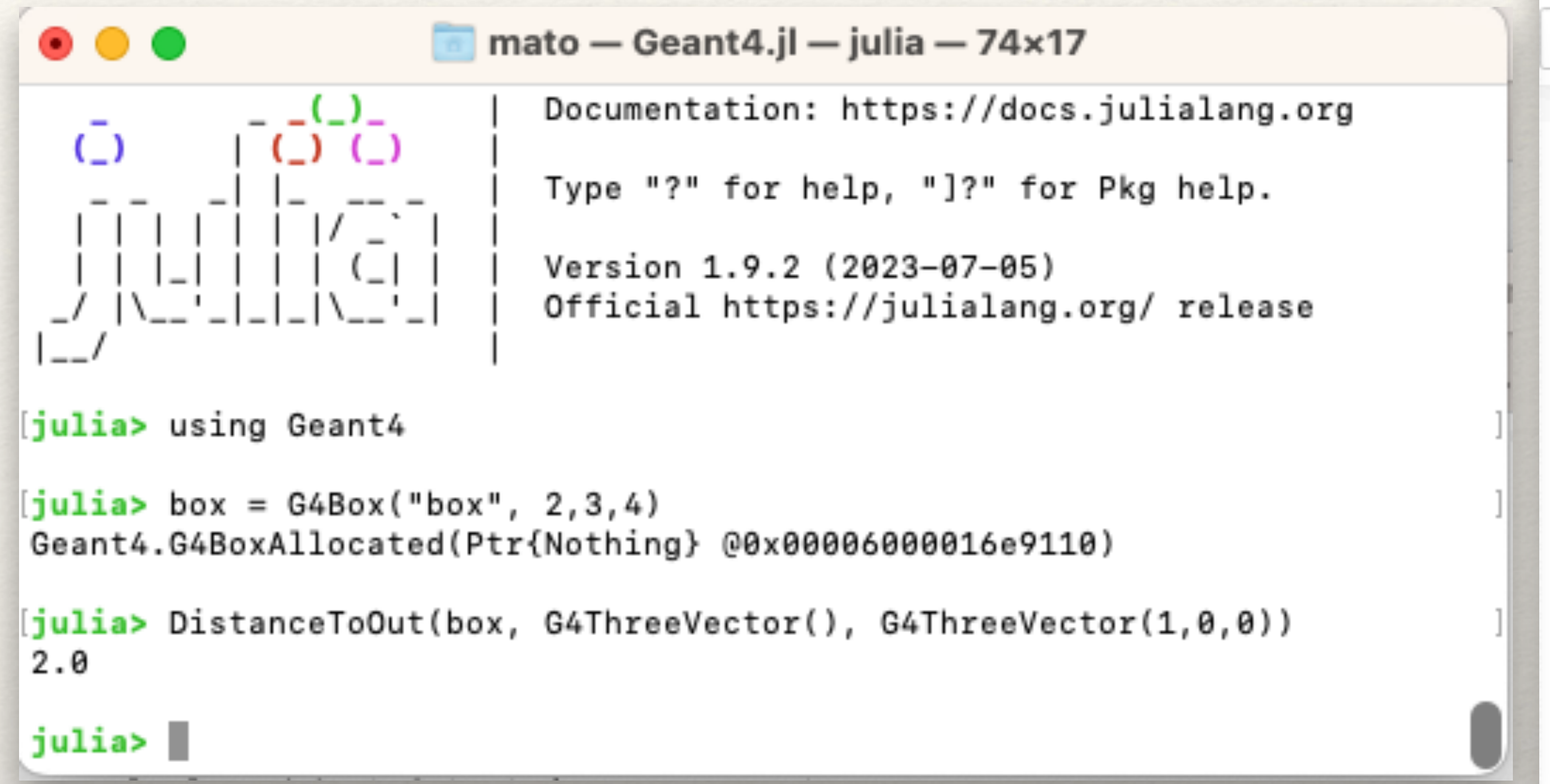
TestEm3 example - display results

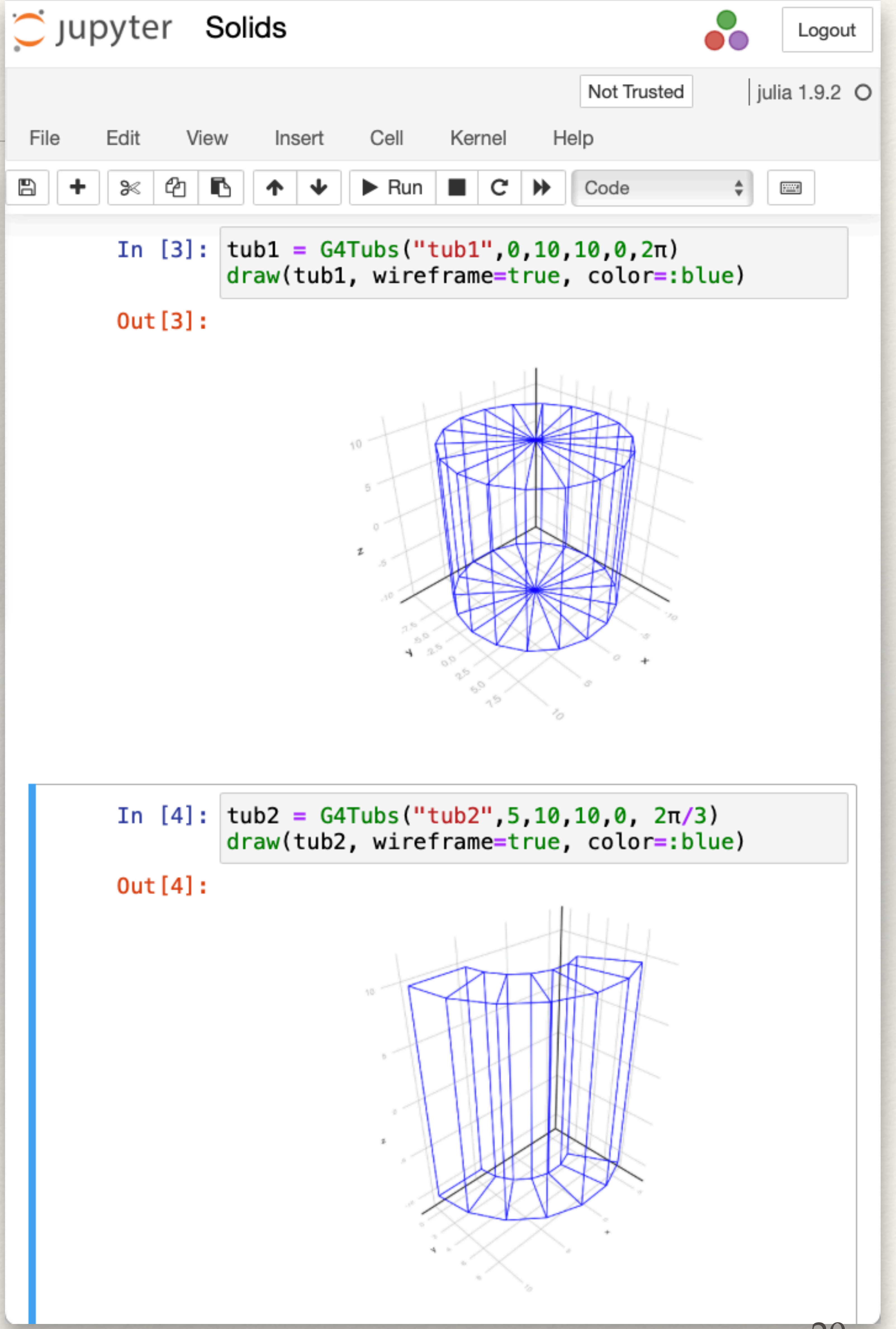
- After running the desired number of events, the simulation data structure can be passed a the plotting function or an analysis code
- Changes can be made interactively and a new run can be started
  - E.g. new detector with different parameters, new gun parameters, different callbacks, etc




```
function do_plot(data::TestEm3SimData)
    (;fEdepHistos, fEdepEventHistos, fTrackLengthChHistos, fAbsorLabel) = data
    lay = @layout [°; ° °]
    plot(layout=lay, show=true, size=(1400,1000))
    for (h, l) in zip(fEdepHistos, fAbsorLabel)
        plot!(subplot=1, h, title="Energy Deposition",
              xlabel="layer #", label=l, show=true)
    end
    ...
end
```

Interactivity





- Julia comes with a powerful and modern REPL (Read-Eval-Print Loop)
  - history, line completion, help, etc.
- Very good support for notebooks (Jupyter, Pluto)
  - see examples in Geant4.jl documentation
- Both are very well integrated in IDEs such as VS Code

Performance

- Performance should be equivalent to the C++ application
- Julia user actions (callbacks from C++ to Julia) do not add any significant overhead and can be executed very efficiently (JIT and with less abstraction layers)
- Julia suffers from a larger startup time (final type inference and JIT compilation)
  - big improvement since Julia version 1.9
- Perhaps the MT performance is not optimal, mainly due to enabling/disabling garbage collector (GC)

	B2a (C++)	B2a.jl
events = 1	0.9 s	6 s
events =100k	106 s	109 s
events =100k (MT)	23 s	27 s

- Simple benchmark of B2a example
  - with protons @ 3 GeV
  - running on a Mac-mini with the M1 processor (8 cores = 4 performance and 4 efficiency)
- C++ and Julia are basically identical taking the initial overhead (serial) into account

Adding more Complete and Realistic Examples

- The package Geant4.jl comes with a number of examples
  - basic/B1 (native interface) and B2a (sensitive detector)
  - extended/RE03 (scoring meshes)
  - TestEm3 (user actions with data analysis integration)
  - WaterPhantom (scoring meshes, special particle generator, ploting results)
  - HBC30 (bubble chamber with event display and online trigger)
  - Scintillator (optical photons and customised physics list)
- Recently added ATLTileCalTB.jl converting L. Pezzotti's C++ example to validate G4 with the ATLAS TileCal TB data
  - sensitive detector, actions, signal processing
  - ~3000 lines (C++) versus ~1000 lines (Julia)

Conclusions

- The package **CxxWrap** works nicely and scales relatively well
  - Callbacks from C++ to Julia are essential for Geant4 . Measured very small overhead
  - Did not find any limitation in the C++ interfaces used by G4 (*, const *, &, const &, …) modulo object ownership peculiarities of G4
- Julia **BinaryBuilder** is a powerful tool to streamline the installation and deployment of C++ projects and make it easier for users to get started with Julia-based applications
- **Geant4.jl** can be a very useful add-on to the Geant4 project
  - Tutorials (very easy to setup and portable), interactive development (notebooks), connection to other powerful packages in the Julia ecosystem (visualization, analysis, etc.)
- Geant4.jl is still in a **prototype state** with probably missing functionality but **very promising**
  - Exploiting the tooling of Julia ecosystem (CI, documentation, registration and deployment, etc.)

If you want to try…

1. Install Julia version > 1.9
   - just download the binary (`https://julialang.org/downloads`) and `untar` it
   - include in `PATH` the `julia-1.9.3/bin` directory
2. clone Geant4.jl for the examples
   - `git clone https://github.com/JuliaHEP/Geant4.jl.git`
   - `cd Geant4.jl`
3. install locally all the needed packages and dependencies by the examples
   - `julia --project=examples -e 'import Pkg; Pkg.instantiate()'`
4. run an example (e.g. TestEm3)
   - `julia --project=examples -i examples/TestEm3/TestEm3.jl`