Monte Carlo simulation in Geant4 for complex models on the Govorun supercomputer

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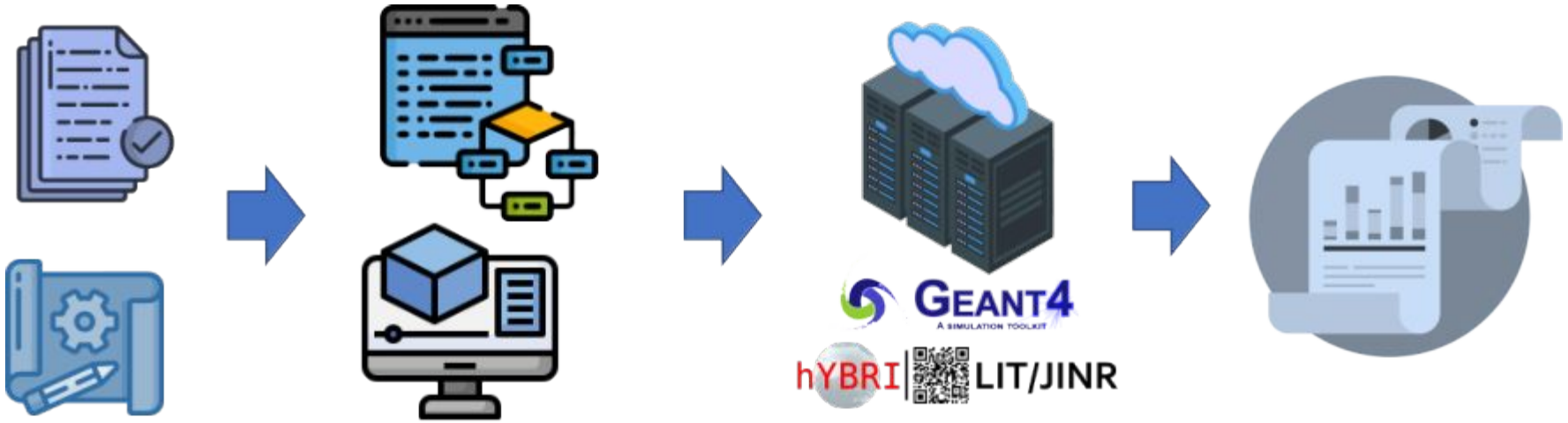
HybriLIT WORKSHOP 2025: Towards Efficient Scientific Computing (25-26.11.2025)

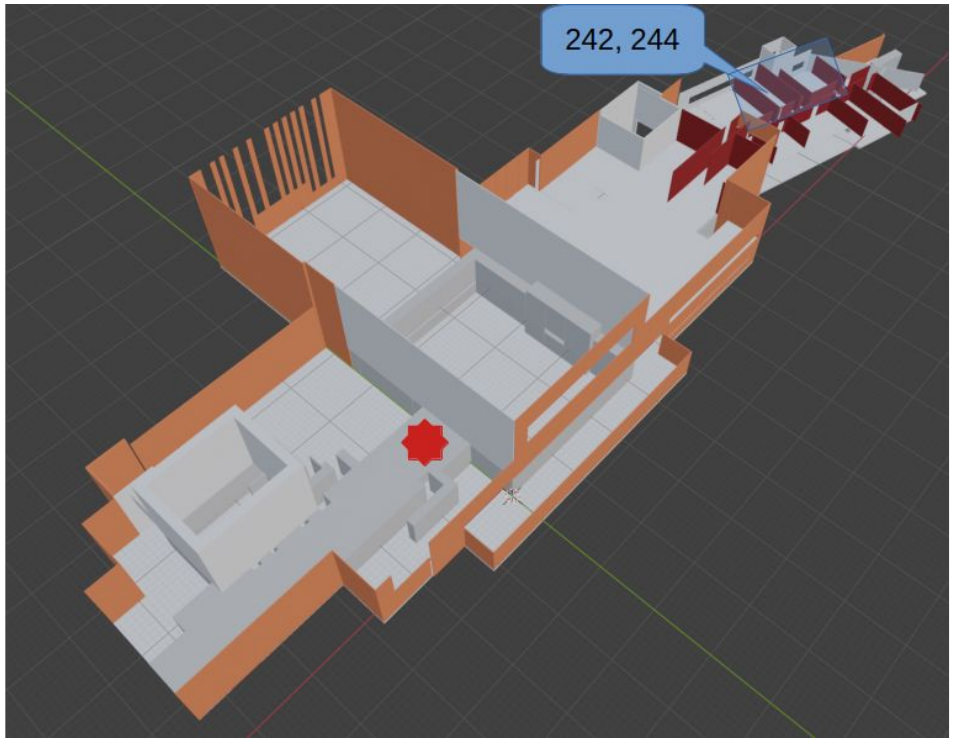
Task overview

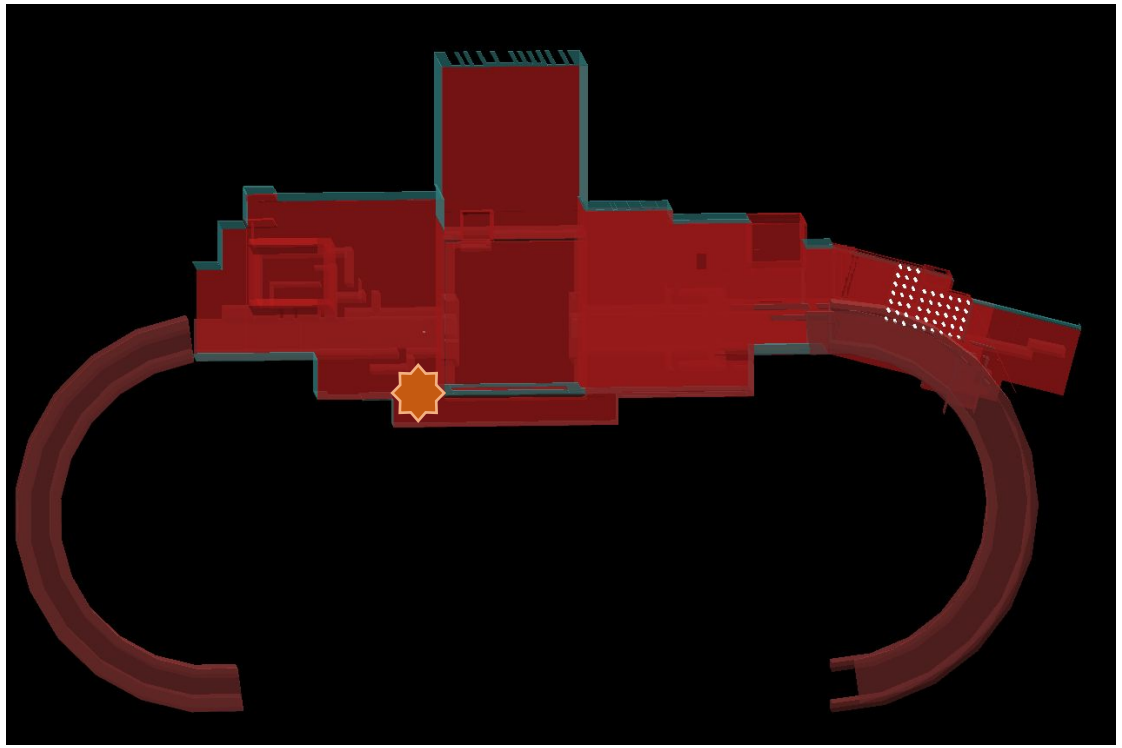
1. Obtain source data (maps, diagrams, materials) for constructing the geometry.
2. Construct the geometry in CAD systems.
3. Create a geometry converter from CAD to the Geant4 format.
4. Determine the main radiation sources and the radiation type.
5. Prepare the Geant4 code for supercomputer calculations.
6. Optimize the calculations.
5. Evaluate the spectra in the selected rooms.



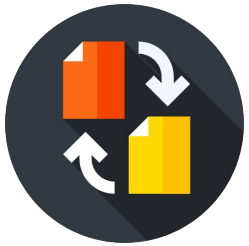
Main sources and detectors

calculation for one source: a collimator.



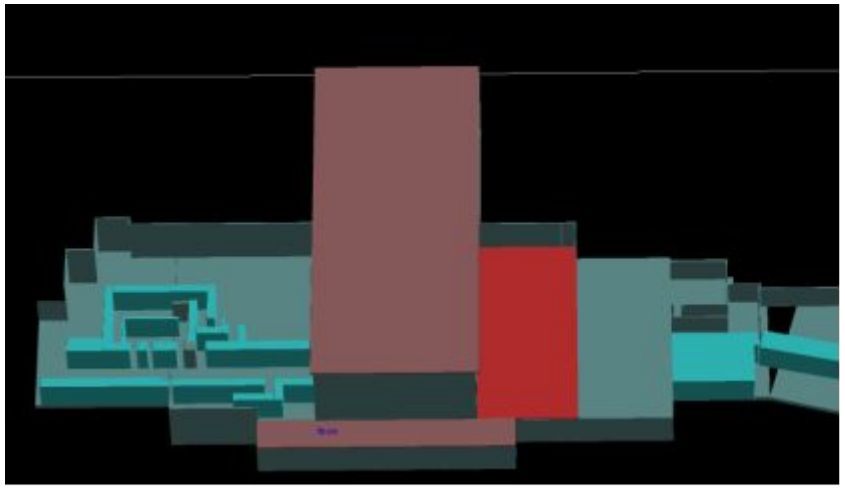


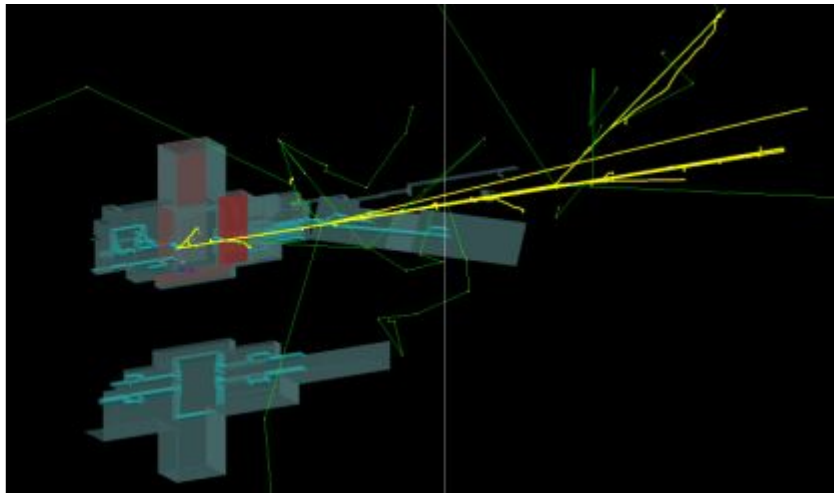
NICA model in Geant4, white dots indicates detectors in the Temporary control room.



Developed CAD to Geant4 converter for box geometry

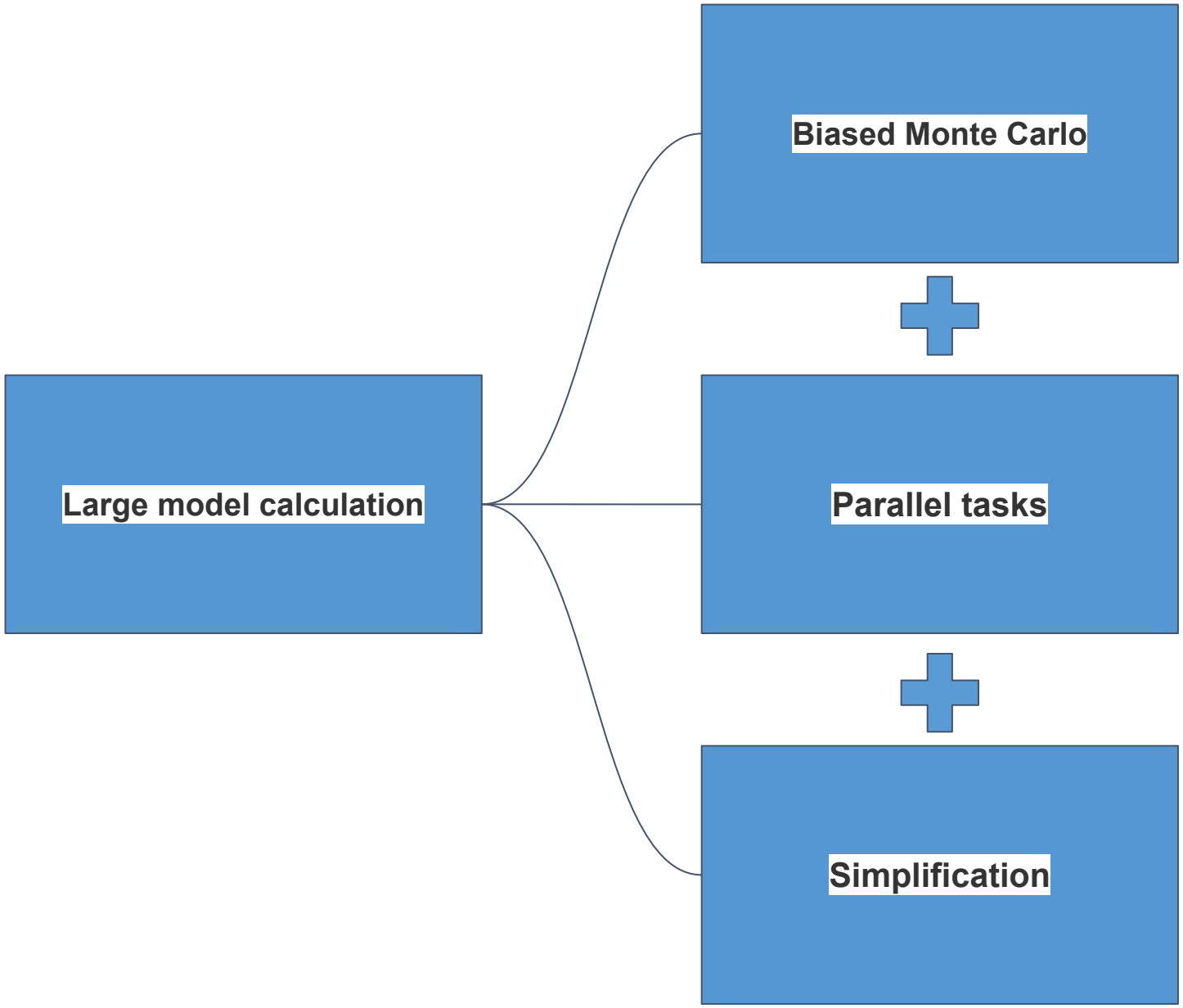
Geant4 GUI





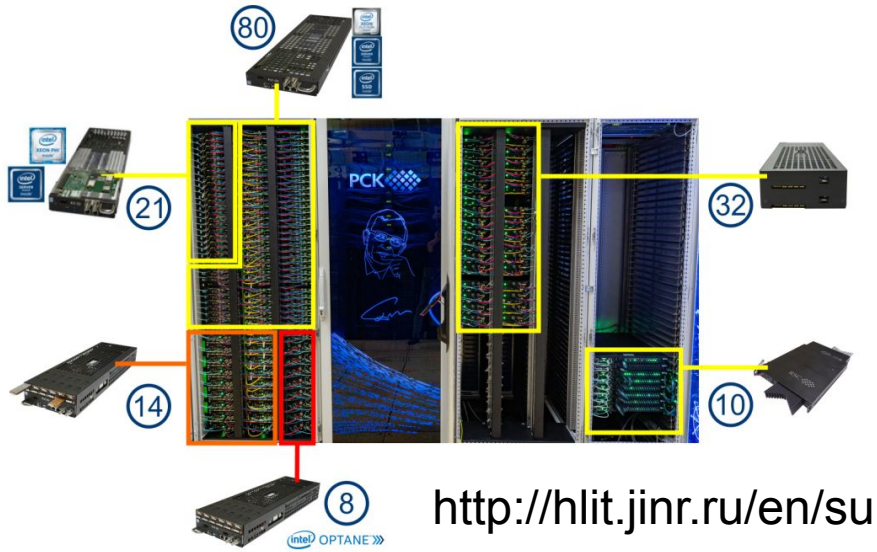
```
...
G4Box* plate = new G4Box("LeadPlate", 10*cm, 10*cm, 5*cm);
G4LogicalVolume* platelv =
new G4LogicalVolume(plate, Lead, "LeadPlate");
new G4PVPlacement(0, G4ThreeVector(0.,0.,0.),
platelv, "LeadPlate",
worldlv, false, 0, checkOverlaps);
G4double density = 2.700*g/cm3;
G4double a = 26.98*g/mole;
G4Material* Al = new G4Material(name="Aluminum",a, z=13.);
...
```

Task optimization



Calculations

- Calculations were done in the “Govorun” supercomputer of the Multifunctional information and computing complex, Mescheryakov Laboratory of Information Technologies (JINR).
- Calculations for large geometry required selection of the optimal number of CPUs (Intel(R) Xeon(R) Platinum 8268 CPU @ 2.90GHz) and allocated memory.
- Sofware version and physics list: Geant4 v.4-11.2.2, FTFP_BERT_HP.
- The Slurm Workload Manager was used to manage tasks.
- The spectrum calculation was done in two stages:
  1. A neutron spectrum was generated from a ion beam striking a steel-copper collimator, accounting for scattering from concrete walls. Time for calculations = 24 hours.
  2. A flat source with the spectrum obtained in the 1st stage, 6x12 m in size, normal directed to the TCR. Time for calculations = 180 hours.



http://hlit.jinr.ru/en/supercomputer_govorun_eng/

Preparation

You need to build the executive files.
You can run several independent calculations and then sum up the results.

```
mkdir build01
cd build01
cmake ..
make -j2
```

```
mkdir build02
cd build02
cmake ..
make -j2
```

<...>

SLURM

Access to “Govorun” is not available by default, ask for access (module add GVR/v1.0-1).
Example for *cascade* partition:

```
#!/bin/bash

#SBATCH -p cascade
#SBATCH -n 80                          # Number of CPU
#SBATCH --mem-per-cpu=28G              # memory
#SBATCH -t 30-00:00:0                  # days-hours

#SBATCH --mail-type=END                # Send email at job completion
#SBATCH --mail-user=kchizhov@jinr.ru   # Email address for notifications


module add CMake/v3.29.2
module add gcc/v11.2.0
module add openmpi/v4.1.1_gcc1120
module add GEANT4/v11.1.3_gcc1120-mt
module add ROOT/v6-18-00

./Geant4task ./run.mac
```

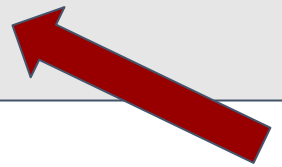
SLURM - Optimizing Memory Usage

If your program consumes a lot of memory, it's best to limit the number of tasks per node.

Parameters:

- **-n (--ntasks)** - total number of tasks
- **-N (--nodes)** - number of nodes
- **--tasks-per-node** - tasks per node
- **-c (--cpus-per-task)** - cores per task

```
/tmp/slurmd/job9203092/slurm_script: line 33: 266558 Killed                ./ddxTask ./run-new.mac

slurmstepd: error: Detected 1 oom-kill event(s) in step 9203092.batch cgroup. Some of your processes may have been killed by the cgroup out-of-memory handler.
```



Geant4 main.cc

```
NumberOfThreads = 2 * NumberOfCores
```

```
#ifdef G4MULTITHREADED
#include "G4MTRunManager.hh"
#else
#include "G4RunManager.hh"
#endif


int main(int argc, char **argv) {

#ifdef G4MULTITHREADED
 G4int nThreads = 160;
 runManager->SetNumberOfThreads(nThreads);
#else
 G4RunManager * runManager =new G4RunManager;
#endif
}


#ifdef G4MULTITHREADED
 G4MTRunManager * runManager = new G4MTRunManager;
 runManager->SetNumberOfThreads(G4Threading::G4GetNumberOfCores()/2);
#else
 G4RunManager * runManager =new G4RunManager;
#endif
  G4cout << " Number of CPU used: " << G4Threading::G4GetNumberOfCores();
```

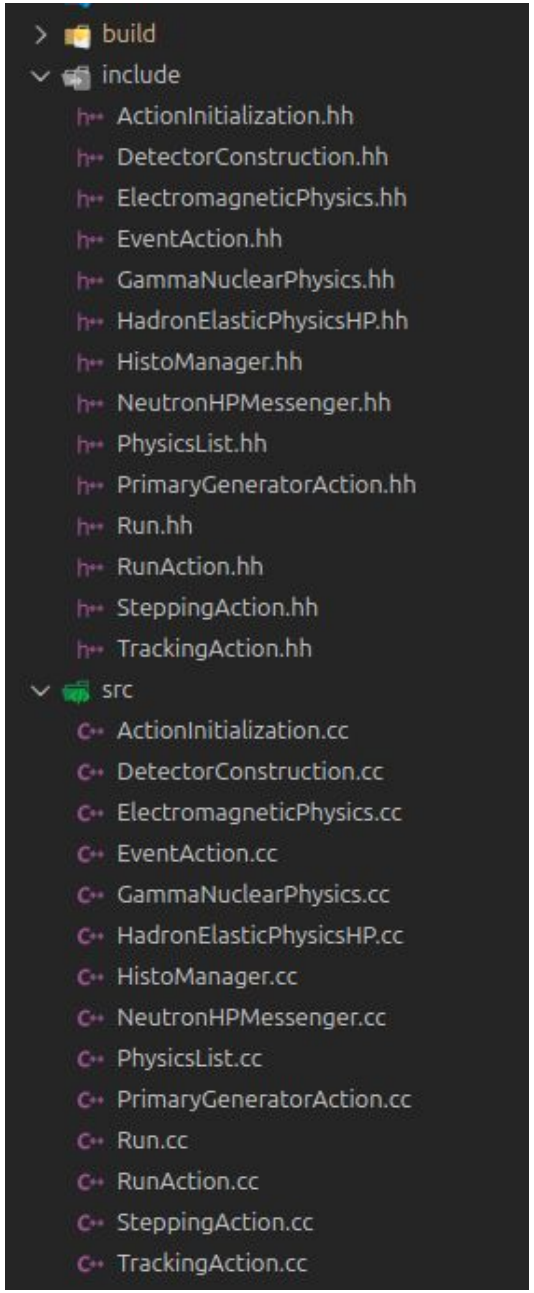
#SBATCH -n 80

indicates the number of processes (MPI tasks), not threads

run.mac

use “./” If you use a separate file with initial spectrum

```
/run/initialize

/control/verbose 1
/run/verbose 1
/process/list

/gps/verbose 0

/gps/particle neutron

#enegy spectrum after the wall of collimator with reflection of orther walls

/gps/ene/type Arb
/gps/hist/file ./Energyspectrum.dat
/gps/hist/inter Log

<...>

/run/printProgress 10000
/run/beamOn 100000000 #1E8
```



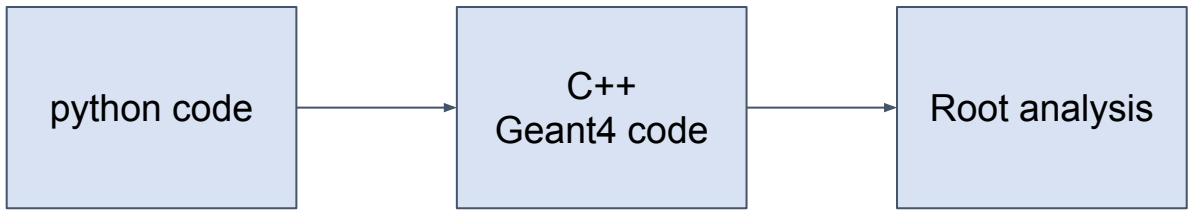
Commands for terminal

- module avail - check available modules
- sinfo - view information about Slurm nodes and partitions.
- sbatch **script.sh**
- squeue - view information about jobs located in the Slurm scheduling queue
- scancel <jobid> - kill the task

Batch script: Automatization for several tasks

```
for (( i=1; i <= 6; i++ ))
do
    source .venv/bin/activate
    python3 gpsmaker.py &
    deactivate

    if [ -d "build" ]
    then
        rm -r build
    fi
    mkdir build
    cd build
    cmake ..
    make -j2

    # Run for different particles and energies:
    sbatch ../slurmcalc.sh --wait
    until [ -f result3RS_n.ascii ]
    do
            sleep 5
    done

    cp "result3RS_n.ascii" "../result3RS/Result_n_"$i".ascii"
    echo "file copied - result3RS_n.ascii"
    cd ..
done
```

example:

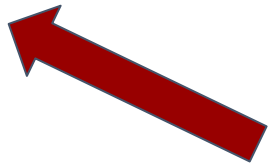


SLURM output

n01p001
Architecture: x86_64
CPU op-mode(s): 32-bit, 64-bit
Byte Order: Little Endian
CPU(s): 288
On-line CPU(s) list: 0-287
Thread(s) per core: 4

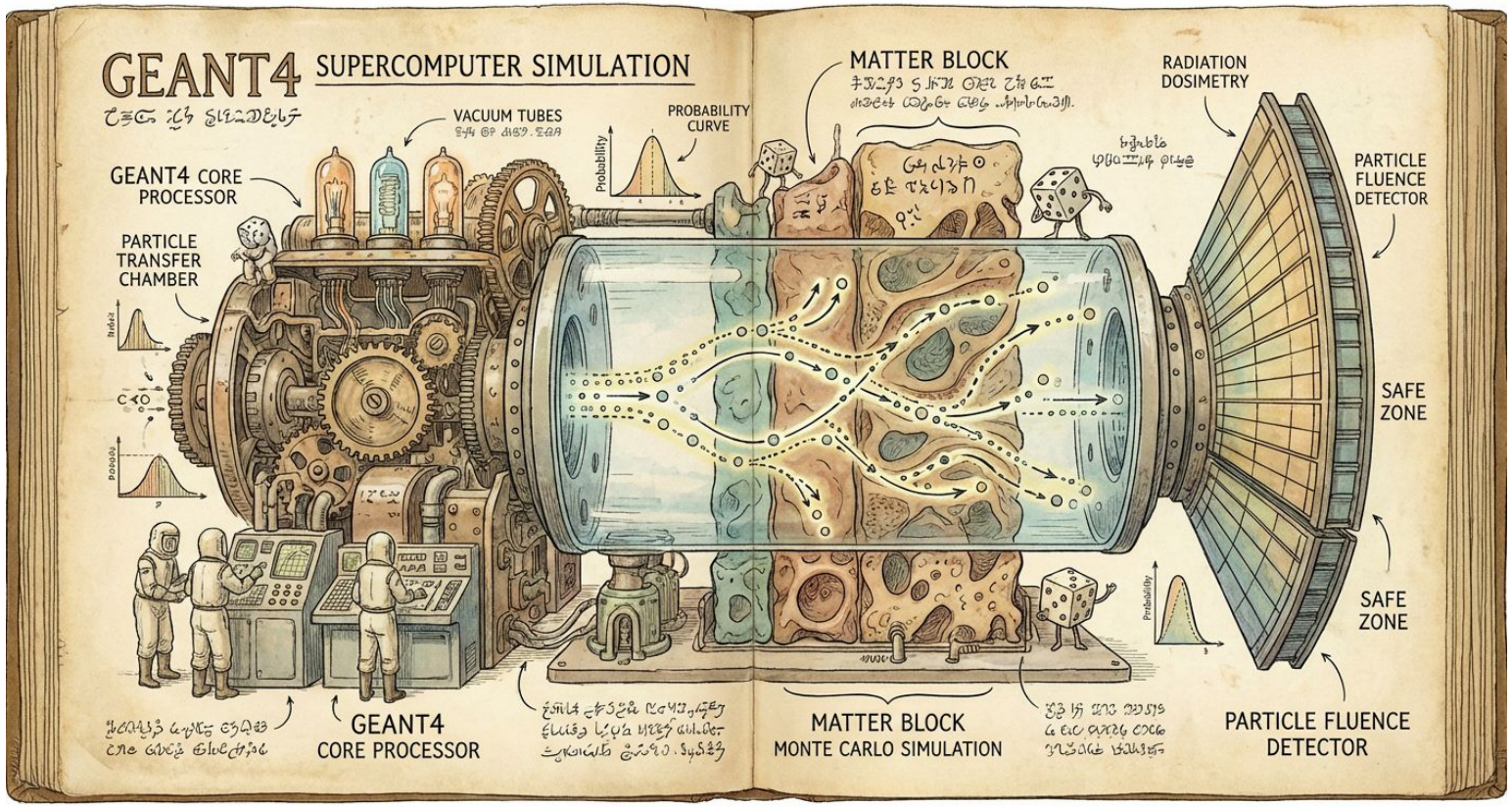
	total	used	free	shared	buff/cache	available
Mem:	94G	9.6G	78G	114M	5.8G	83G
Swap:	4.0G	1.2G	2.8G			

```
*************************************************************
 Geant4 version Name: geant4-11-01-patch-03 [MT]   (10-November-2023)
  << in Multi-threaded mode >>
                       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/
*************************************************************
```



Conclusions

1. First, test on a local computer.
2. Run the finished code on the server via SLURM.
3. Automate repetitive steps using batch scripts.
4. Read logs and fix erros.
5. Run again.



Thank you!

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References

1. Chizhov K et al. Monte-carlo simulation of the radiation environment in the temporary control room at the NICA Accelerator Complex, 16th Vietnam Conference on Nuclear Science and Technology (VINANST-16), Da Nang, Vietnam, October 8th – 10th, 2025.