OAK RIDGE National Laboratory

Celeritas physics validation

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HPC Methods for Nuclear Applications

HSF Detector Simulation on GPU Community Meeting
May 3-6, 2022

ORNL is managed by UT–Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

***Celeritas* core team:**

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BNL	Vincent Pascuzzi

Validation phases

- Geant4 verification
  - Test physics, geometry, EM fields
  - experiment-independent

- Community-driven performance test-problems **More on this in tomorrow's session**

- Experiment integration **More on this in tomorrow's session**
  - Incorporate *Celeritas* into real workflows starting with *Acceleritas*
    - e.g. CMSSW, Athena, *art* (e.g. LArSoft)
  - LCF-experiment integration

Geant4 verification status

- Currently a **single *Geant4 app*** manages the whole process:
  - Performance
    - MT, only outputs wall/cpu times (total; simulation run)
  - Physics verification
    - Comprehensive ROOT output (serial-only)
  - Export geometry to GDML for *Celeritas*

https://github.com/celeritas-project/benchmarks/tree/master/geant4-validation-app

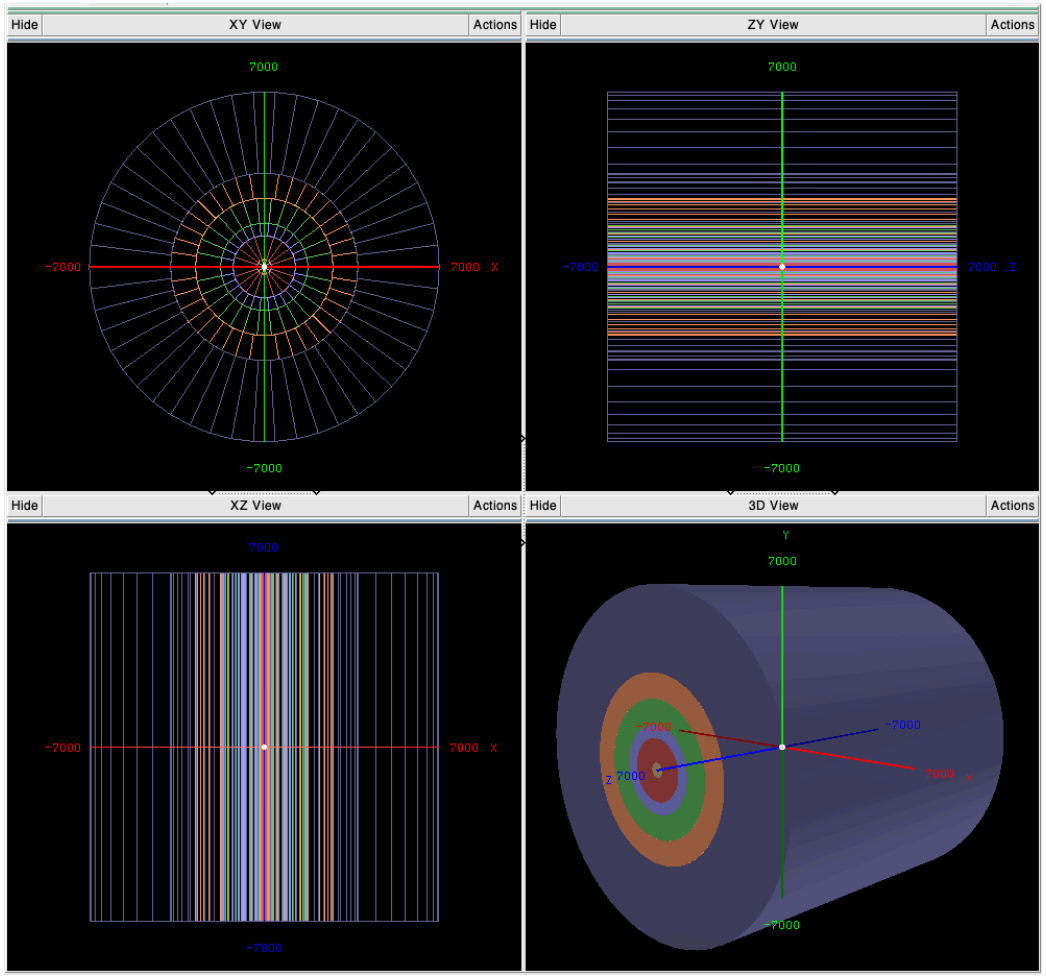
Geant4 verification status

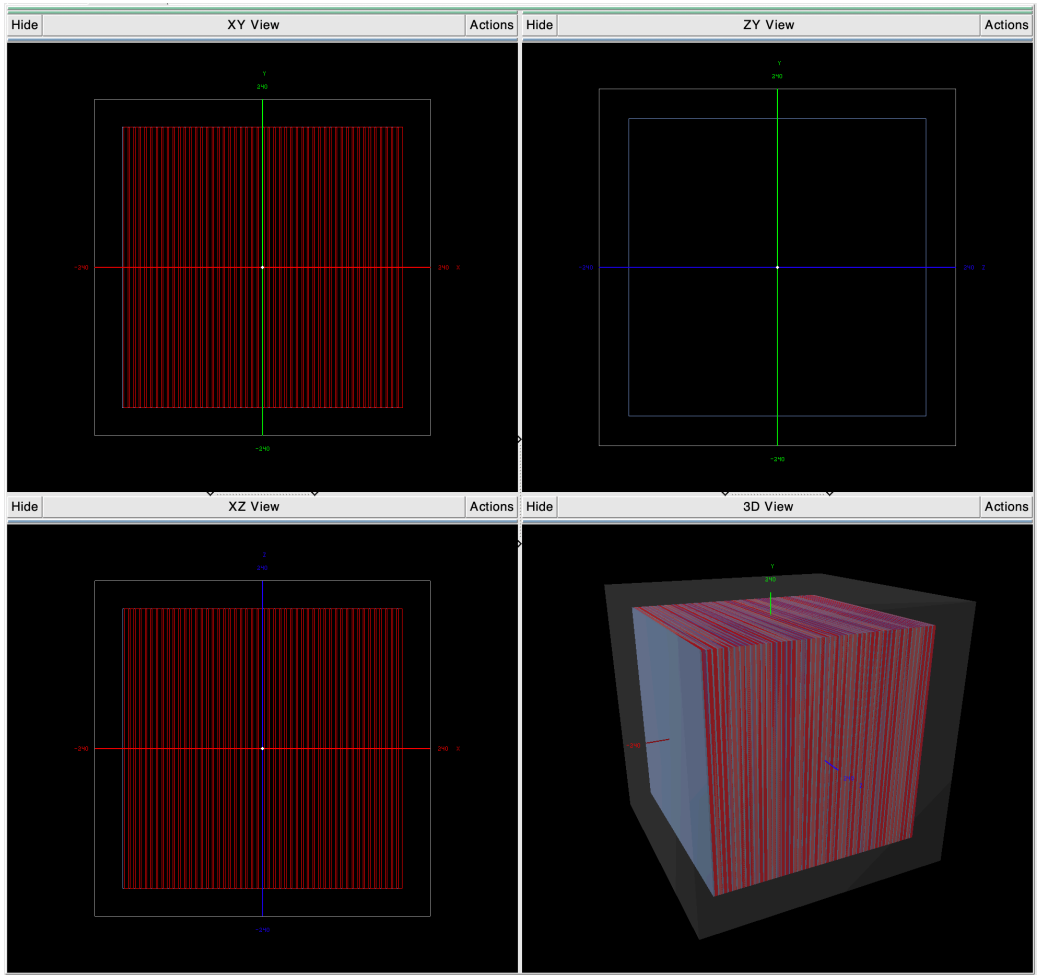
- Currently a **single *Geant4 app*** manages the whole process:

```
{
    "simulation": {
        "geometry": 0,
        "range_cuts": 0.7,
        "hepmc3": "",
        "particle_gun": {
            "events": 1,
            "pdg": 22,
            "energy": 10,
            "vertex": [0, 0, 0],
            "direction": [1, 1, 1]
        },
        "cores": 4,
        "performance_run": false,
        "step_info": true,
        "random_seed": false,
        "spline": true,
        "kill_secondaries": false
    },
    "physics": {
        "compton_scattering": true,
        "photoelectric": true,
        "rayleigh_scattering": true,
        "gamma_conversion": true,
        "positron_annihilation": true,
        "bremsstrahlung": true,
        "e_ionization": true,
        "coulomb_scattering": false,
        "multiple_scattering": false
    },
    "verbosity": {
        "RunManager": 0,
        "RunAction": 0,
        "EventAction": 0,
        "PhysicsList": 0,
        "PrintProgress": 1000
    },
    "GUI": false,
    "vis_macro": "vis.mac",
    "export_gdml": false
}
```

Geant4 verification status

- Current geometries: Simple CMS and Adept's version of TestEm3





Geant4 verification status

- Comprehensive ROOT output (particle/SD data)

```
struct Event
{
    size_t                                id;
    std::vector<Track>                    primaries;
    std::vector<Track>                    secondaries;
    std::vector<SensitiveDetectorScore>   sensitive_detectors;
};

struct Step
{
    ProcessId process_id;
    double    kinetic_energy; //!< [MeV]
    double    energy_loss;    //!< [MeV]
    Vector3   direction;      //!< Unit vector
    Vector3   position;       //!< [cm]
    double    global_time;    //!< [s]
};
```

```
struct Track
{
    int               pdg;
    size_t            id;
    size_t            parent_id;
    double            length;             //!< [cm]
    double            energy_dep;         //!< [MeV]
    double            vertex_energy;      //!< [MeV]
    double            vertex_global_time; //!< [s]
    Vector3           vertex_direction;   //!< Unit vector
    Vector3           vertex_position;    //!< [cm]
    size_t            number_of_steps;
    std::vector<Step> steps;
};
struct SensitiveDetectorScore
{
    SDProcessMapUL process_counter;   //!< Count processes
    SDProcessMapD  process_edep;      //!< Tally edep per process
    double         energy_deposition; //!< [MeV]
    size_t         number_of_steps;
};
```

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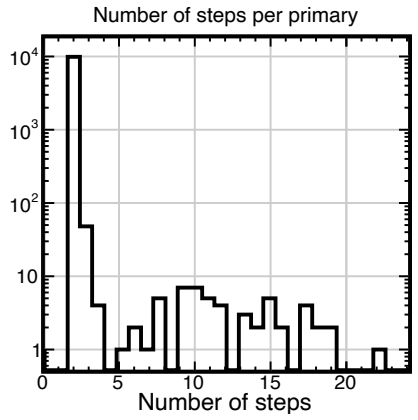
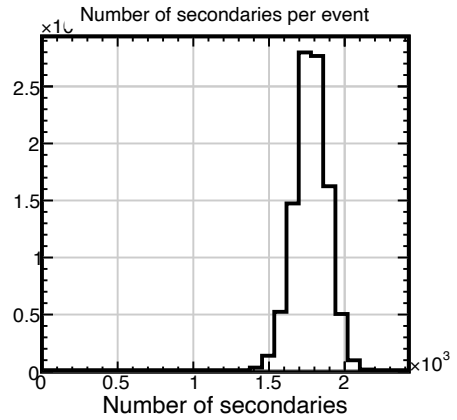
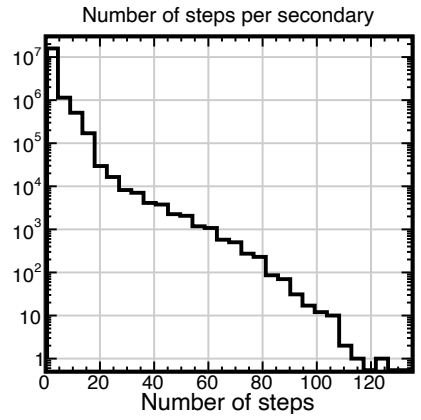
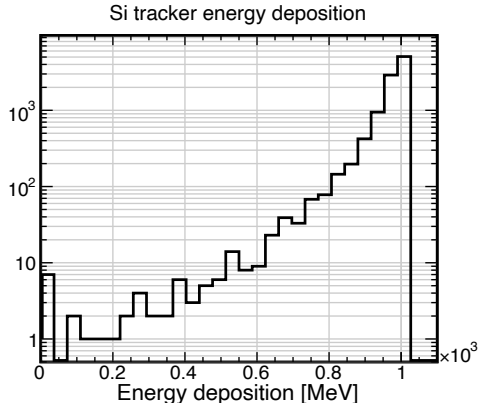
Geant4 verification status

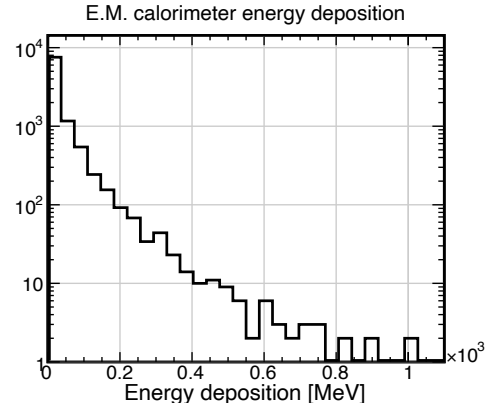
- Comprehensive ROOT output (particle/SD data)

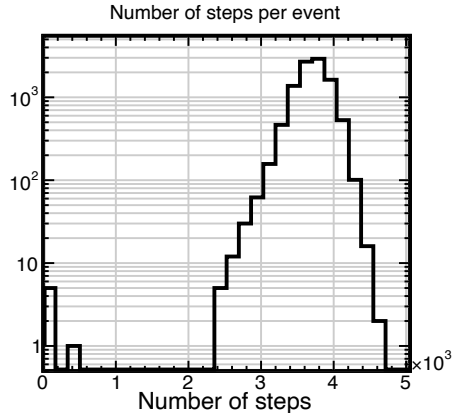


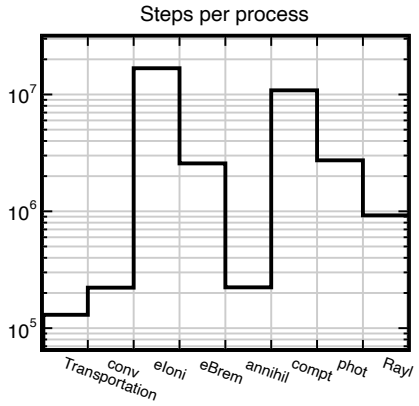


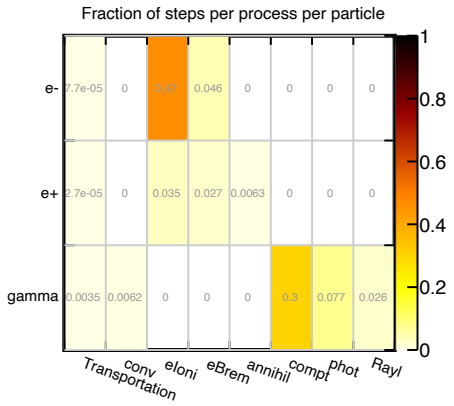


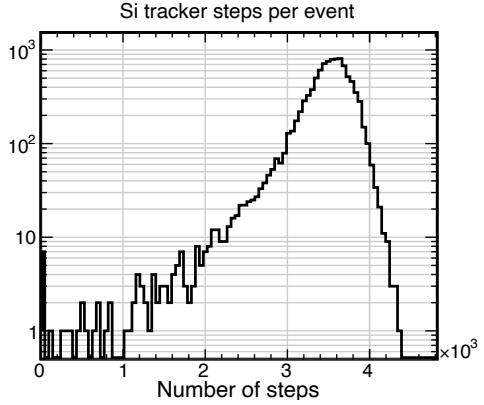


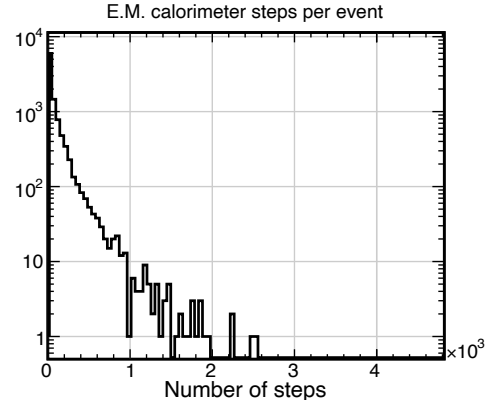












Geant4 verification status

- Comprehensive ROOT output (performance/input information)

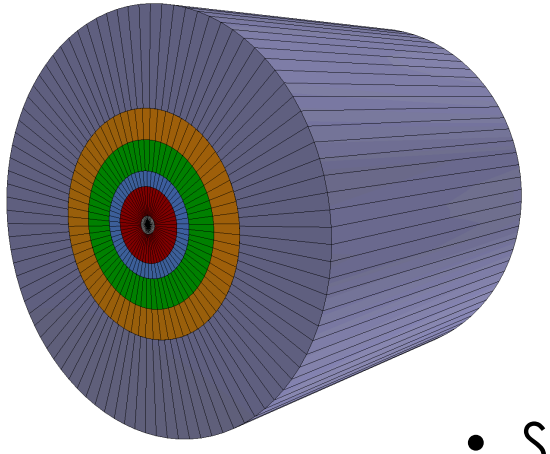
```
struct ExecutionTime
{
    double wall_total;
    double cpu_total;
    double wall_sim_run;
    double cpu_sim_run;
};
```

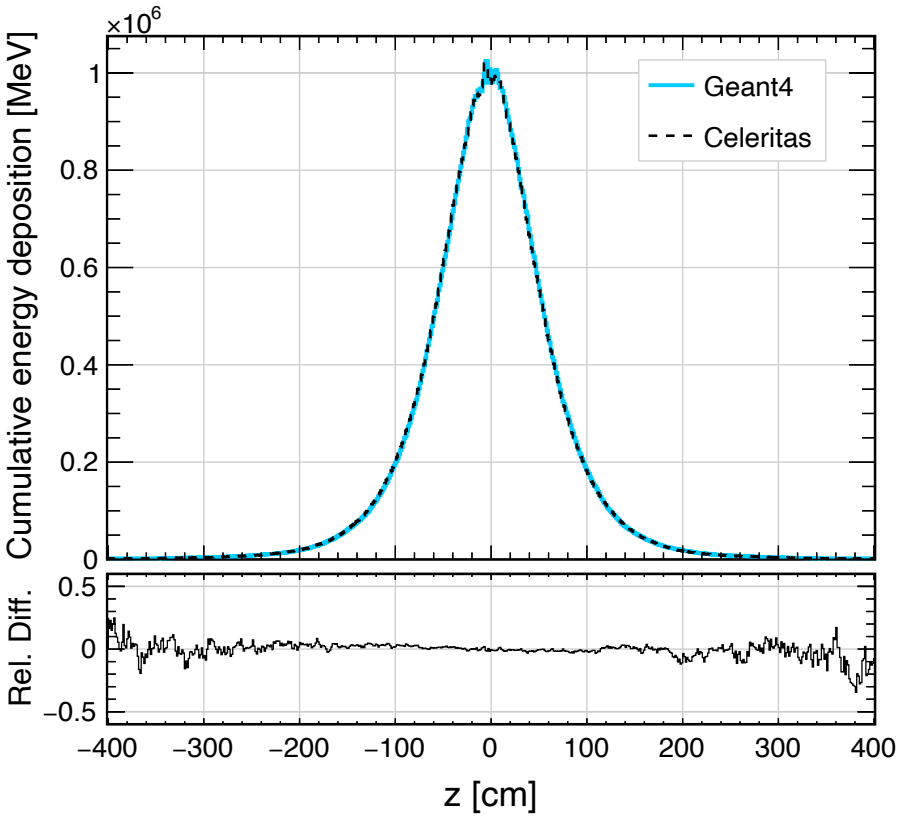
```
root [1] input->Show(0)
======> EVENT:0
 version          = 1072
 geometry         = simple_cms
 simulation       = particle_gun
 range_cuts       = 0.7
 events           = 1
 pdg              = 22
 energy           = 10
 vertex           = 0,
                    0, 0
 direction        = 1,
                    1, 1
 cores            = 1
 seed             = 1
 rng              = MixMaxRng
 spline           = 1
 kill_secondaries = 0
 compton_scattering = 1
 photoelectric    = 1
 rayleigh_scattering = 1
 gamma_conversion = 1
 positron_annihilation = 1
 bremsstrahlung   = 1
 e_ionization     = 1
 multiple_scattering = 0
 coulomb_scattering = 0
```

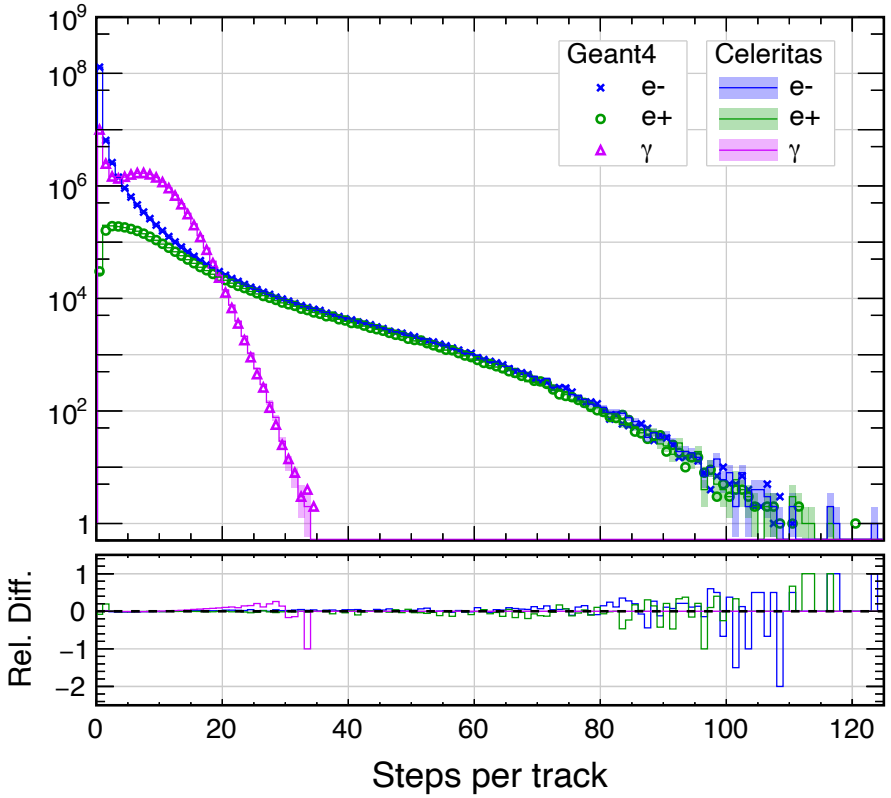
- ROOT input info stores more than just the json parameters
  - G4 version
  - RNG engine
  - Seed

Simple CMS

- Isotropic source
- 100k gammas
- 1 GeV each
- Vertex at (0, 0, 0)



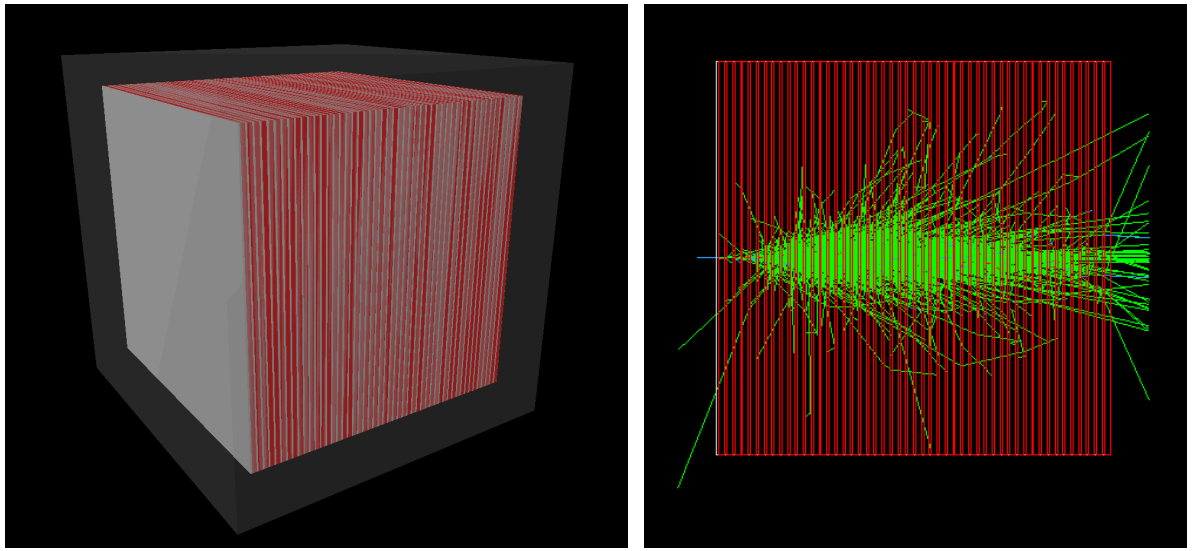




- Single-element concentric cylinders of **Si**, **Pb**, **C**, **Ti**, and **Fe**

AdePT's TestEm3: first "community-based" test

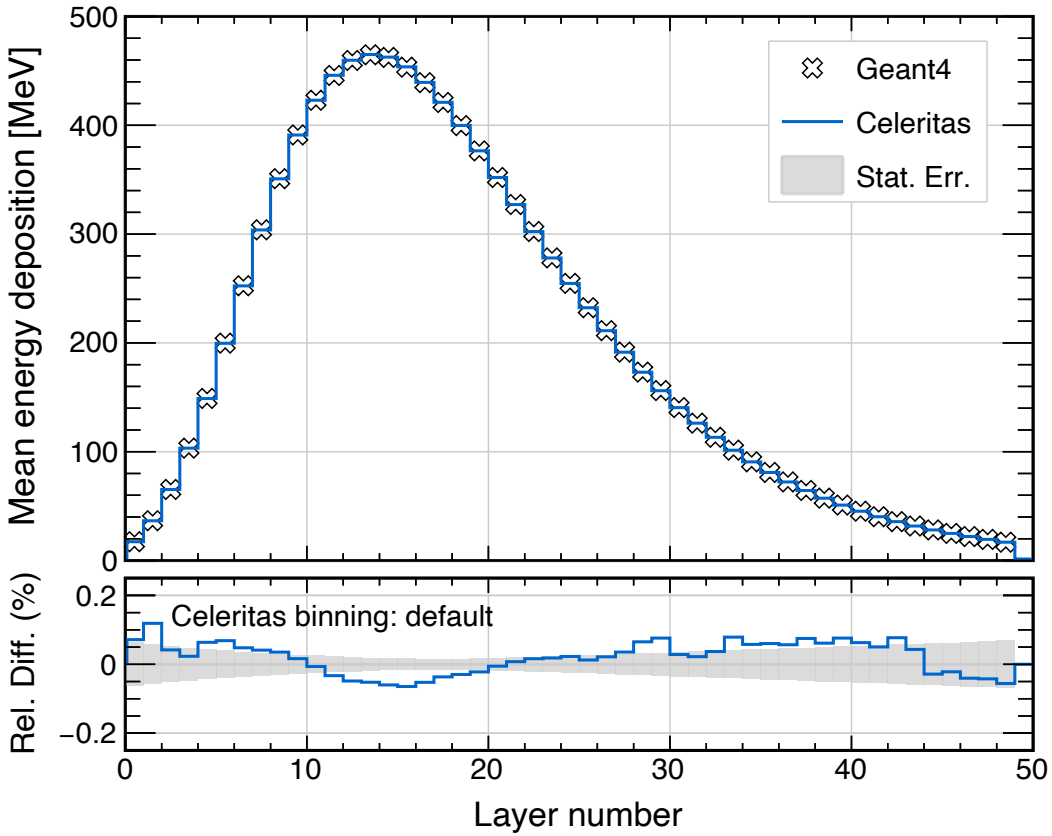
- 50 layers of G4_LAr + G4_Pb
  - 1E6, 10 GeV, e^- primaries
  - Vertex before 1st layer (–22, 0, 0) [cm]
  - Momentum direction: (1, 0, 0)
  - 1 mm secondary production cuts

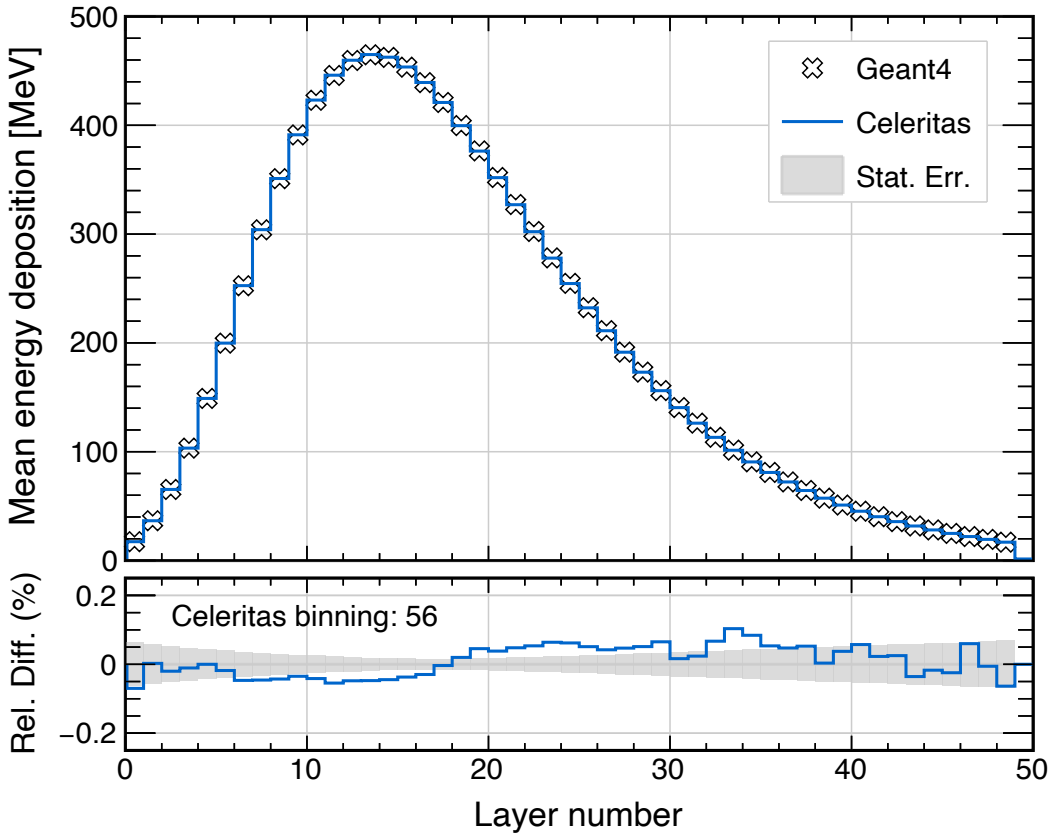


- Manually converted geometry defined in **AdePT**/examples/TestEm3 to a Geant4 programmatic geometry
  - https://github.com/celeritas-project/benchmarks/blob/master/geant4-validation-app/src/testem3/TestEm3Detector.cc

AdePT's TestEm3: first "community-based" test

- *Celeritas* vs. Geant4 v10.7.3 (1E6 primaries each)
- *Celeritas* has no spline interpolation; 8× cross-section table binning increase





Future work

Further discussions in tomorrow's session

- *Celeritas* verification
  - Streamline the verification process with an automated toolchain
  - Simulation runs → outputs → validation plots → documentation
  - Recurring process
    - More thorough during early stages and new implementations...
    - Standardized and streamlined for tag release comparison
  - Metrics/criteria for successful physics verification are open for discussion

- Community-driven problems should
  - Solidify results
  - Provide performance assessments

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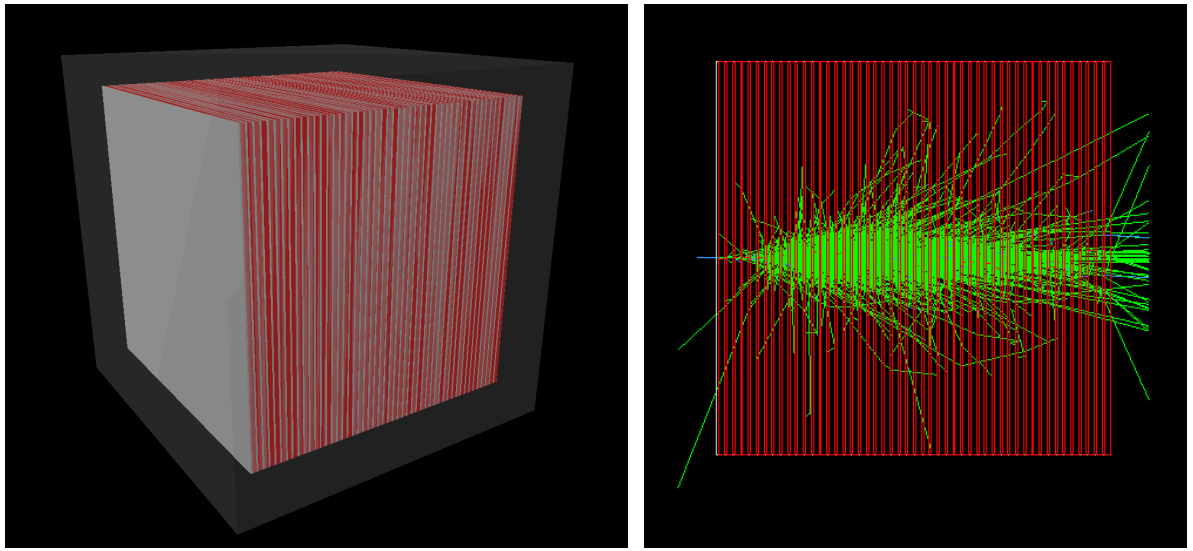
BACKUP

AdePT's TestEm3: first comparison test



- Ported geometry to G4
- Produced GDML for *Celeritas*' run
- Input
  - 1E6, 10 GeV, e^- primaries
  - 1 mm secondary production cuts
  - AdePT: Changed capacity to $\mathbf{2^{21}}$ and batching to **235**
    - TestEm3.cu::196: `constexpr int Capacity = 2048 * 1024;`
    - TestEm3.cpp:202: `OPTION_INT(batch, 235);`
    - electrons.cu::4: `#define NOMSC`

https://github.com/stognini/AdePT/tree/summit
https://github.com/celeritas-project/benchmarks/tree/master/geant4-validation-app

AdePT TestEm3: first comparison test

- *Celeritas* vs. Geant4 v10.7.3 vs. AdePT (1E6 primaries each)
- *Celeritas* has no spline interpolation; 8× cross-section table binning increase