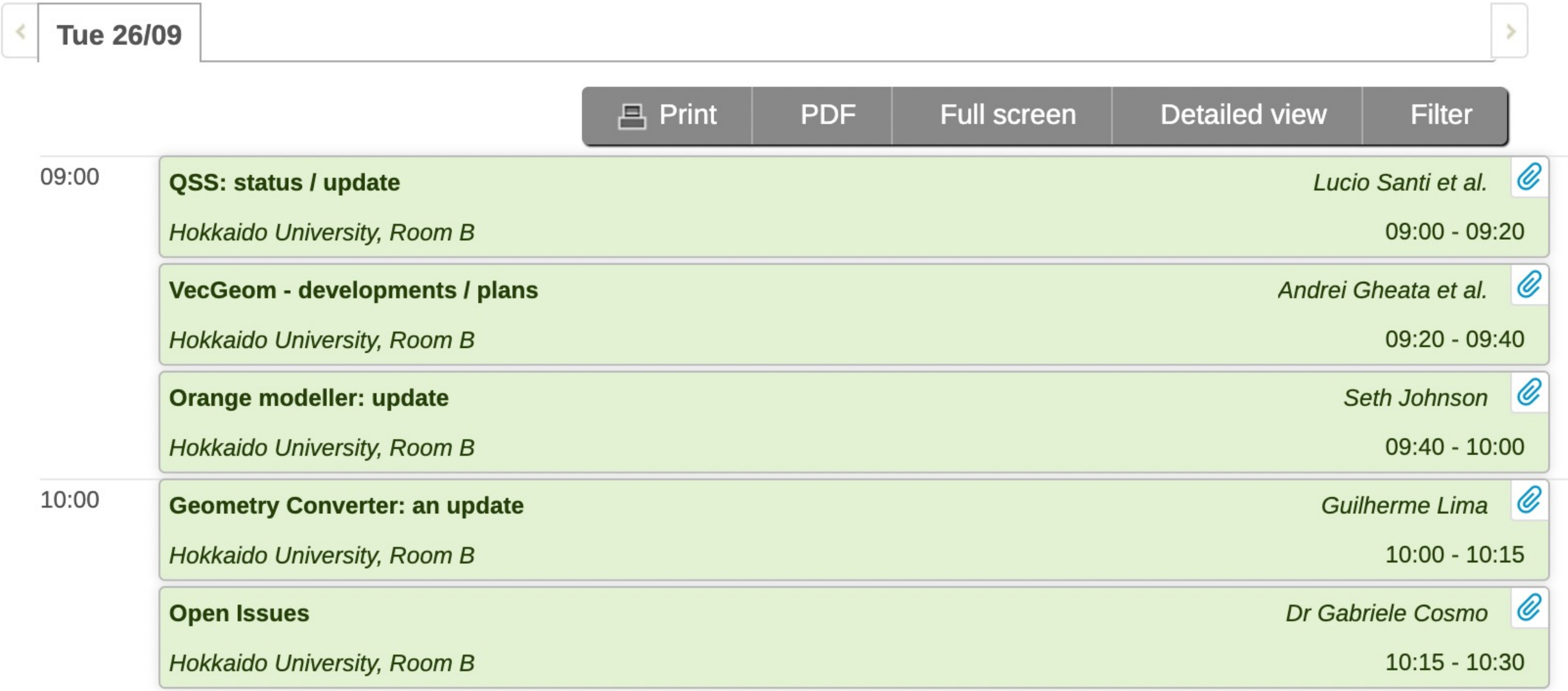
Summary of
Parallel 2B: Geometry

J. Apostolakis



Tue 26/09

09:00

QSS: status / update — *Lucio Santi et al.*
Hokkaido University, Room B — 09:00 - 09:20

VecGeom - developments / plans — *Andrei Gheata et al.*
Hokkaido University, Room B — 09:20 - 09:40

Orange modeller: update — *Seth Johnson*
Hokkaido University, Room B — 09:40 - 10:00

10:00

Geometry Converter: an update — *Guilherme Lima*
Hokkaido University, Room B — 10:00 - 10:15

Open Issues — *Dr Gabriele Cosmo*
Hokkaido University, Room B — 10:15 - 10:30

UBA
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Facultad de Ciencias Exactas y Naturales - UBA

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Progress in adapting the QSS Stepper to the current version of Geant4

Testing and benchmark results

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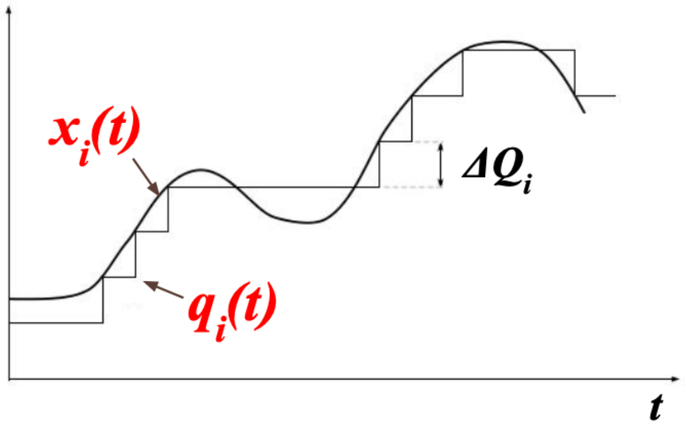
Quantized State System (QSS) numerical methods

- Based on **state variables quantization**
- QSS methods discretize the system **state variables** as opposed to classical solvers which discretize the **time** (e.g. family of Runge-Kutta methods)
- ***Continuous* state variables** approximated by ***Quantized* state variables**
  - A **quantization function** is in charge of controlling **error and accuracy** throughout the simulation

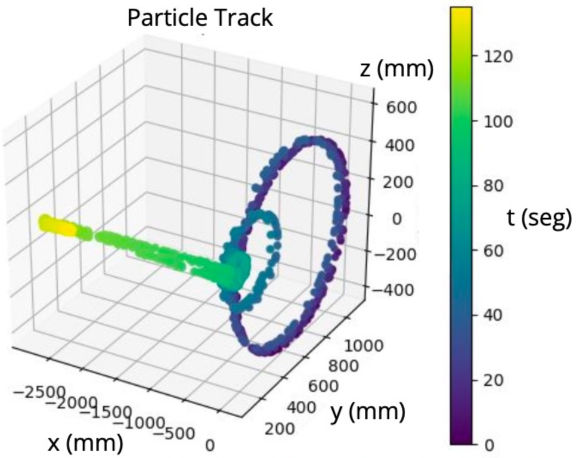
$$\underbrace{\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(\mathbf{t}))}_{\text{ODE system}} \Rightarrow \underbrace{\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{q}(\mathbf{t}))}_{\text{ODE quantized system}}$$



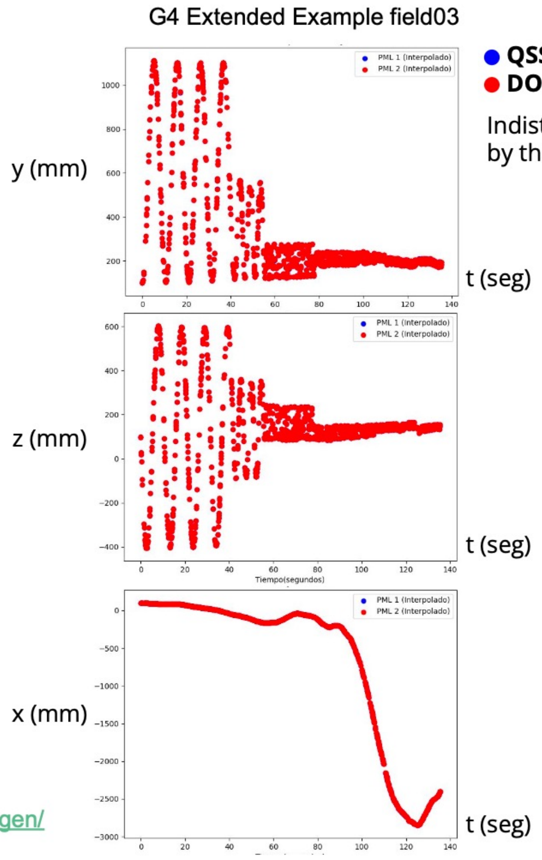
New: Logging of time series for error assessment

- Calculation of the Mean Square Error (MSE) for x(t),y(t),z(t) and the Track Length L(t)
- Thorough systematic comparison of deviation between methods for **different accuracies**
- Interpolation of asynchronous time series
- E.g.: QSS2 vs DOPRI

```
dQRel=1e-5, dQMin=1e-6
X_MSE = 1.64
Y_MSE = 0.00072
Z_MSE = 0.0014
L_MSE = 0.0
```



https://geant4-userdoc.web.cern.ch/Doxygen/examples_doc/html/Examplefield03.html


G4 Extended Example field03

- ● QSS2
- ● DOPRI

Indistinguishable by the naked eye

Results highlights

- 11 examples tested and verified successfully:
    - **Basic** (B2a, B2b, B4c, B4d, B5), **Extended** (with magnetic field: 01, 02, 03, 06), **Advanced** (ams_ECAL)
    - **FullSimLight**, a lightweight standalone Geant4 simulation tool that supports the full ATLAS geometry and the ATLAS magnetic field map
- Benchmarks made against G4 (ver. 11.0.0-ref-02) default stepper (DOPRI with Interpolation Driver)
- In 5 cases *there exist* ***QSS accuracy parameters*** that can outperform DOPRI
    - **However**, the ratio of geometry intersections per G4 step remains below 19% in all tested examples (typically around 5%) => these are **not** "QSS-friendly" scenarios (not too many intersections per step)
- Particle trajectories were compared visually using Paraview and VTK output files
- Benchmarking software: we continue developing a **toolset for repeatable benchmarking** that can be parameterized to produce systematic performance comparisons across G4 Steppers

Benchmark computing platform

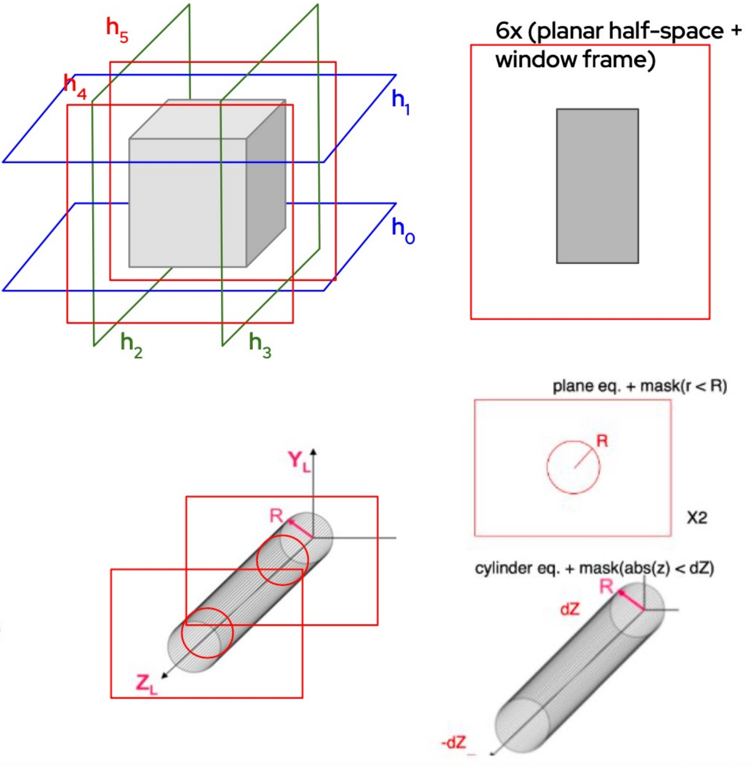
- All experimentations carried out in CERN's OpenLab (controlled environment)
- Hardware specs: Intel(R) Xeon(R) CPU E5-2683 v4 @ 2.10GHz (64 CPUs) 64 GB RAM

Surface-based GPU model in VecGeom

Slides prepared by Andrei Gheata for the AdePT team

Bounded surface modeling

- 3D bodies represented as Boolean operation of half-spaces*
  - First and second order, infinite
  - Just intersections for convex primitives
    - e.g. box = h_0 & h_1 & h_2 & h_3 & h_4 & h_5
  - Similarities with the Orange model
    - Evaluated Orange to start with
- Storing in addition the solid imprint (frame) on each surface: FramedSurface
  - Similarities with detray (ACTS)
  - The frame information allows avoiding to evaluate the Boolean expression for distance calculations to primitive solids



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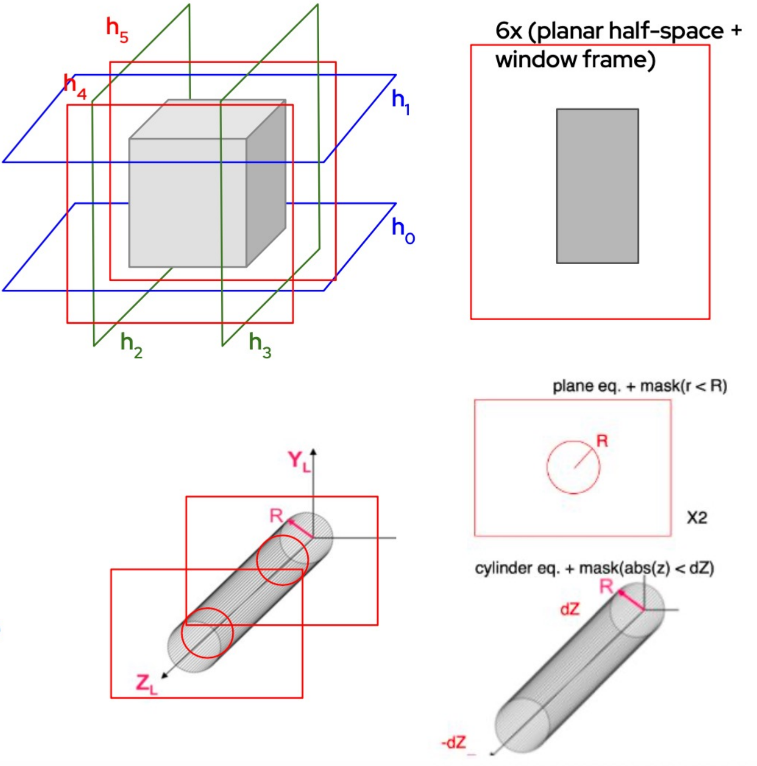


Outlook

- As GPU simulation gains in weight and geometry is on critical path, VecGeom develops dedicated surface-based GPU support
  - Surface model enriched with solid frame information
  - Collaboration with Celeritas/ORANGE team on commonalities and convergence paths
  - Transparent implementation, better work-balanced and friendlier to GPU
- Currently implemented all the features required by particle transport, for a subset of solids
  - Locate, relocate, distance and safety calculation
  - Promising preliminary numbers
- Working on extending the model, memory and performance optimization
  - Targeting cms_2018 setup working in AdePT/Celeritas by the end of the year

ORANGE surface geometry progress

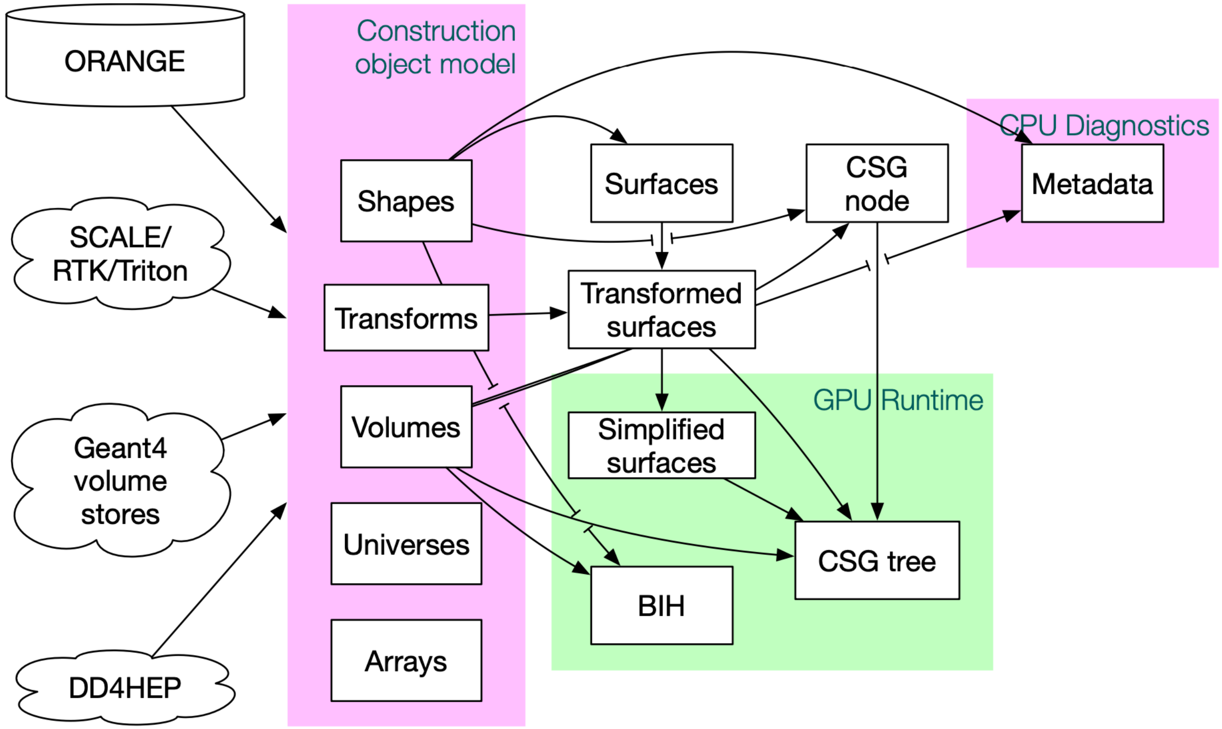
Seth R Johnson, Elliott Biondo, Tom Evans

Celeritas/ORANGE/Shift developers

Background

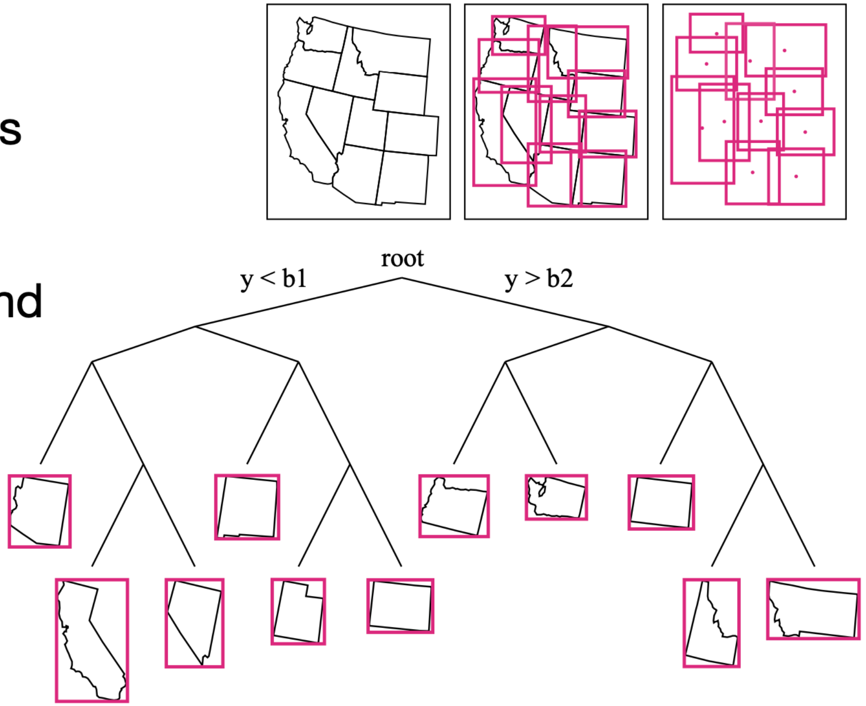
- Many nuclear engineering codes use “unbounded” surfaces and constructive solid geometry
  - MCNP, KENO, earlier codes: >40 years of history
  - Quadric surface cards, CSG cell cards
  - Neutral particles or no magnetic fields
- 2017: Shift GPU code (part of ECP) uses simple but efficient surface-based reactor model (nested cylinders and arrays)
- 2021: Initial GPU port for Celeritas
- 2023: GPU port integrated into Shift

User-to-runtime construction



Acceleration: bounding interval hierarchy

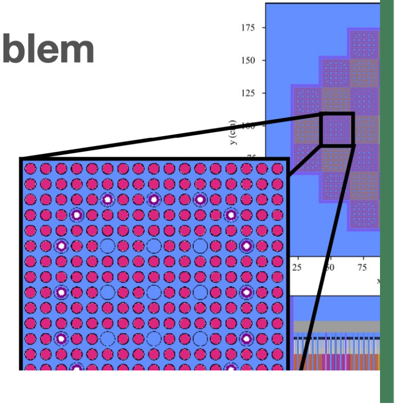
- Inputs: volume bounding boxes
- Recursive partitioning scheme
- Tree traversal at initialization and surface crossing
- Low memory requirements
  - Single-precision bounding boxes
  - Tree nodes are ~16B



Results

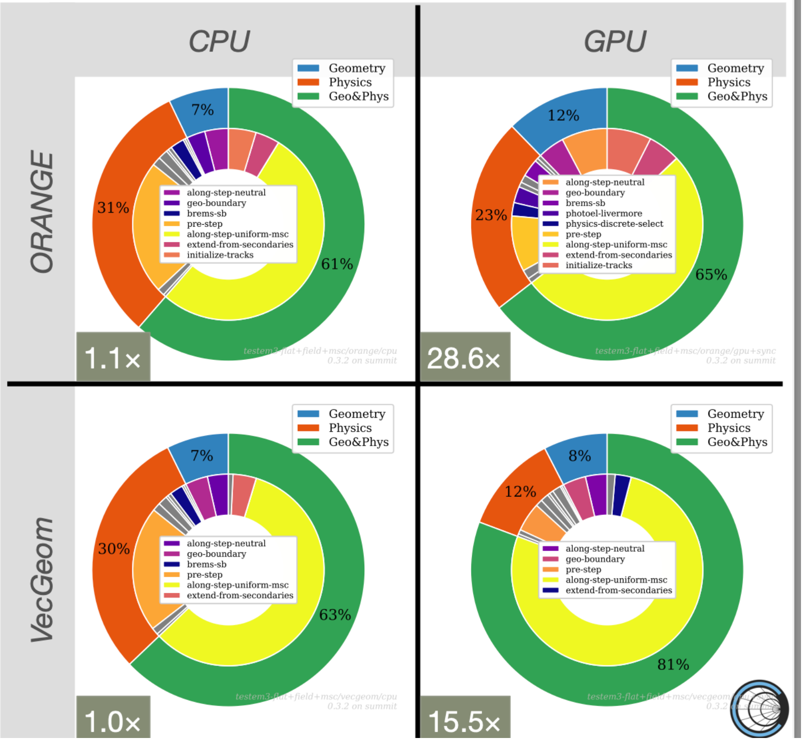
Small Modular Reactor problem

- Array of array of “pin cells”
- Water and uranium
- Neutron-only physics



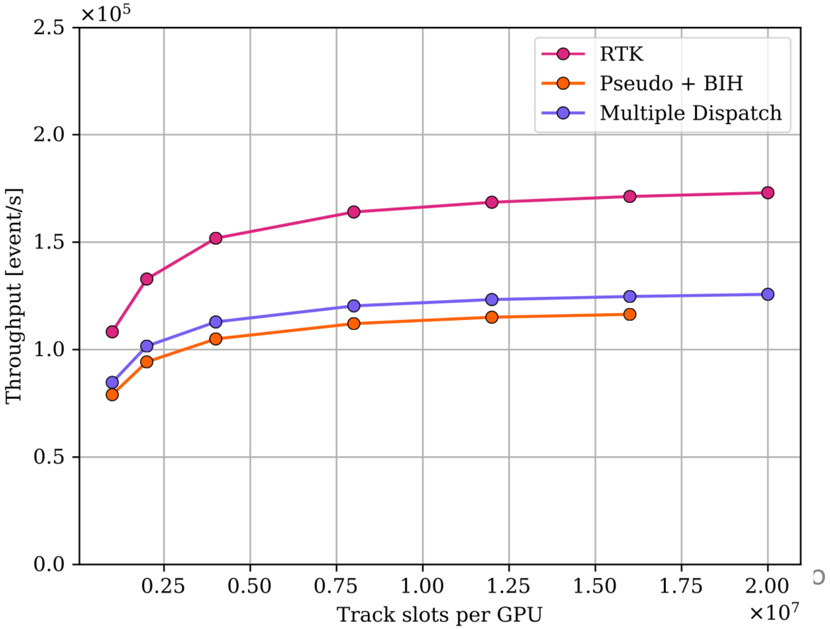
Current ORANGE/VecGeom performance for TestEM3

- VecGeom 1.x navigation on GPU known to be suboptimal
- Results from Summit
  - 7 CPU Power9 cores vs 1 V100 GPU
  - 1T uniform field
  - 1300 × 10 GeV e- per event × 7 events
  - Speedup relative to CPU VecGeom



SMR on Frontier (AMD MI250)

- Template metaprogramming “multiple dispatch” faster on AMD for this problem
- ORANGE is 30% slower than “reactor toolkit” geometry
  - RTK is extremely limited
  - Highlights performance/functionality tradeoff



Next Steps

- Optimisation
  - Reduce memory use by recognising “same” surface
  - Precalculating information for quadratic surfaces
- Extension of capabilities
  - Tracking simultaneously at multiple levels
  - Safety calculation (to determine if beneficial or needed)
  - Aggregate “poly” shapes (e.g. polygon)

In-memory Geometry Converter

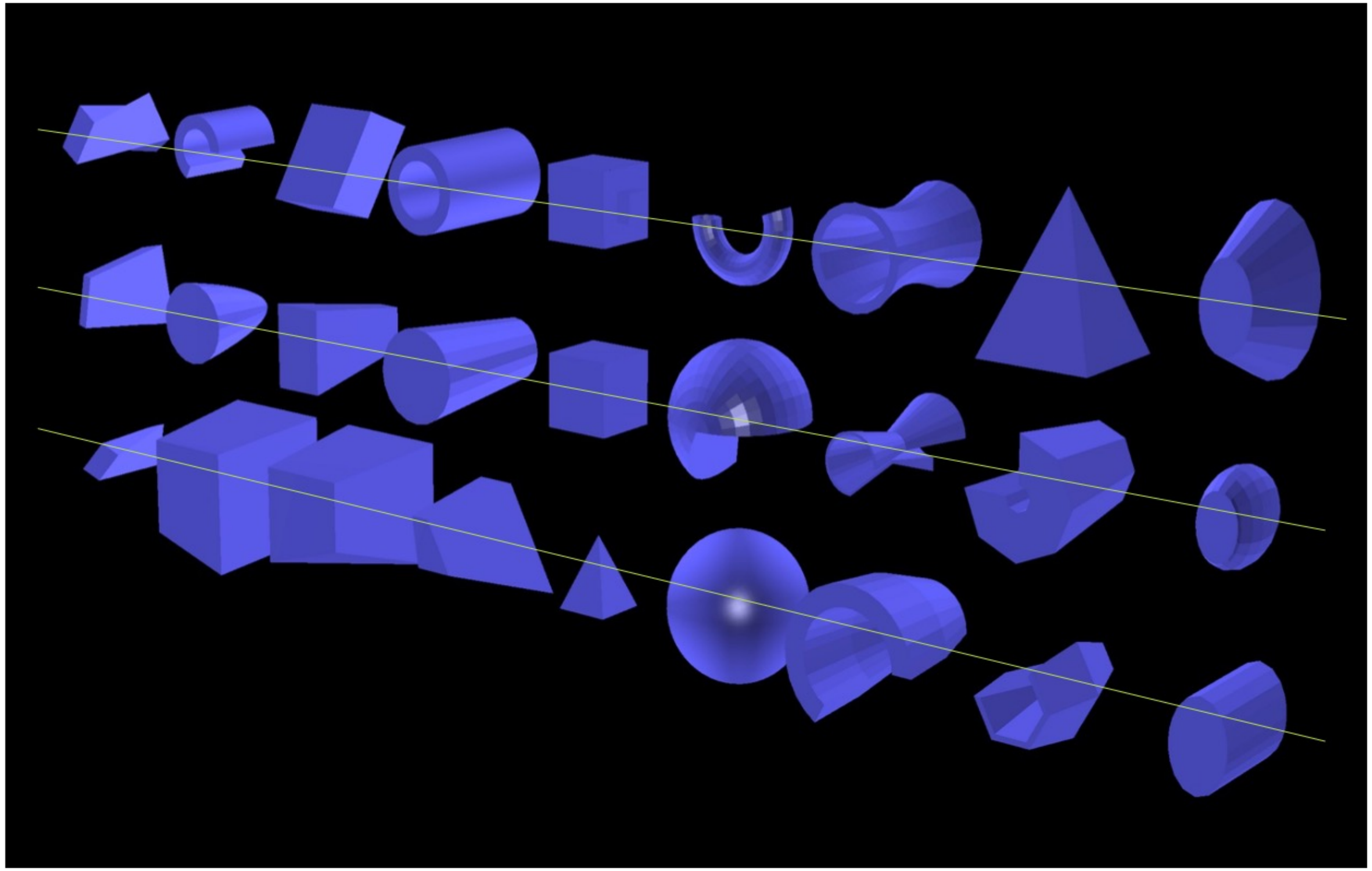
Guilherme Lima

Geometry converter: what is it?

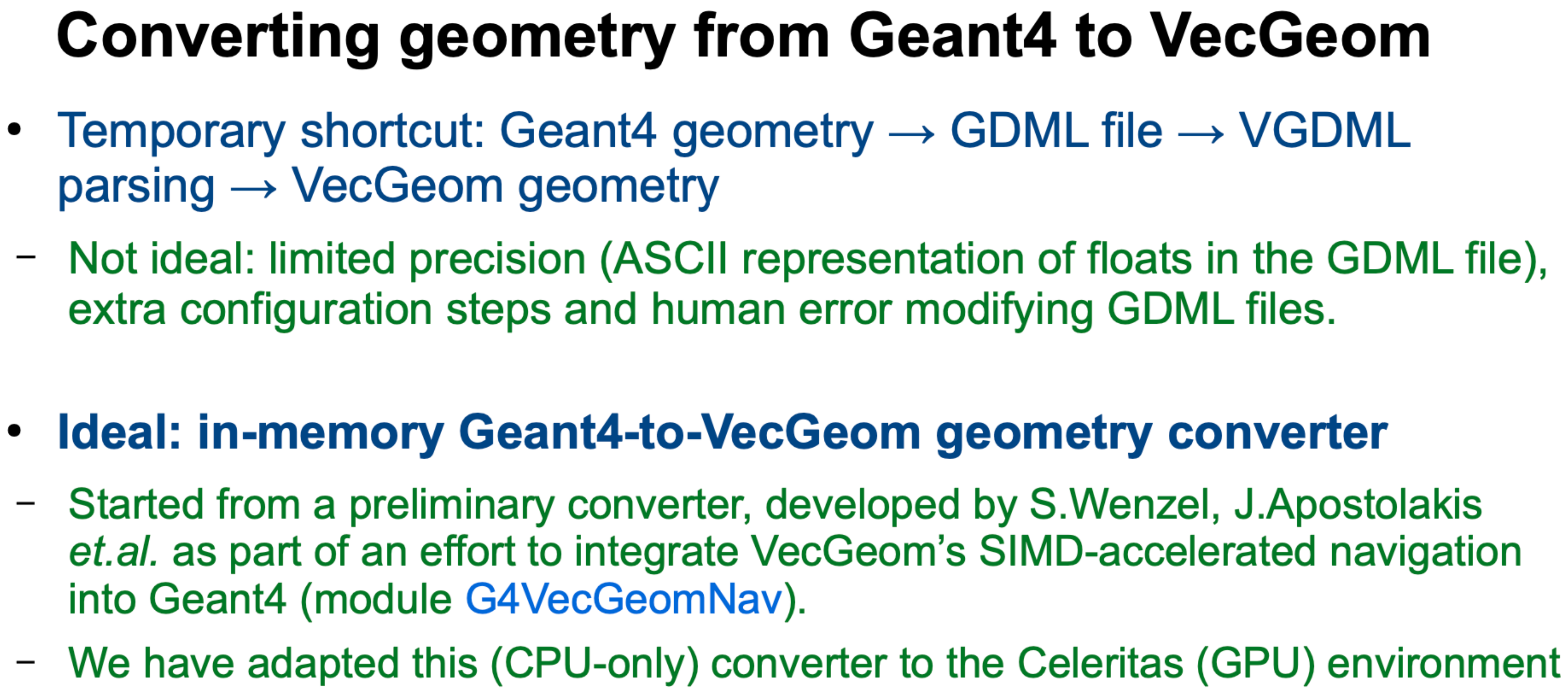
- Converter developed within the context of Celeritas, which goal is to allow a Geant4 job to offload some of the tracking to a GPU device
  - see Seth Johnson's talk for more details on the Celeritas project
- VecGeom (VECtor GEOMetry) was developed to promote SIMD-vectorized algorithms. Since its algorithms could also run well on GPGPUs, it became a natural choice for HEPsim-on-GPU prototypes like Celeritas and AdePT.
  - Celeritas uses VecGeom v1.x for now, at least while surface-based systems (VecGeom 2.x and ORANGE) are being developed
- In order to offload some tracking to the GPU, the Geant4 geometry needs to be made available in VecGeom.

Validation: current status of solids.gdml

- Added support to several shapes
- Similar shape dimensions and adequate positioning and spacing
- Detailed tracking, comparing coordinates of each boundaries crossed



What?



Converting geometry from Geant4 to VecGeom

- Temporary shortcut: Geant4 geometry → GDML file → VGDML parsing → VecGeom geometry
  - Not ideal: limited precision (ASCII representation of floats in the GDML file), extra configuration steps and human error modifying GDML files.

- **Ideal: in-memory Geant4-to-VecGeom geometry converter**
  - Started from a preliminary converter, developed by S.Wenzel, J.Apostolakis *et.al.* as part of an effort to integrate VecGeom's SIMD-accelerated navigation into Geant4 (module G4VecGeomNav).
  - We have adapted this (CPU-only) converter to the Celeritas (GPU) environment

Geometry converter: status and plans

- In-memory Geant4-to-VecGeom geometry converter is now available
  - From a preliminary prototype in G4VecGeomNav, further developed under the Celeritas environment
  - Debugged, fixed, validated and released: produces in-memory VecGeom model
  - The VecGeom model is readily available for tracking in the GPU
  - Has been (partly) ported back into the G4VecGeomNav module
    - Still to be ported: reflected shapes, multi-union, simplifying refactoring

- Prospects:
  - New: surface-based geometry approach, still under development – see previous talks

    → expected to be supported by this converter, no roadblocks anticipated
  - More shapes to be added as needed (e.g. triggered by other complex GDML files used)
  - TBD: long-term repository (requirements, dependencies, constraints)