UBA Universidad de Buenos Aires

SED Discrete Event Simulation Lab

ICC Instituto de Ciencias de la Computación

CONICET

DEPARTAMENTO DE COMPUTACION
Facultad de Ciencias Exactas y Naturales - UBA

Efficient discrete-event based particle tracking simulation for high energy physics

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GEANT4 A SIMULATION TOOLKIT

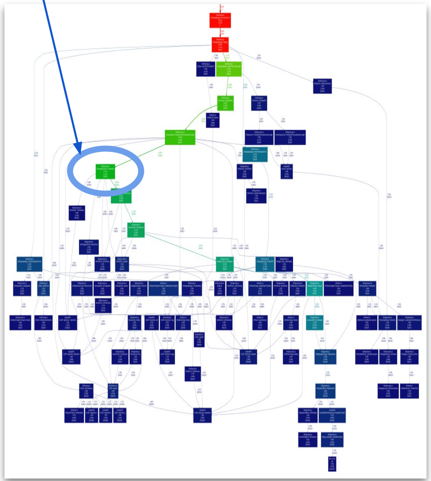
Agenda

1. Introduction to Quantized State methods
2. Main properties of QSS
3. Relevant features for HEP problems
4. Proof of Concept QSStepper for Geant4
    - High level architecture
    - High level sequence diagram
5. CMS reference application: a Benchmark
6. ATLAS as a next reference model
7. Plans for integration into the Geant4 release
8. Summary

Introduction

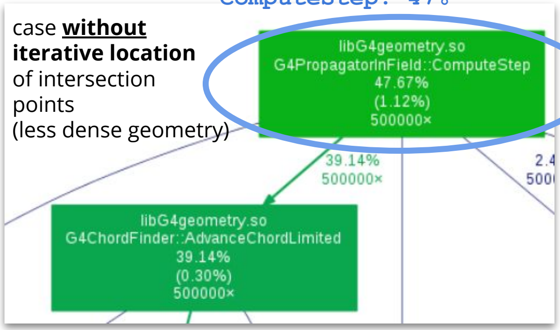
- Simulation domain: Tracking of subatomic particles
  - Undergoing physics processes within complex detector geometries
- **Key issue:** Handling of boundary crossings across discrete volumes
  - Can require **CPU-intensive, ad-hoc iterative algorithms**
  - **Can we do better?**
- **Approach:** Family of hybrid (continuous/discrete-event) integrators
  - **Quantized State System (QSS) numerical methods**
  - Attractive performance features for HEP applications

G4PropagatorInField::ComputeStep

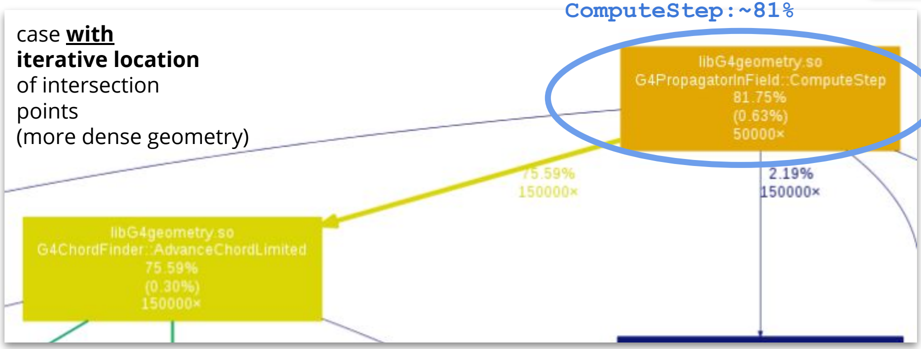


callgrind performance analysis

ComputeStep:~47%



ComputeStep:~81%



Synthetic benchmark
Perfect 2D particle oscillator
radius: 45 mm
Geometry: Parallel planes
G4 params:
epsilon = 1E− 7
deltaChord = 0.25 mm
stepMax = 20 mm
trackLength = 1000 m

QSS solvers for HEP applications

- Started as a collaboration with the Detector Simulation Group in Fermilab
  - w/Daniel Elvira & Team, Software for Physics Applications Dept., Scientific Computing Div.
- Since 2015 - Research on Efficient simulation of particle systems (HEP and other apps.)
- 2 completed Master's Thesis
- 1 PhD Thesis
- 5 peer-reviewed publications
- Successful case of a HEP/Computer Science interdisciplinary collaboration
  - Results relevant and innovative both for the Physics and the Computer communities

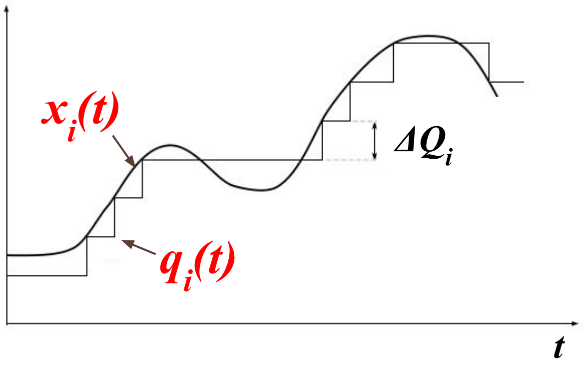
Latest manuscript:
Efficient discrete-event based particle tracking simulation for high energy physics
L. Santi, L. Rossi, and R. Castro
https://doi.org/10.1016/j.cpc.2020.107619

Discrete
Event
Simulation Lab

Quantized State System (QSS)

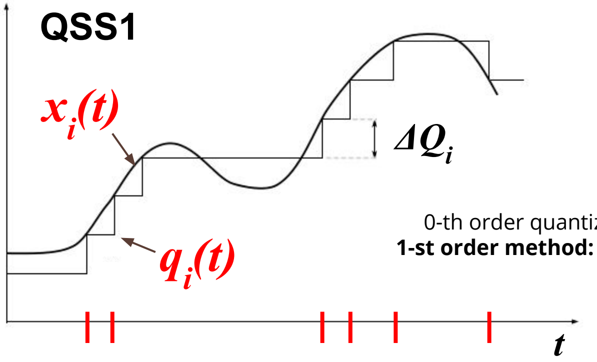
- Based on **state variables quantization**
- QSS methods discretize the system **state variables** as opposed to classical solvers which discretize the **time** (e.g. family of Runge-Kutta methods)
- ***Continuous*** **state variables** approximated by ***Quantized*** **state variables**
  - A **quantization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

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



Higher order QSS methods

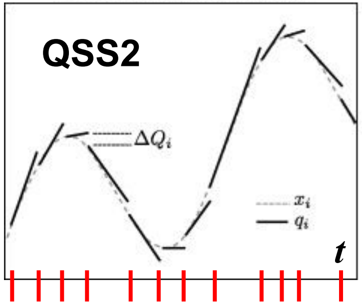
$$q_i(t) = \begin{cases} x_i(t) & \text{if } |q_i(t^-) - x_i(t)| \geq \Delta Q_i \\ q_i(t^-) & \text{otherwise} \end{cases}$$



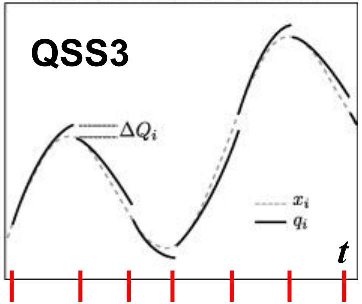
0-th order quantizer
1-st order method: QSS1

- ΔQ_i is the **quantum**
  - **Maximum deviation allowed** between x_i and q_i (error control)
  - Derived from the **accuracy** demanded by the user
- **Higher order QSS methods** (**QSSn**) follow a similar principle
  - In a **QSS1** method, $q(t)$ follows piecewise constant trajectories
  - In a **QSSn** method, $q(t)$ follows piecewise *(n-1)-th* order polynomial trajectories

1-st order quantizer
2-nd order method: QSS2



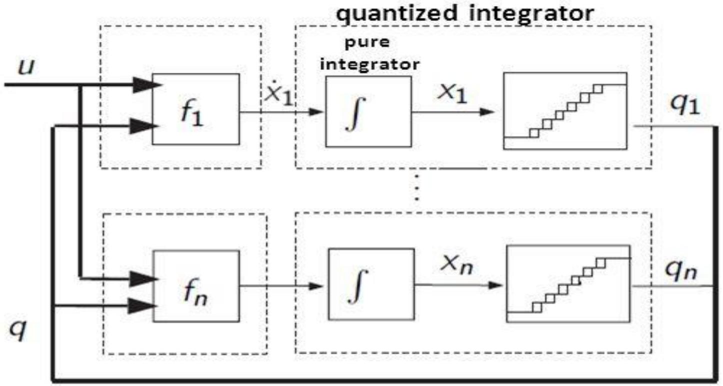
2-nd order quantizer
3-rd order method: QSS3

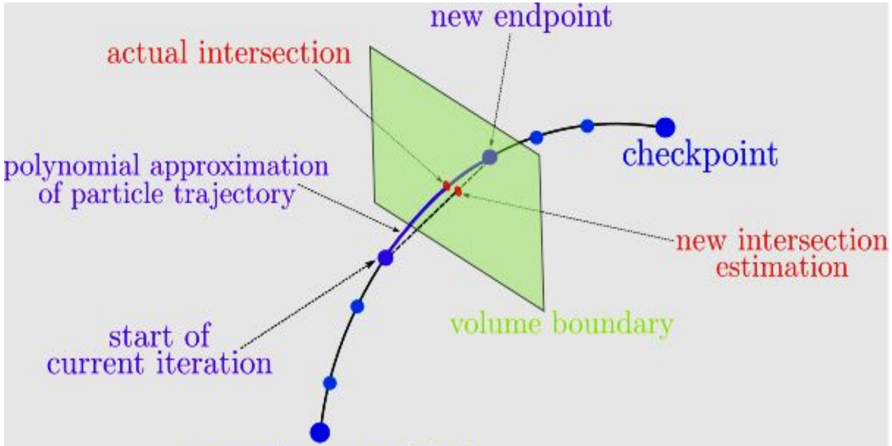


asynchronous **discrete events**
no regular time step

Main QSS features for HEP problems

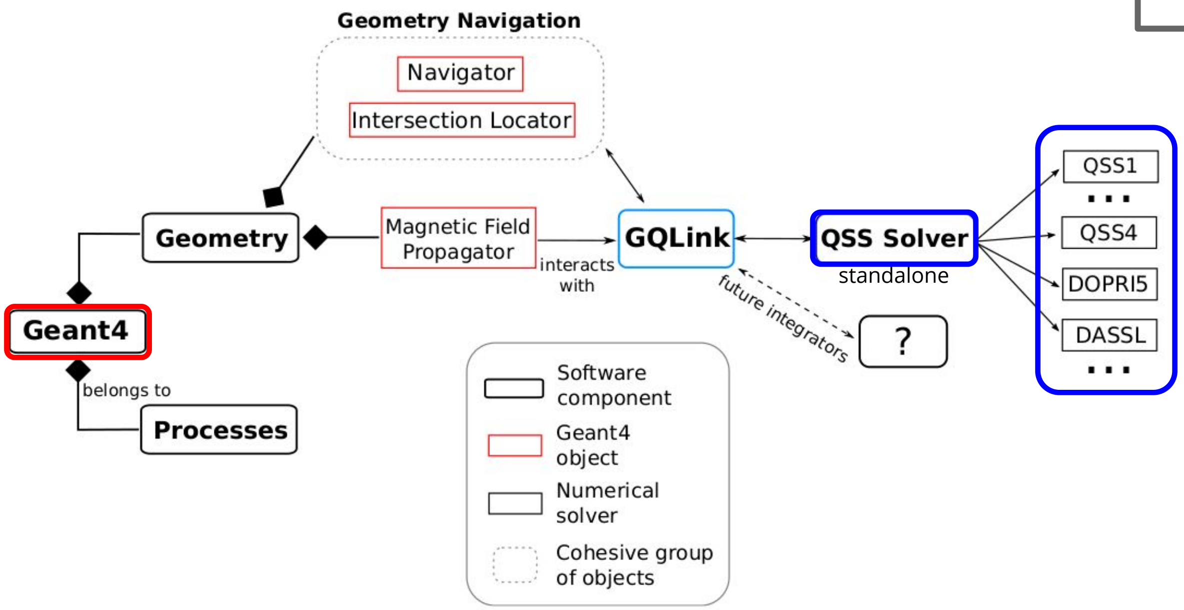
- **Inherent asynchronicity**
  - Decoupled, independent computation of changes in states variables (no “global clock”)
- **Dense trajectory output**
  - Supported by piecewise polynomial approximations of trajectories
- **Lightweight discontinuity handling**
  - Boundary crossings detected by finding roots of simple polynomials

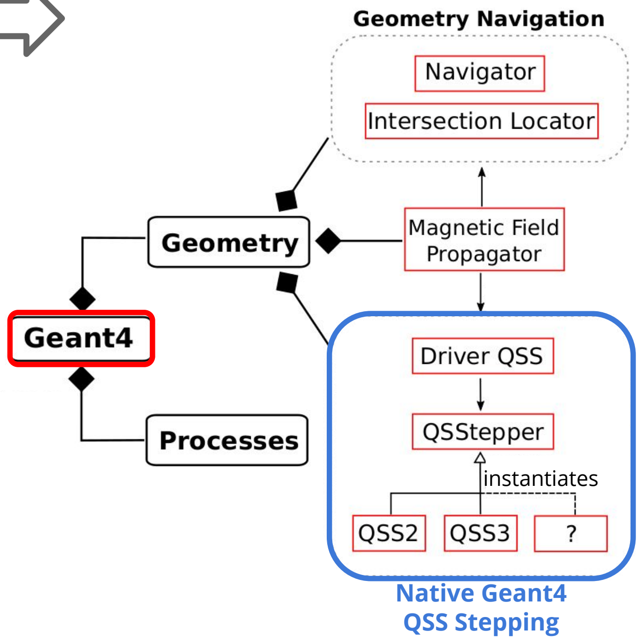




particle trajectory

Integration with G4: High Level architectures



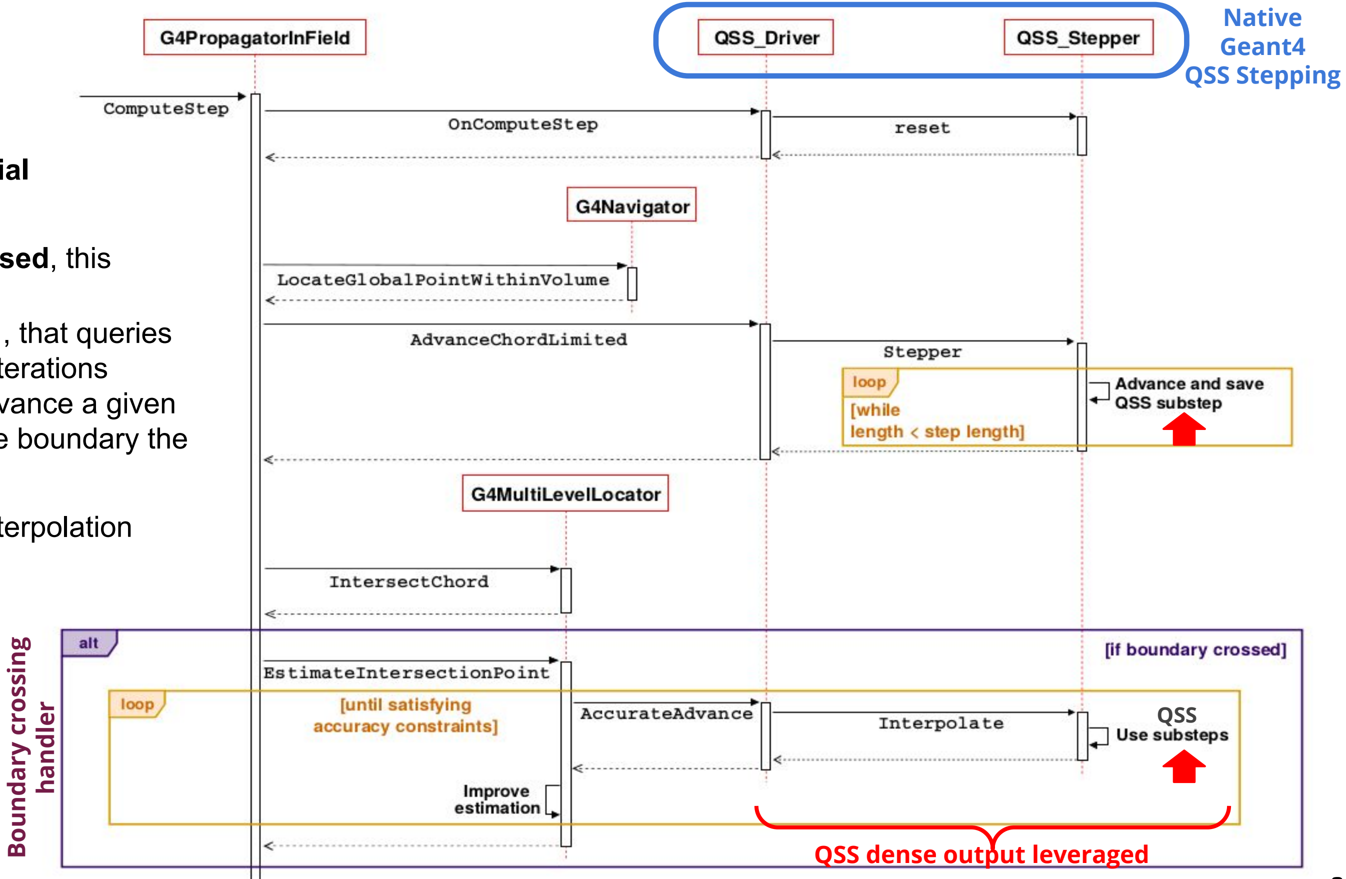


Strategy 1: "Co-Simulation"
- **GQLink** (Geant4 to QSS Solver **Link**)
- Both simulation toolkits preserve their responsibilities

Strategy 2: "Embedded QSS"
- **QSStepper** for Geant4
- New native G4 Steppers

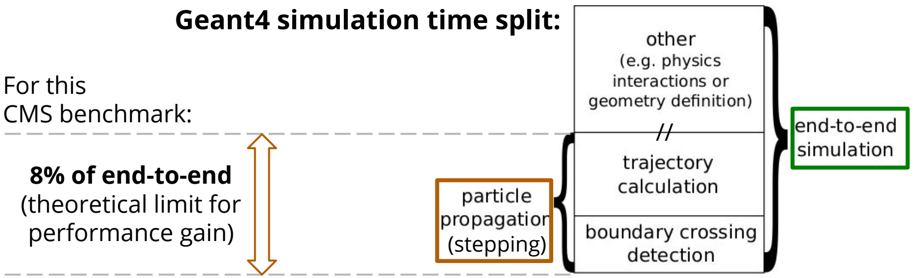
QSS-based step computation sequence in Geant4

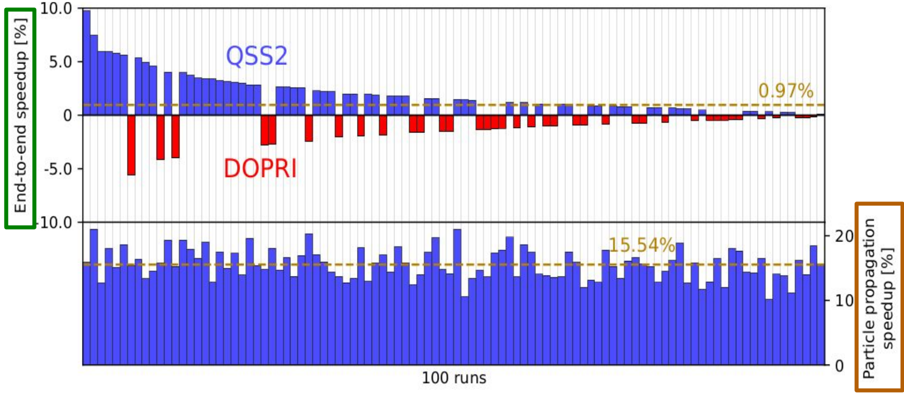
- The **intersection-finding algorithm** starts with a quick test using a linear segment joining the step endpoints (`IntersectChord`) yielding an **initial estimation** of the intersection point
- In case a **volume boundary is crossed**, this estimation is progressively improved (`EstimateIntersectionPoint`) , that queries the Integration Driver on each of its iterations (`AccurateAdvance`) in order to advance a given length and then test which side of the boundary the particle lies in
- The **QSS Driver**, by means of the Interpolation Driver's custom behavior, issues an `Interpolate` call to the **QSS Stepper**
- `Interpolate` **is handled very efficiently** using the **polynomial QSS Substeps** computed previously at each substep



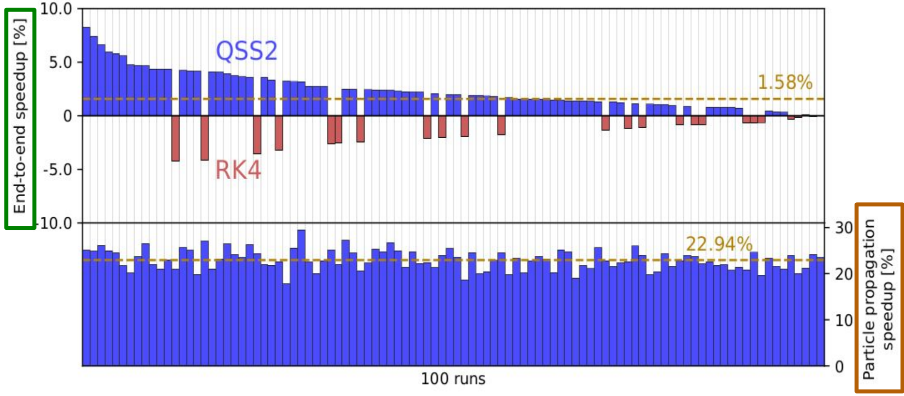
CMS Benchmark results

- Experimental results
  - CMS full Run 1 geometry
    Single π⁻ particles, Physics list FTFP_BERT
  - 100 independent runs, 2000 particle gun events
- QSS2 vs. DOPRI
  - 62 runs favorable for QSS; 38 for Geant4
  - Avg. End to End speedup: **~1%** (max. ~10%)
  - Avg. Stepping speedup: **~15%** (max. ~20%)
- QSS2 vs. RK4
  - 77 runs favorable for QSS; 23 for Geant4
  - Avg. End to End speedup: **~1.5%** (max. ~8%)
  - Avg. Stepping speedup: **~23%** (max. ~30%)





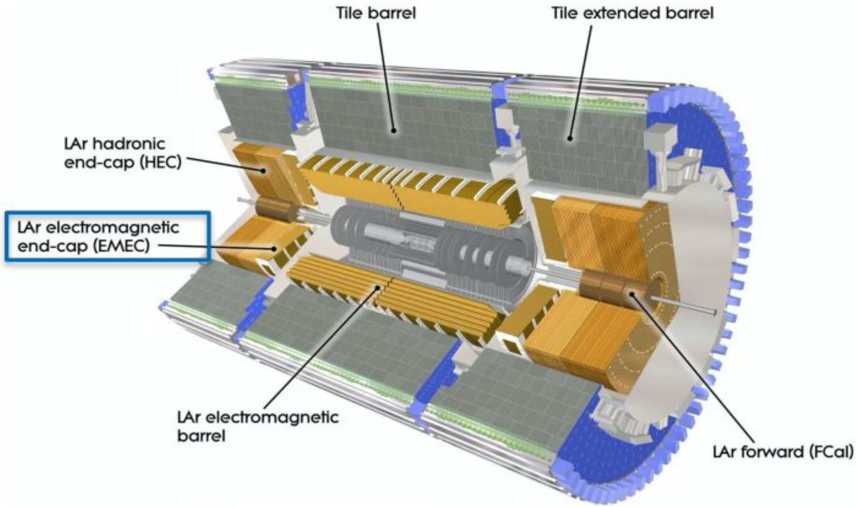
(a) QSS2 vs. DOPRI

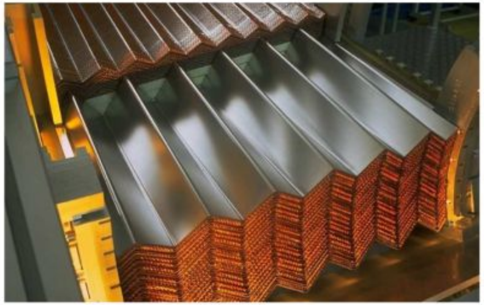


(b) QSS2 vs. RK4

ATLAS as a next reference model

- **ATLAS experiment** as next reference model for QSS methods
- Explore simulation scenarios that use QSS methods integrated into the recently developed **FullSimLight** simulation prototype [1][2], a lightweight standalone Geant4 simulation tool that supports the full ATLAS geometry and the ATLAS magnetic field map
- Of particular interest is the simulation of the **EMEC** detector
- The **EMEC (ElectroMagnetic End-Cap) [3]** is a lead-liquid argon sampling calorimeter with interleaved accordion-shaped absorbers and electrodes.
  - The accordion fold amplitude varies with the radius from the wheel center leading to a varying gap size
  - It has been implemented as a **custom solid *(GeoSpecialShape)*** in GeoModel and in Geant4





Picture of an electromagnetic end-cap module during stacking, showing the accordion structure of the ATLAS EM calorimeters.

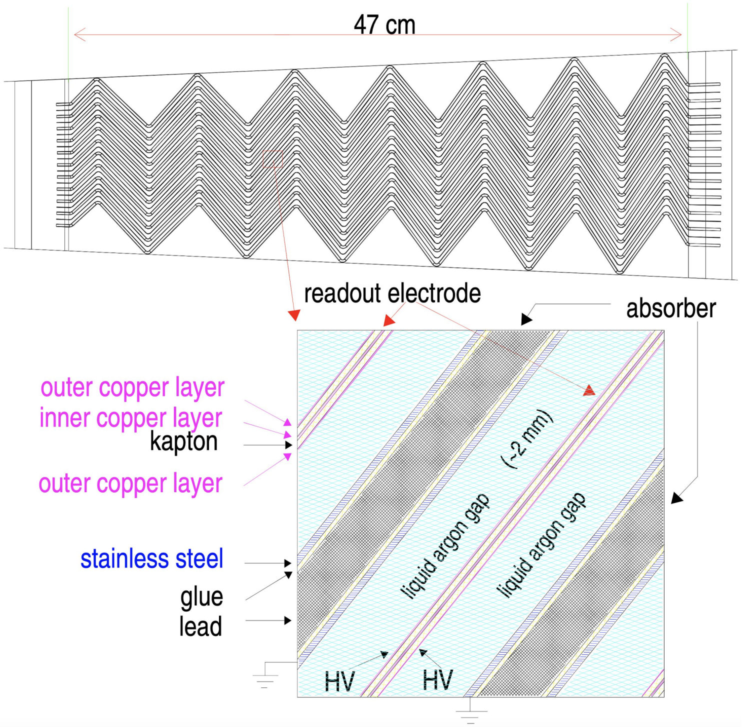
Contributed by Marilena Bandieramonte, U. of Pittsburgh

ATLAS as a next reference model

- The EM calorimeters comprise accordion-shaped copper-kapton electrodes positioned between lead absorber plates and kept in position by honeycomb spacers while the system is immersed in LAr [1]

- The **EMEC** special shape is a well-known hotspot in the ATLAS simulation:
  - takes a significant amount of the total full Geant4 simulation CPU time: **~11.5%**

- The research hypothesis is that the **EMEC's densely layered geometry** is a very **suitable** application case where the efficient discontinuity handling property of QSS can be effectively leveraged.



Module / Class / Source Function / Call Stack	CPU Time ▼	Instructions Retired	Microarchitecture Usage	CPI Rate
			Microarchitecture Usage	
▸ libG4geometry.so	27.0%	26.9%	40.2%	0.665
▸ libG4processes.so	24.2%	21.4%	32.2%	0.693
▾ libGeoSpecialShapes.so	11.5%	14.2%	53.9%	0.571
▸ LArWheelCalculator_Impl::DistanceCalculatorSaggingOff	6.7%	8.9%	50.1%	0.563
▸ LArWheelCalculator	2.4%	3.3%	66.7%	0.570
▸ LArWheelCalculator_Impl::WheelFanCalculator<LArWheelCalculator_Impl::SaggingOff_t>	2.1%	1.8%	45.5%	0.610

Contributed by Marilena Bandieramonte, U. of Pittsburgh

Plans for QSS integration into the Geant4 release

- March/April
  - Goal: Integrate the already developed QSS capabilities (last integration: v10.5)
  - Incorporate members of the UBA Team (Simulation Lab, CS Dept.) to the Geometry and Transport WG
  - Initial tests, code housekeeping, documentation for final users.
- June/July/August
  - Goal: Include QSStepper into the Geant4 Quality Assurance regular procedures (collab. with Soon Yung Jun, Fermilab)
  - Reproduce benchmarks already run by the UBA Team in Argentina
  - Start adding more applications (based on the success of previous benchmarks)
- September/October
  - Goal: QSStepper in the next *development version*
  - Assess performance, identify bottlenecks and opportunities for improvements
  - Design/start new projects for extensions/refinements/enhancements
    - Typically advanced undergrad students, Master's Thesis, 6mo-1yr. Potentially a new PhD student
- November/December
  - Goal: QSStepper in the next *release version*
  - Design/start maintenance procedures/plan
  - More goals TBD according to the progresses made so far

Summary

- Performance gains in Geant4 achievable by QSS methods are a fact
  - But also largely application-dependent

- We are entering a new phase of more comprehensive benchmark-based performance characterizations
  - CMS continues to serve as a reference model (add more test cases)
  - ATLAS to be soon added to the list, bringing in new particular challenges

- HEP as a provider of challenging applications for continued Simulation-specific R&D

Thanks!

Questions?