Progress in adapting the QSS Stepper to the current version of Geant4
Testing and benchmark results

Rodrigo Castro and Lucio Santi

University of Buenos Aires and
ICC-CONICET, Argentina.
rcastro@dc.uba.ar

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Goals of the current stage (work in progress)

- Test the QSS Stepper in a relevant subset of typical examples
- Verify the correct functioning of the examples (for the latest Geant4 version)
- Benchmark the QSS Stepper against the default Geant4 Stepper
- *For a quick background on QSS, see the Backup Slides at the bottom*

Results highlights

- 9 examples tested and verified successfully: **Basic** (B2a, B2b, B4c, B4d, B5) and **Extended** (with magnetic field: 01, 02, 03, 06)
- 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 developed a **toolset for repeatable benchmarking** that can be parameterized to produce systematic performance comparisons between 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

Summary of results: QSS vs. DOPRI

Example	Method	QSS accuracy parameters		% of Intersections per G4 Step	QSS Substeps per G4 Step	User Time (seg)	System Time (seg)	Real Time (seg)	Average Time per G4 Step (seg)	Speedup (QSS vs. DOPRI) Real Time
		dQrel	dQmin							
B2a	DOPRI	N/A	N/A	3.79%	N/A	2.052	0.175	2.614	1.3E-04	N/A
B2a	QSS	1.0E-02	1.0E-03	3.75%	10.191	2.067	0.176	2.654	1.3E-04	-1.53%
B2b	DOPRI	N/A	N/A	3.73%	N/A	2.081	0.178	2.651	1.3E-04	N/A
B2b	QSS	1.0E-02	1.0E-03	3.77%	10.209	2.107	0.178	2.680	1.3E-04	-1.09%
B4c	DOPRI	N/A	N/A	4.31%	N/A	1.623	0.180	2.202	1.1E-03	N/A
B4c	QSS	1.0E-02	1.0E-03	4.02%	2.517	1.603	0.182	2.170	2.1E-03	1.43%
B4d	DOPRI	N/A	N/A	4.31%	N/A	1.637	0.183	2.217	1.1E-03	N/A
B4d	QSS	1.0E-03	1.0E-04	4.19%	5.026	1.605	0.178	2.164	1.1E-03	2.39%
B5 SingleBeam	DOPRI	N/A	N/A	2.78%	N/A	3.442	0.257	4.004	1.1E-01	N/A
B5 SingleBeam	QSS	1.0E-03	1.0E-04	2.78%	1,494.940	3.259	0.245	3.841	1.1E-01	4.06%
Extended Field 01	DOPRI	N/A	N/A	6.51%	N/A	1.020	0.096	1.347	7.4E-04	N/A
Extended Field 01	QSS	1.0E-02	1.0E-03	5.99%	37.787	1.014	0.096	1.333	6.7E-04	1.03%
Extended Field 02	DOPRI	N/A	N/A	19.17%	N/A	1.270	0.124	1.612	9.7E-04	N/A
Extended Field 02	QSS	1.0E-02	1.0E-03	19.17%	3.056	1.265	0.128	1.610	9.7E-04	0.07%
Extended Field 03	DOPRI	N/A	N/A	14.76%	N/A	1.375	0.186	1.783	1.9E-04	N/A
Extended Field 03	QSS	1.0E-02	1.0E-03	9.99%	62.279	2.608	0.451	3.281	8.2E-05	-83.95%
Extended Field 06	DOPRI	N/A	N/A	0.08%	N/A	0.030	0.010	0.037	3.1E-05	N/A
Extended Field 06	QSS	1.0E-02	1.0E-03	0.08%	1.190	0.032	0.012	0.040	3.3E-05	-7.27%

(*)

Note: In all cases (*) where **QSS is able to outperform DOPRI**, only the best combination of QSS accuracy parameters is shown (**rel**ative and **min**imum **Q**uantum **d**elta sizes, **dQrel** and **dQmin**). Other combinations may exist that could even perform worse than DOPRI.

4

Example visualizations

QSS

B5

DOPRI

Extended 02

Extended 01

Extended 03
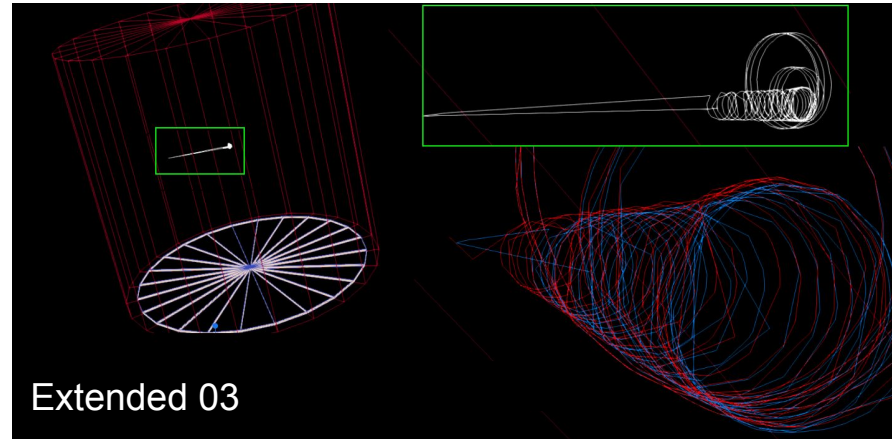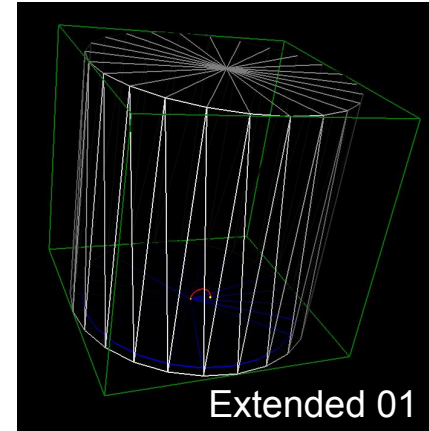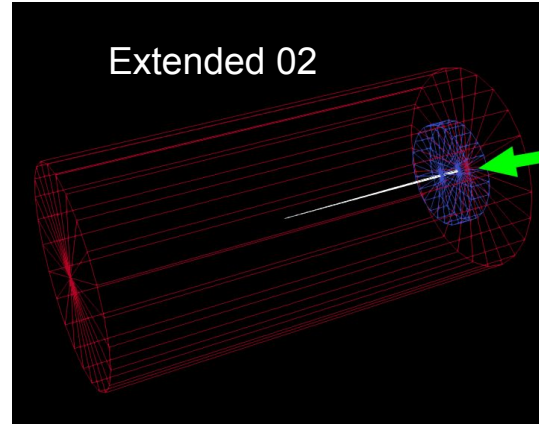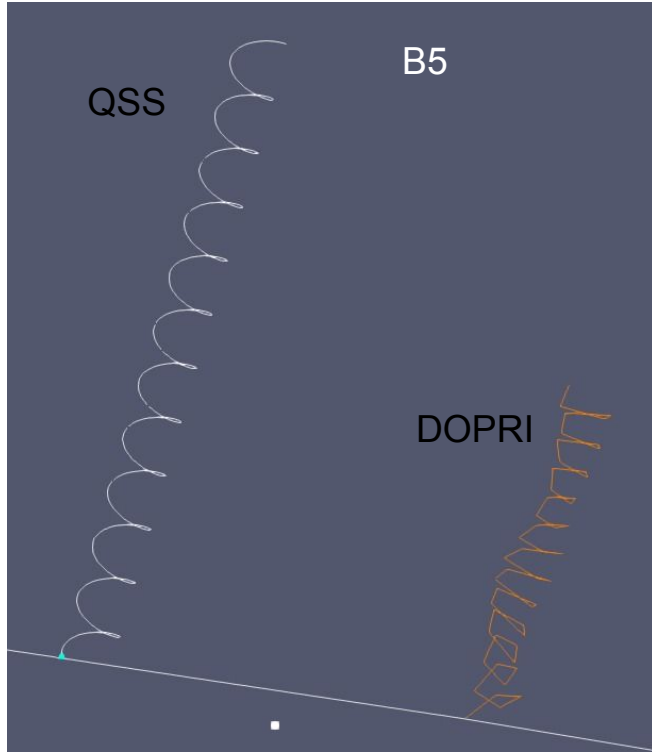
Backup Slides

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**
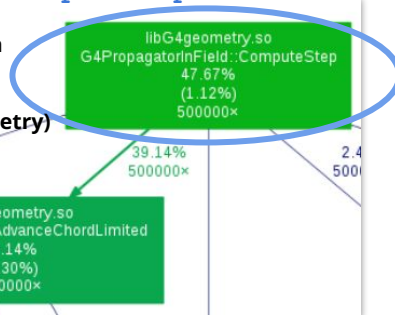 - Attractive performance features for HEP applications

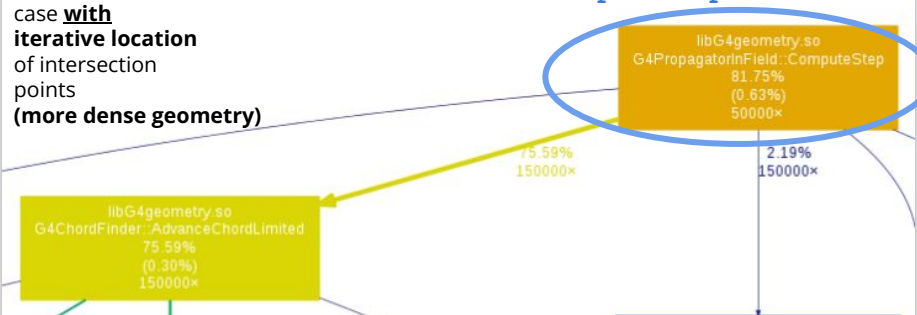**G4PropagatorInField::ComputeStep**
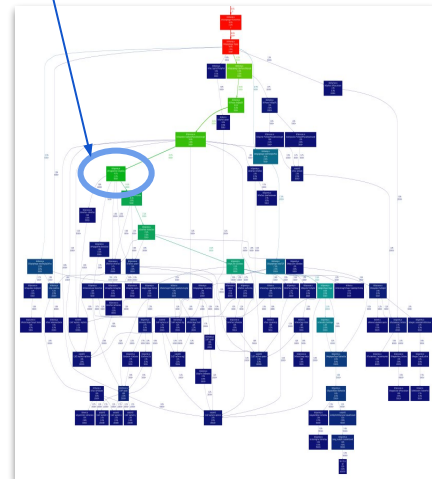
callgrind performance analysis

ComputeStep:~47%

case **without** iterative location of intersection points **(less dense geometry)**

libG4geometry.so
G4PropagatorInField::ComputeStep
47.67%
(1.12%)
500000×

39.14%
500000×

2.4
500

libG4geometry.so
G4ChordFinder::AdvanceChordLimited
39.14%
(0.30%)
500000×

ComputeStep:~81%

case **with** iterative location of intersection points **(more dense geometry)**

libG4geometry.so
G4PropagatorInField::ComputeStep
81.75%
(0.63%)
50000×

75.59%
150000×

2.19%
150000×

libG4geometry.so
G4ChordFinder::AdvanceChordLimited
75.59%
(0.30%)
150000×

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
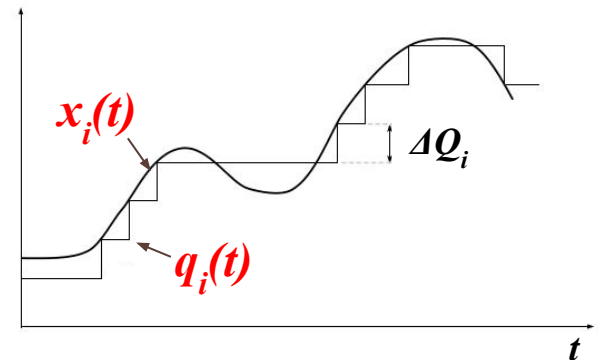L. Santi, L. Rossi, and R. Castro
https://doi.org/10.1016/j.cpc.2020.107619

SED Discrete Event Simulation Lab

GEANT4
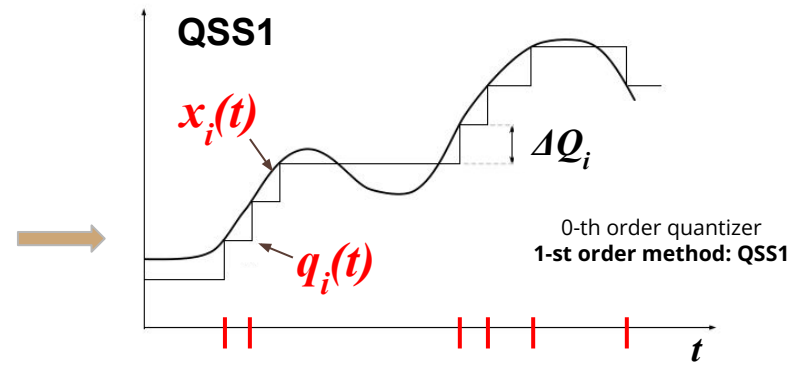A SIMULATION TOOLKIT

Fermilab

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

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

$x_i(t)$

ΔQ_i

$q_i(t)$

t

Higher order QSS methods

QSS1

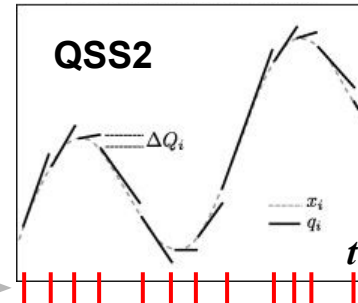$x_i(t)$

ΔQ_i

$q_i(t)$

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

$$q_i(t) = \begin{cases} x_i(t) & \text{if } |q_i(t^-) - x_i(t)| \geq \Delta Q_i \\ q_i(t^-) & \text{otherwise} \end{cases}$$
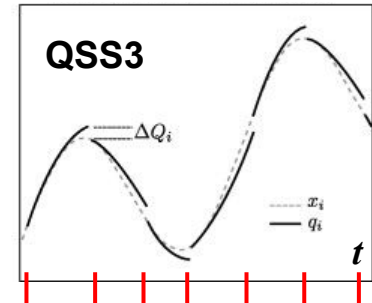
- ΔQ_i is the **quantum**
  - **Maximum deviation allowed** between x_i and q_i (error control)
  - Derived from the **accuracy** demanded by the user
- **Higher order QSS methods** (**QSSn**) follow a similar principle
  - In a **QSS1** method, $q(t)$ follows piecewise constant trajectories
  - In a **QSSn** method, $q(t)$ follows piecewise (n-1)-th order polynomial trajectories

asynchronous **discrete events**
no regular time step

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

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

QSS2

ΔQ_i

x_i
q_i

t

QSS3

ΔQ_i

x_i
q_i

t

11

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
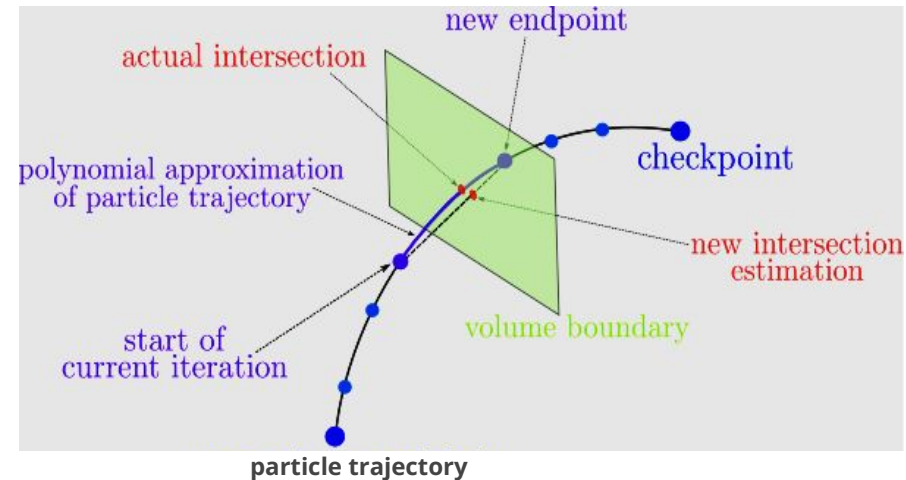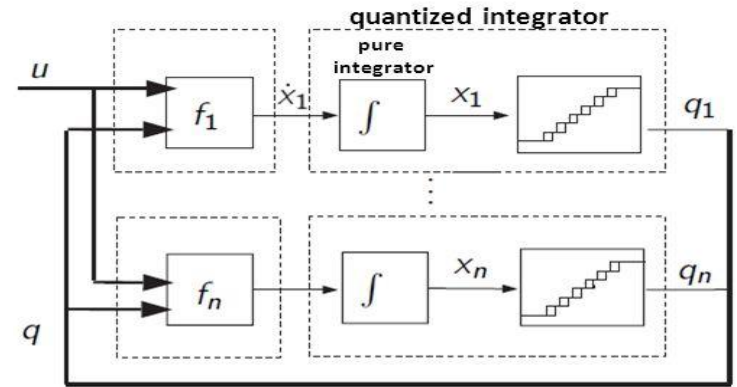
Integration with G4: High Level architectures
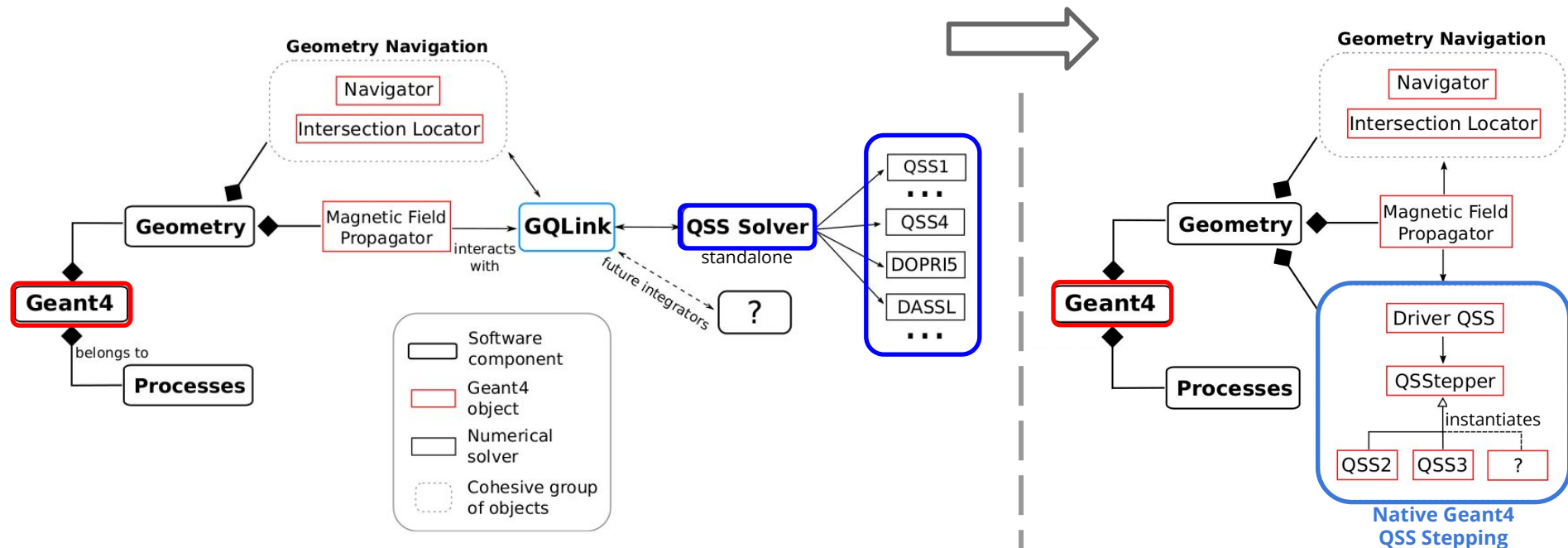
**Strategy 1**: "Co-Simulation"
- **GQLink** (Geant4 to QSS Solver **Link**)
- Both simulation toolkits preserve their responsibilities

Strategy 2: "Embedded QSS"
- **QSSStepper** 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
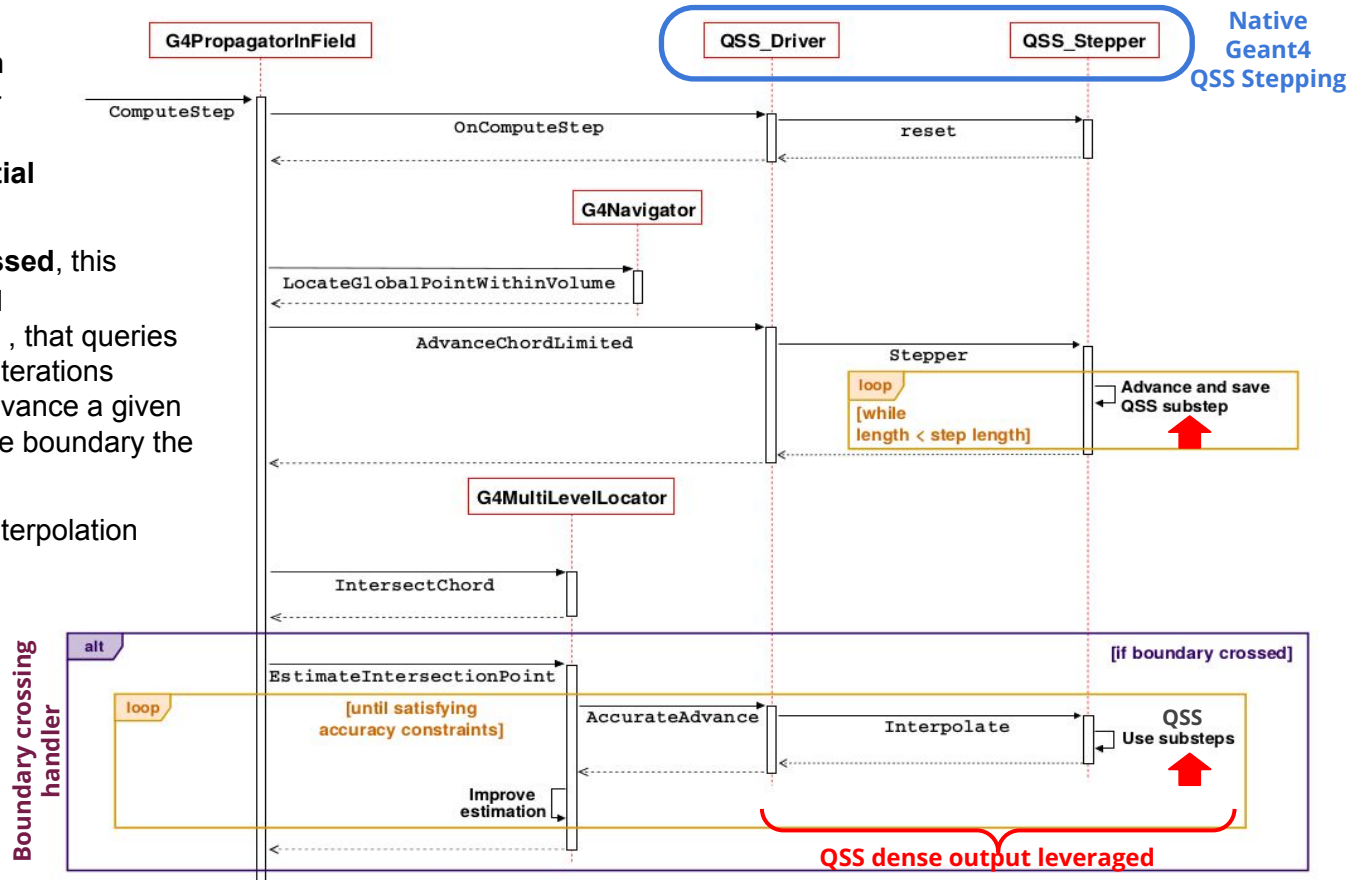
CMS Benchmark results

- **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%)
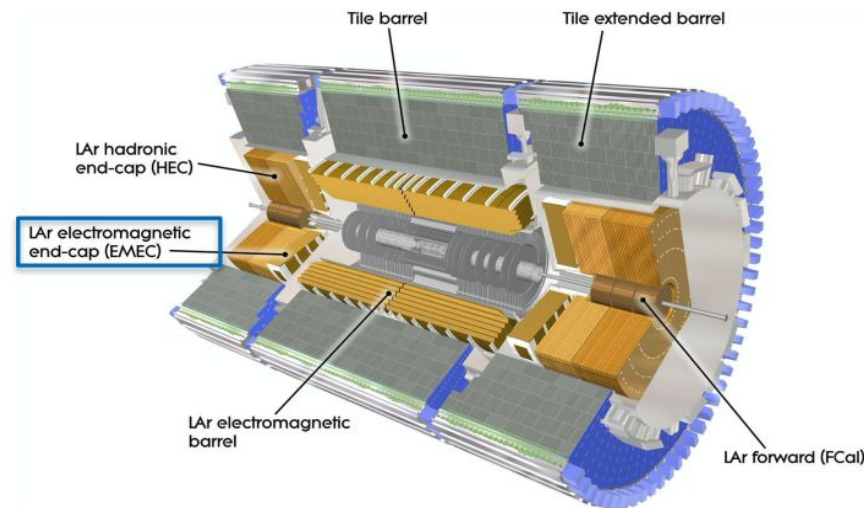
Geant4 simulation time split:

8% of end-to-end (theoretical limit for performance gain)
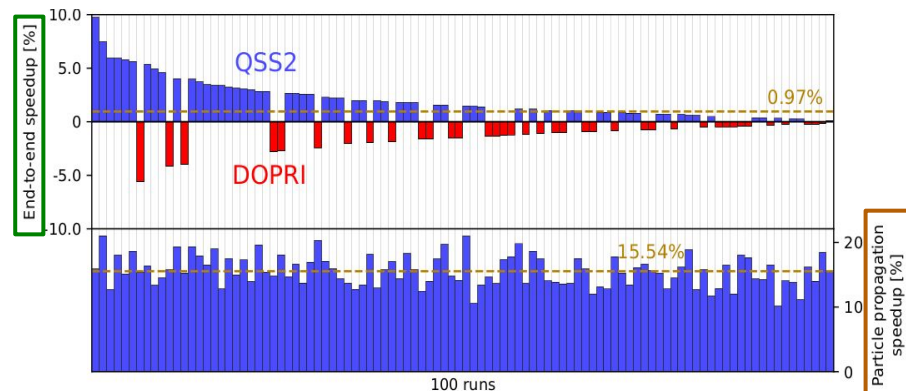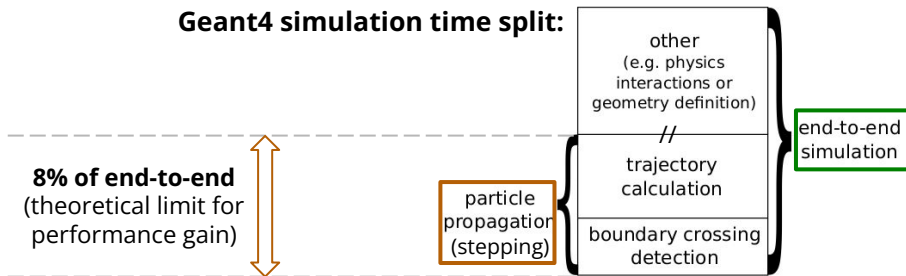
(a) QSS2 vs. DOPRI
(comparison with "DOPRI with Interpolation" is work in progress)
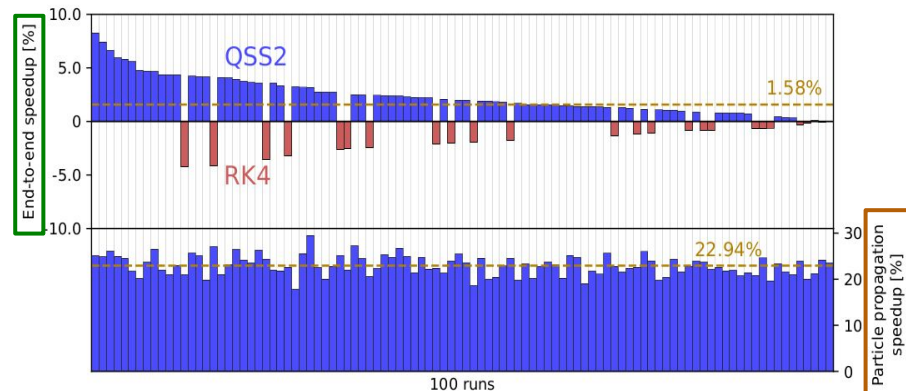
(b) QSS2 vs. RK4

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

Tile barrel
Tile extended barrel
LAr hadronic end-cap (HEC)
LAr electromagnetic end-cap (EMEC)
LAr electromagnetic barrel
LAr forward (FCal)

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

ATLAS as a next reference model

47 cm

readout electrode

absorber

outer copper layer
inner copper layer
kapton
outer copper layer

liquid argon gap (~2 mm)
liquid argon gap

stainless steel
glue
lead

HV   HV

- 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.
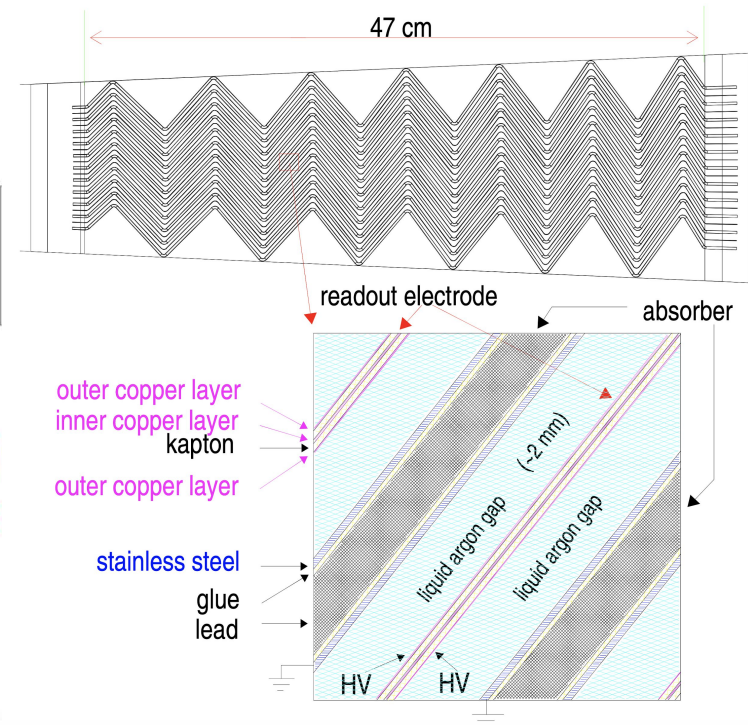
Module / Class / Source Function / Call Stack	CPU Time ▼	Instructions Retired	Microarchitecture Usage	CPI Rate
▶ libG4geometry.so	27.0%	26.9%	40.2%	0.665
▶ libG4processes.so	24.2%	21.4%	32.2%	0.693
▼ libGeoSpecialShapes.so	11.5%	14.2%	53.9%	0.571
▶ LArWheelCalculator_Impl::DistanceCalculatorSaggingOff	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?