Application of State Quantization-Based Methods in HEP Particle Transport Simulation

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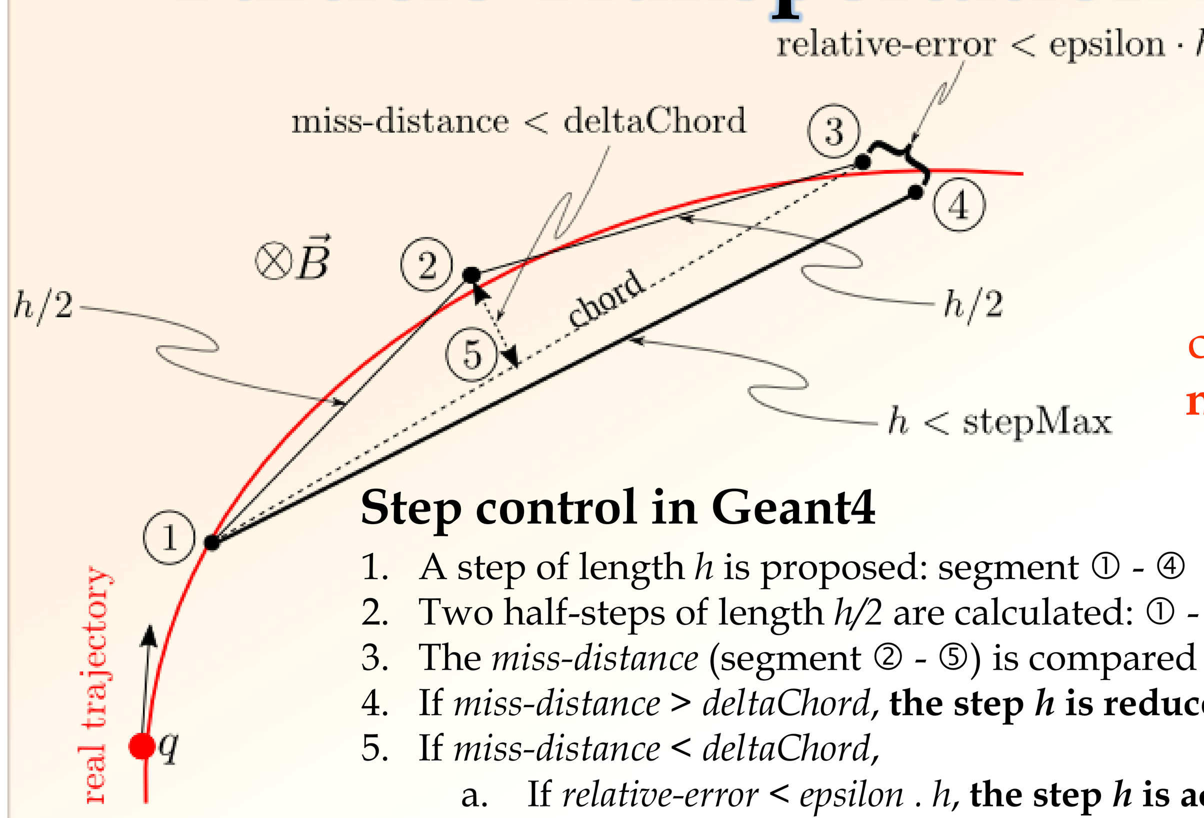
Abstract

Simulation of particle-matter interactions in complex geometries is one of the main tasks in high energy physics (HEP) research. An essential aspect of the task is an accurate and efficient handling of particle transport and crossing volume boundaries within a predefined (3D) geometry and a magnetic field.

The Quantized State Systems (QSS) family of numerical methods [2,4] provide attractive features for these types of problems, such as a dense output, which consists in sequences of polynomial segments whose coefficients change only at discrete events, and lightweight detection and handling of boundary crossings based on explicit root-finding of polynomial functions.

In this work we present a performance comparison between a QSS-based standalone solver [3] and combinations of standard fixed step 4th order Runge-Kutta (RK4) and adaptive step RK4/5 methods in the context of Geant4 [5]. Results showed speedups up to 8x in case studies for a single particle oscillating harmonically in the x-y plane with a uniform B field in the z plane, with up to 200 crossing planes.

Particle Transportation in Geant4



Simulation performance depends strongly on the computing effort needed by the **numerical integration methods**

Step control in Geant4

1. A step of length h is proposed: segment ① - ④
2. Two half-steps of length $h/2$ are calculated: ① - ② and ② – ③ (as typical for RK4)
3. The *miss-distance* (segment ② - ⑤) is compared against *deltaChord*
4. If *miss-distance* > *deltaChord*, **the step h is reduced** and the process starts again from 1
5. If *miss-distance* < *deltaChord*,
   a. If *relative-error* < *epsilon* . h, **the step h is accepted** and the particle is moved to ③
   b. If *relative-error* > *epsilon* . h, **the step h is rejected and reduced** using an adaptive step RK4/5 to improve accuracy
6. If segment ① - ③ crosses a volume, Geant4 computes the **boundary crossing intersection point using a custom iterative algorithm based on RK4/5**

Quantized State Systems (QSS) methods

Efficient boundary crossing detection with dense output

QSS Solvers for ODEs [2,4]

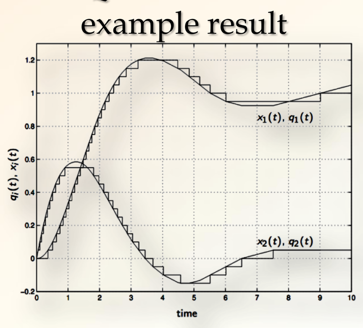
$$\dot{\mathbf{x}}(t) = f(\mathbf{x}(t))$$

$$\dot{\mathbf{x}}(t) = f(\mathbf{q}(t))$$

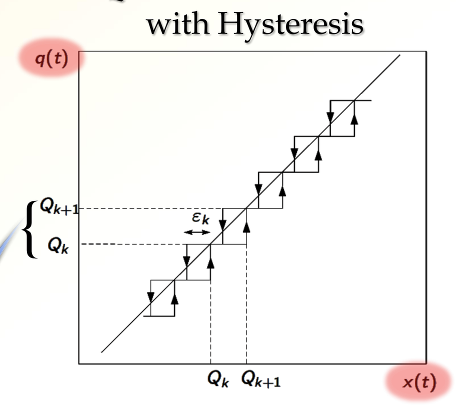
State Quantization

- Discretize (**Quantize**) **state variables** $x(t)$ instead of time slicing (as in classical Discrete Time Systems like the Runge-Kutta family)
- Keep time axis **continuous**
- Results in a Discrete-Event System

A QSS1 simulation example result



Quantization function with Hysteresis



Quantum ΔQ → **Accuracy control**

QSS Main Features

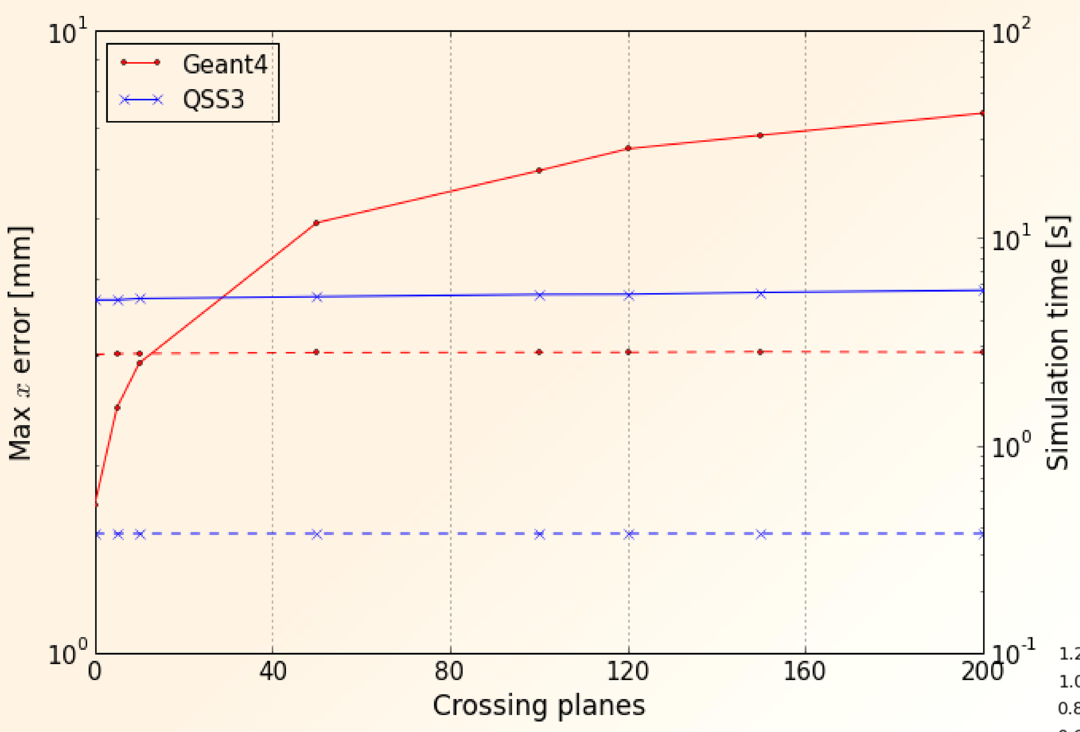
- **Naturally asynchronous:** Decoupled handling of changes in different state variables.
- Intrinsically **exploits system's sparsity:** Only related variables affect each other
- Remain **practically stable** and the **global integration error** can be estimated.
- Efficient **handling of discontinuities:** Polynomial dense output on a continuous time base

QSS in HEP simulation [1]

- **Boundary crossings** modeled as discontinuities (Discrete Events).
- **Efficient detection and handling:** Lightweigth root-finding of explicit polynomial functions.

Simulation results using QSS Solver

Tracking only scenario

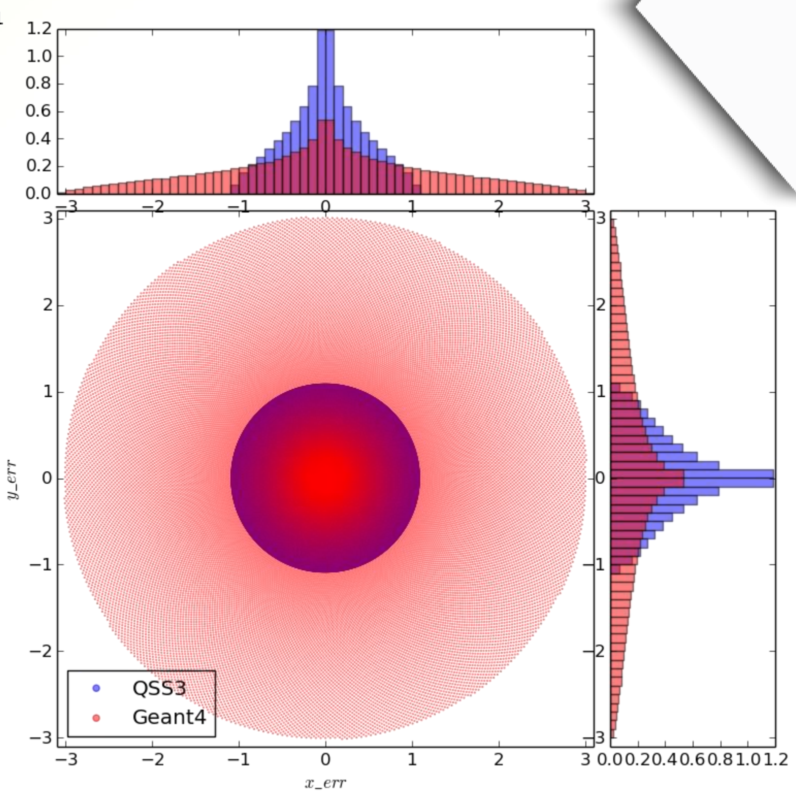


Error (left y axis, dashed lines) and **Simulation Time** (right y axis, solid lines) vs. **Number of Crossing Planes**

Experimental setup

- **Track length**: 1 km
- **Relative accuracy**: 10^{-5}
- Other Geant4 parameters
  - *deltaOneStep*: 10^{-2} mm
  - *epsilonMin*: 10^{-5}
  - *epsilonMax*: 10^{-5}
  - *stepMax*: 20 mm
  - *deltaChord*: 0.25 mm
  - *deltaIntersection*: 10^{-5} mm

- Third Order QSS (QSS3) in **QSS Solver** **scaled better** than RK4/5 in **Geant4** with an increasing number of planes
  - **Up to 8x faster for 200 planes**
- **Smaller errors** in $x(t)$ and $y(t)$ trajectories



Distribution of errors in $x(t)$ and $y(t)$ for Geant4 and QSS3

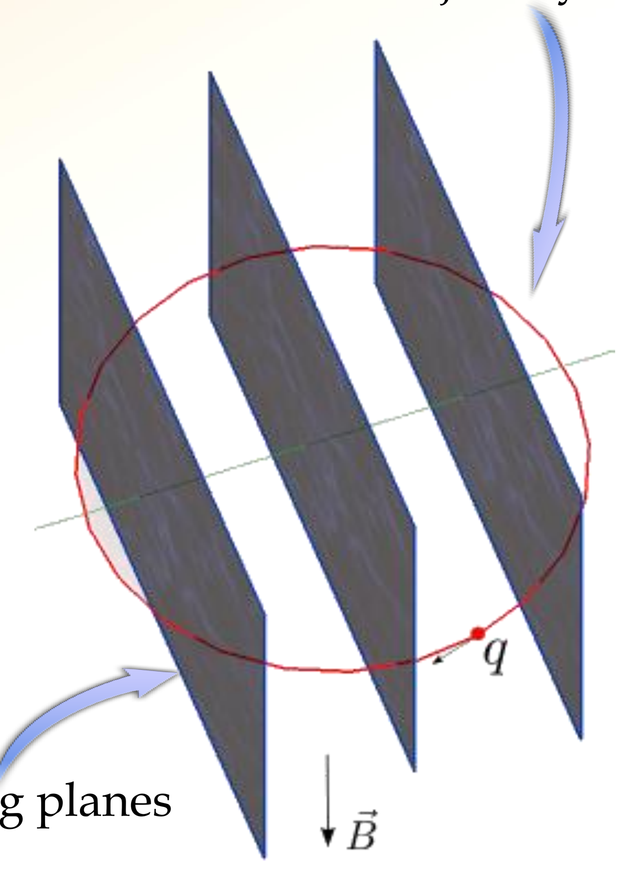
Case study

- Circular motion of a single electron in the x-y plane
- Uniform magnetic field in the z plane
- Equidistant parallel crossing planes
- Physics processes turned off

Known analytic solution facilitates **error analysis**

$$\begin{cases} x(t) &= x_0 + R\sin(\omega\, t) \\ y(t) &= y_0 + R\cos(\omega\, t) \\ v_x(t) &= R\,\omega\cos(\omega\, t) \\ v_y(t) &= -R\,\omega\sin(\omega\, t) \end{cases}$$

Particle trajectory



Crossing planes

$\vec{B}$

GQLink: QSS methods within Geant4

Work in Progress

- We are currently embedding QSS into Geant4 through an abstract interface: **GQLink**
- **GQLink** can be fully integrated into Geant4's building process to provide three new shared libraries:
  - `libqss`: QSS core functionality
  - `libgqlink`: API interfacing Geant4 and QSS
  - `libmodel`: model definition and structure (e.g., Lorentz equations)
- **GQLink** is **not a new Geant4 stepper** but an **abstract, clean, single entry point interface** to the QSS Solver library, provided by the QSS Solver simulation engine [3]
- Early results based on Geant4 10.02.p01: Statistically consistent simulations for a CMS application featuring full detector geometry, volume base magnetic field and Pythia $pp \rightarrow H \rightarrow ZZ$ events (Z to all channels; $\sqrt{s}$ = 14 TeV).

Conclusions and future work

- We studied how QSS3, an asynchronous, discrete event based, third order accurate integration method performs in the context of a basic HEP model.
- We compared QSS3 as implemented in the standalone tool QSS Solver [3] against fourth order Runge-Kutta as implemented in Geant4.
- Our results showed that QSS3 performance scales significantly better in situations with increasing number of volume crossings, as it was expected due to its efficient discontinuity handling property (dense output).
- An implementation of the QSS family of methods within Geant4 (GQLink) is currently being tested on a realistic HEP application. Performance studies are underway.

References

[1] N. Ponieman and R. Castro, *Application of state quantization based-methods in the particle simulator Geant4*, Master's thesis, School of Exact and Natural Sciences, University of Buenos Aires, 2015

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