GQLink

An implementation of Quantized State System (QSS) methods in Geant4

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Introduction

Motivation of this work

- Simulation in HEP involves the numerical solution of ODE systems in order to determine the trajectories described by charged particles in a magnetic field.
- As a particle moves through a detector, each volume crossing interrupts the underlying numerical solver.
- Traditional methods can invest considerable computational efforts to handle very frequent discontinuities accurately (detection of intersection points).

Motivation of this work

- **Quantized State System** methods (**QSS**, Kofman 2001 [7]) is a modern family of numerical integration methods exhibiting attractive features for this type of HEP simulation scenarios.
- The goals pursued in this work are:
  - To develop a proof-of-concept implementation of QSS within the Geant4 simulation toolkit.
  - To address its suitability as an alternative production integrator, and
  - To characterize its performance in a realistic HEP application.

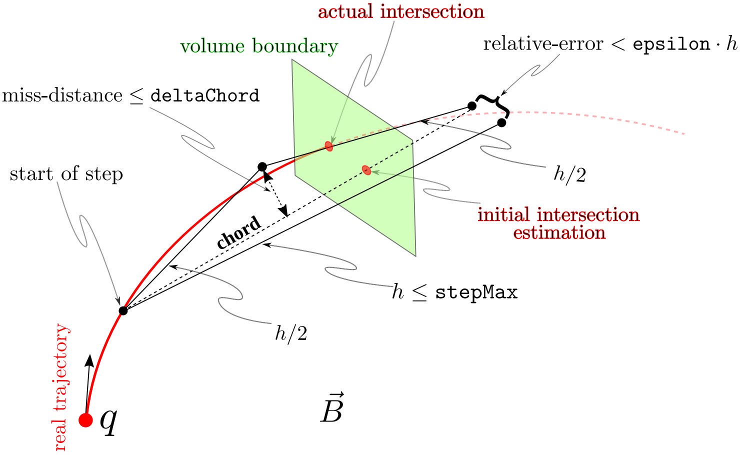
Background information

The Geant4 simulation toolkit

- **Geant4** [1] is the most widely used simulation toolkit in contemporary HEP experiments.
- Provides classical numerical methods based on **time discretization** [3] (variations of the Runge-Kutta family of numerical solvers [4]).
- Uses custom iterative algorithms to approximate the event times of each spatial discontinuity (which mostly occur after a physics interaction).
- When these events are very frequent, they can dominate the CPU time dedicated to the integration method, and reduce considerably its performance.

Geant4: particle transport

Transportation of a charged particle q along a step of length h proposed by a physics process:



⇒ a total of 11 RHS evaluations involved for the 4th order Runge-Kutta.

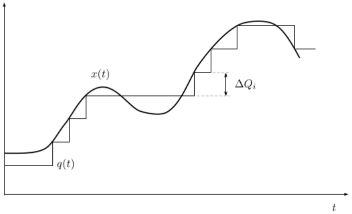
Quantized State System methods

- QSS methods are based on **state variable quantization**.
- As opposed to traditional solvers which discretize **time** (e.g., Runge-Kutta family) QSS methods discretize the system's **state variables**.
- **Continuous state variables** are thus **quantized** and approximated by their corresponding **quantized variables**.
- The relation between both is given by a **quantization function** which is in charge of the **error control** and **accuracy control**.

ODE system		Quantized system
$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t))$	$\Rightarrow$	$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{q}(t))$

QSS1: first order quantization function

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



- ΔQ_i is the **quantum**.
  - **Maximum deviation allowed** between x_i and q_i (error control).
  - Derived from the **precision** demanded by the user.
- Higher order methods (**QSS**n) follow essentially the same principle.
  - From the definition above, in QSS1 $q(t)$ follows piecewise constant trajectories.
  - In QSSn, $q(t)$ is composed of piecewise $(n-1)$-th order polynomials.

QSS features

- QSS features attractive for HEP problems
    - **Asynchronicity**
      Decoupled, independent computation of changes in states variables.
    - **Lightweight discontinuity handling**
      Boundary crossings detected by finding roots of polynomial equations.
    - **Dense trajectory output**
- Selected speedups reported for QSS vs. time-slicing methods modeling processes in various domains [6][2]

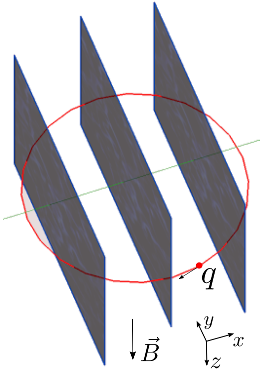
Model	Features	Speedup
advection-reaction	10^4 state variables	30x
spiking neurons	10^3 state variables	35x
logic inverters chain	4000 neurons, 80 connections per neuron	100x
cellular division	100 cells, 600 state variables	100x to 1000x

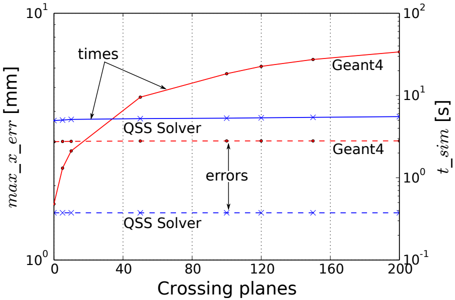
Standalone tool: QSS Solver

- The QSS Solver [5] is an open-source standalone simulation tool.
- Provides C implementations for several QSS methods.
- Provides also implementations of some traditional algorithms (e.g., Dormand-Prince method).
- Our **GQLink interface** partially relies on the QSS Solver's simulation engine.

Preliminary comparison between Geant4 and QSS Solver

- Circular 2D particle motion, uniform magnetic field, crossing equidistant parallel planes.
  - Known exact analytic solution facilitates error analysis.
  - Physics processes turned off.





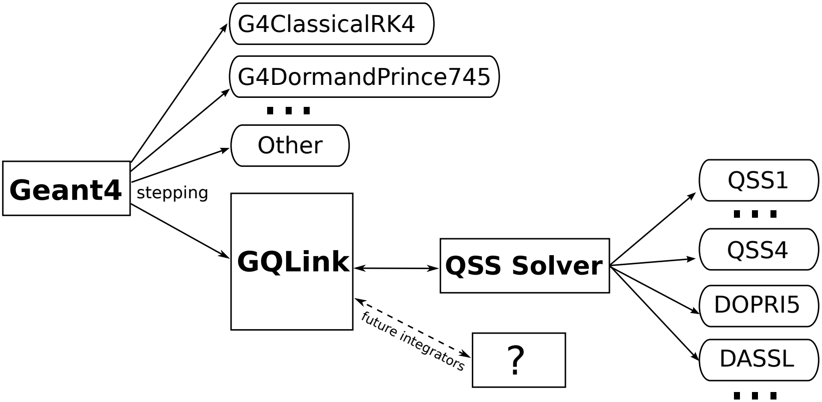
- With 200 plane crossings and a track length of 100 m, QSS Solver is 6x faster than Geant4[9][8].

Geant4 to QSS Link (GQLink): an implementation of QSS within Geant4

GQLink: QSS within Geant4

- GQLink is a proof-of-concept implementation of QSS in Geant4.
  - Geant4 version `10.03.p01` (released February 24, 2017).
  - QSS Solver engine from version 3.0 (as of March 2016).
- Provides three new shared libraries to Geant4:
  - `libqss`: QSS core functionality.
  - `libgqlink`: interface API between Geant4 and QSS.
  - `libmodel`: model definition and structure (i.e., Lorentz equations).
- QSS methods have complete control over the propagation for each Geant4 transportation step.
  - QSS manages accuracy in its own terms (through the control of the quantum ΔQ).

GQLink: high-level diagram



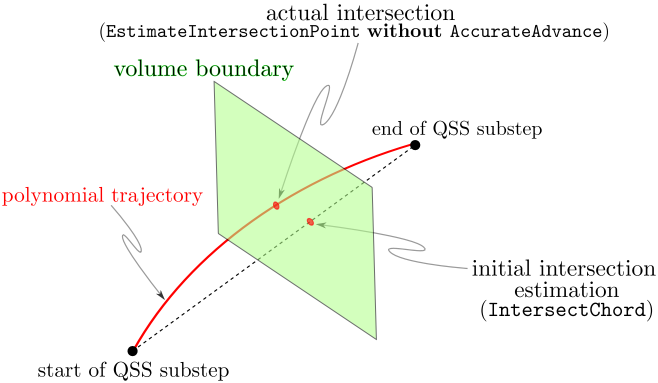
- GQLink: not another Geant4 *stepper*.
- An abstract, clean, single entry point interface to the QSS Solver family of numerical integration methods.

Detection of boundary crossings

- Boundary crossings are detected through Geant4's geometry library.
- Follows same call pattern as in standard Geant4 simulations:
  - `LocateGlobalPointWithinVolume`
    - Notifies the geometry navigator that the particle has moved to a new position inside the current volume.
  - `IntersectChord`
    - Computes an initial estimation of an intersection by means of a linear segment between the endpoints of the step.
  - `EstimateIntersectionPoint`
    - Refines the initial estimation mentioned above through an iterative procedure.

Detection of boundary crossings

Cheaper particle transport until the crossing point using QSS polynomial dense output instead of iterative procedures:



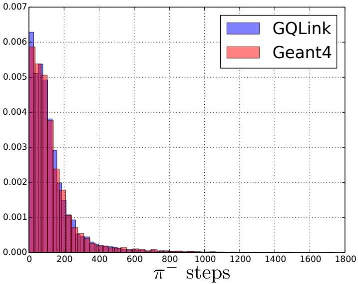
- QSS dense output not fully exploited yet for boundary crossing detection ⇒ main goal driving our current work.

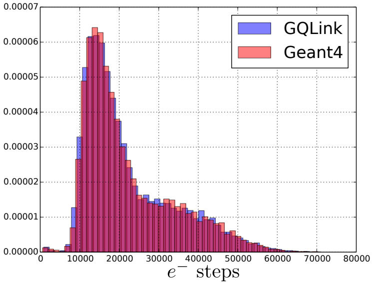
Results

CMS application analysis

- GQLink validation was performed against a standalone Geant4 application featuring:
  - Full CMS (RunI) detector geometry.
  - Volume base magnetic field excerpted from CMSSW.
  - Particle gun shooting π^- particles (10 GeV, 10^4 events).
  - Pythia $pp \to H \to ZZ$ (Z to all channels) ($\sqrt{s} = 14$ TeV, 50 events).

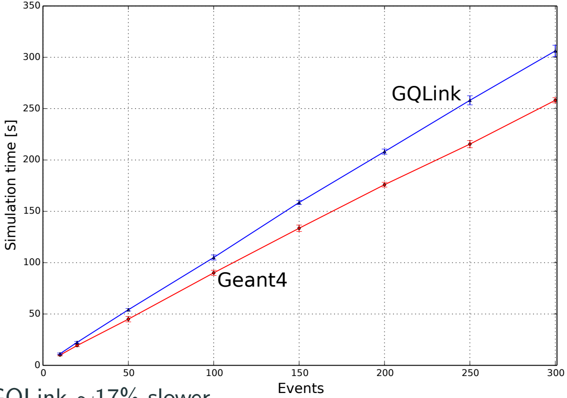
- Step count distribution for π^- (left) and secondary electrons (right) for 10^4 single π^- events, showing equivalency of GQLink simulations:





CMS application: performance comparison

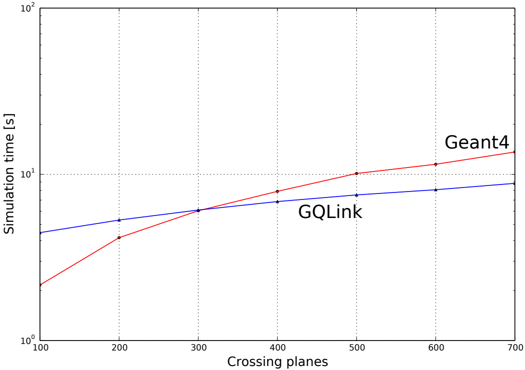
- **Single π^- events**



  - GQLink ~17% slower.
- **Pythia $H \to ZZ$ events**
  - GQLink ~22% slower (5.86 hours vs. 4.8 hours).
- Geant4 stepper: `G4ClassicalRK4` (accuracy set to $\epsilon = 10^{-5}$).

Alternative scenario: helix and parallel planes

- Different scenario: helix trajectory crossing parallel equidistant planes & more frequent boundary crossings.
- Physics processes turned off.
- Using `G4ClassicalRK4` stepper (accuracy set to $\epsilon = 10^{-5}$).

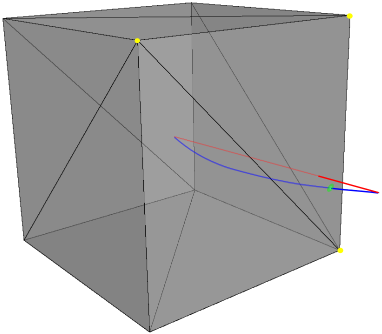


- GQLink outperforms Geant4 when using $\geq$ 300 planes ($\sim$35% faster for 700 planes).

Work in progress

Work in progress

- Exploitation of QSS capabilities for efficient geometry crossing detection:
  - Conversion of Geant4 solids into faceted polyhedrons.
  - Finding intersection points by (analytically) solving a polynomial equation given by the equation of a plane and the QSS polynomials approximating the trajectory.
  - Candidate plane given by the face crossed by the linear segment joining the endpoints of a step.



Conclusions

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- We developed **GQLink**, a prototype for QSS methods within Geant4.
- Validation: number of steps and tracks produced are statistically consistent with Geant4's for both toy examples and realistic HEP applications.
- Performance:
  - We found that GQLink can outperform Geant4 in certain simplified scenarios involving tracking only.
  - Preliminary tests revealed GQLink is currently $\sim$17% slower than standard Geant4 in a full CMS realistic scenario (using single π^- events).
- From an abstract viewpoint, GQLink also opens new possibilities to interface Geant4 with any external stepper.

Thank you!

Questions?

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