-333a33Experiment 3 - Vary deltaQDoc-Start -33a33Experiment 3 - Vary deltaQDoc-Start 43b33Experiment 3 - Vary deltaQDoc-Start 4b33Experiment 3 - Vary deltaQDoc-Start 54a34Experiment 3 - Vary deltaQDoc-Start 5a34Experiment 3 - Vary deltaQDoc-Start 64b34Experiment 3 - Vary deltaQDoc-Start 6b34Experiment 3 - Vary deltaQDoc-Start

Simulation methods for equations of motion in Geant4

Exploring the suitability of Discrete Event driven Quantized State Systems (QSS) methods and the different parameters involved in Geant4

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Fermilab, October 29th 2015

Outline

1. Transportation Chain in Geant4
   - Visual Analysis
   - Parameters Involved
   - Runge-Kutta
2. Quantized State System
   - Introduction to QSS
   - QSS Explained
3. Exploring Geant4 Parameters
   - Vary epsilon
   - Experiment 2 - Vary stepMax
   - Experiment 4 - Vary deltaChord
4. Exploring QSS Parameters
   - Experiment 3 - Vary deltaQ
5. Exploring geometry crossings in Geant4
   - Experiment 5 - Vary number of Planes in $\hat{x}$

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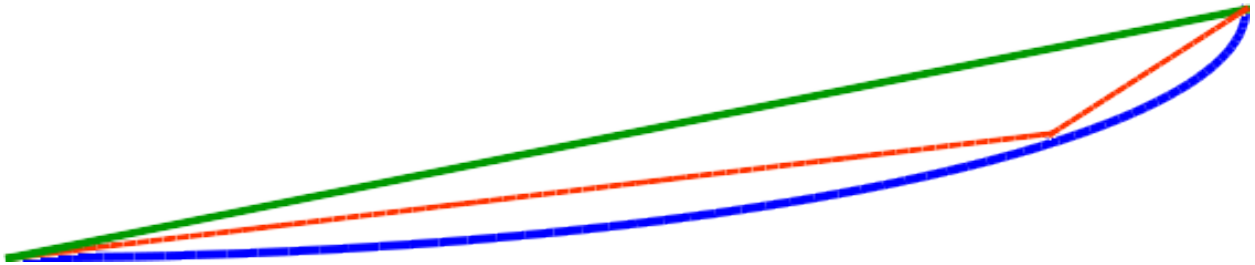
Transportation Chain in Geant4

Visual Analysis

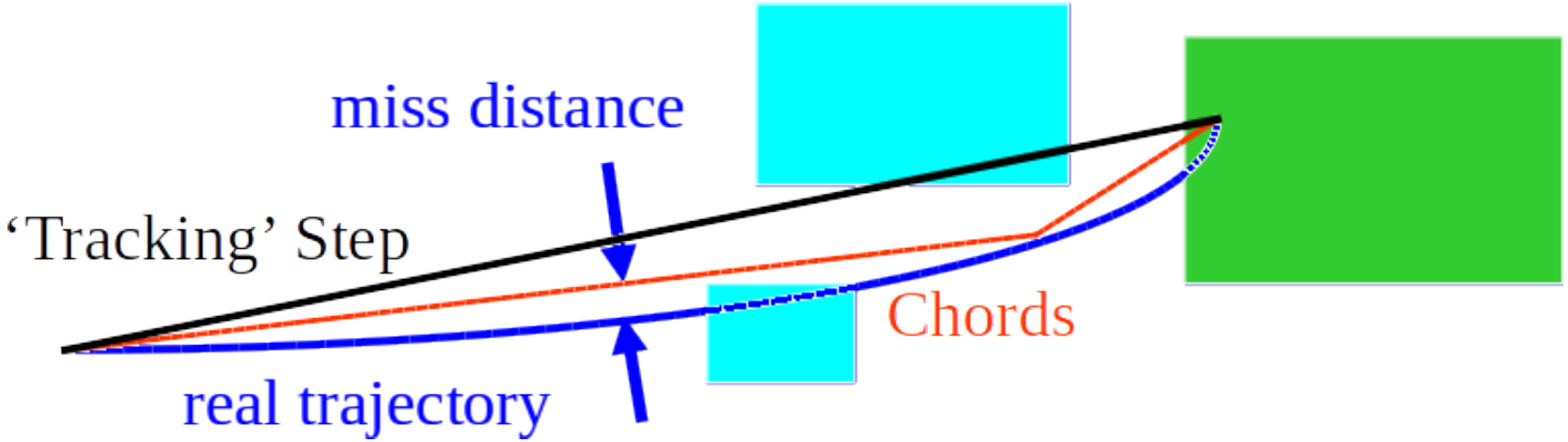
- To propagate a particle inside a field, we solve its equation of motion.
- Geant4 uses Runge-Kutta method to solve the ODE (and other alternatives for specific cases.
- Each step may be divided in smaller steps.
- Geant4 breaks up the curved path into linear chord segments
- Chord segments are determined so that they closely approximate the curved path (if the current error is large, the path uses more segments).



Transportation Chain in Geant4

Visual Analysis

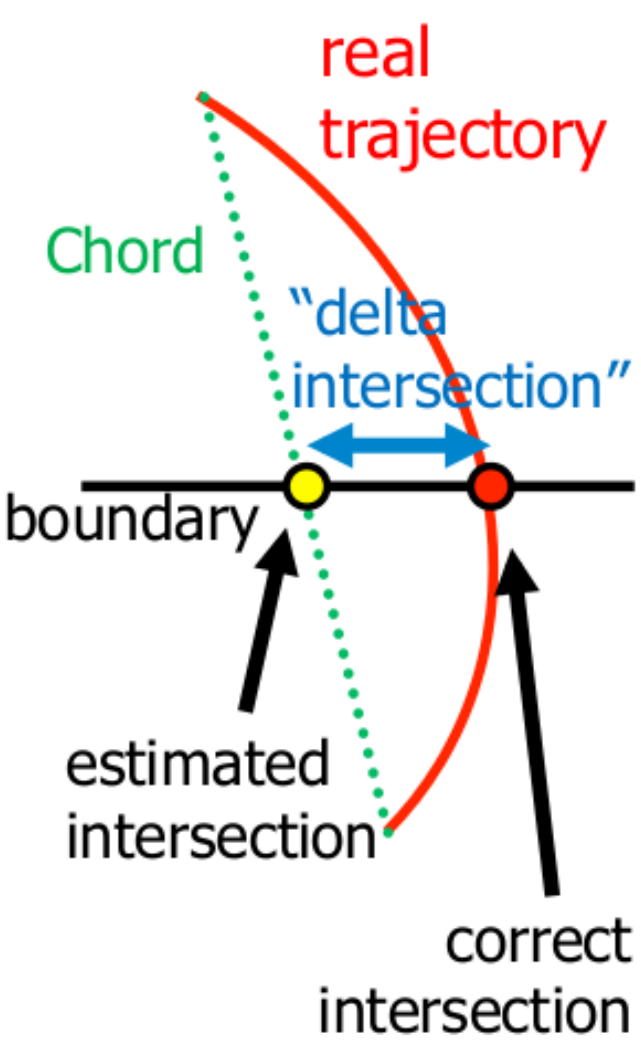
- Using the chords, G4Navigator is interrogated to check if a volume boundary was crossed.
- User can set the accuracy of the volume intersection: the parameter is called *missed distance*. WRONG?
- User can set the maximum distance from the chord: the parameter is called *missed distance*. CORRECT?



Transportation Chain in Geant4

Parameters Involved

- delta intersection controls the accuracy of the intersection with a volume boundary. It limits a bias on the algorithm (intersection point always *inside* of the curve).
- *delta one step* controls the accuracy for the endpoint of an ordinary integration step (not crossing any boundary).
- *epsilonMin* and *epsilonMax* control the local error of each substep.



Transportation Chain in Geant4

Runge-Kutta

We describe here the Runge-Kutta method of 4th order, used by Geant4.

- Let $\dot{y} = f(t, y)$ and $y(t_0) = y_0$ be our initial problem.
- A step size $h > 0$ should be picked, which defines
  $y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$
  $t_{n+1} = t_n + h$
- $k_1 = f(t_n, y_n)$ respresents the increment based on the slope at the initial point
  $k_2 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1)$ increment based on the slope at the midpoint (calculated with h_1)
  $k_3 = f(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2)$ increment based on the slope at the midpoint (now calculated with h_2)
  $k_4 = f(t_n + h, y_n + hk_3)$ increment based on the slope at the end of the interval, using k_3.

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- Consider the following second order system:

$$\begin{aligned} \dot{x_1}(t) &= x_2(t) \\ \dot{x_2}(t) &= -x_1(t) \end{aligned} \tag{1}$$

- We can introduce an approximation by state quantization:

$$\begin{aligned} \dot{x_1}(t) &= floor(x_2(t)) = \lfloor x_2(t) \rfloor = q_2(t) \\ \dot{x_2}(t) &= -floor(x_1(t)) = -\lfloor x_1(t) \rfloor = -q_1(t) \end{aligned} \tag{2}$$

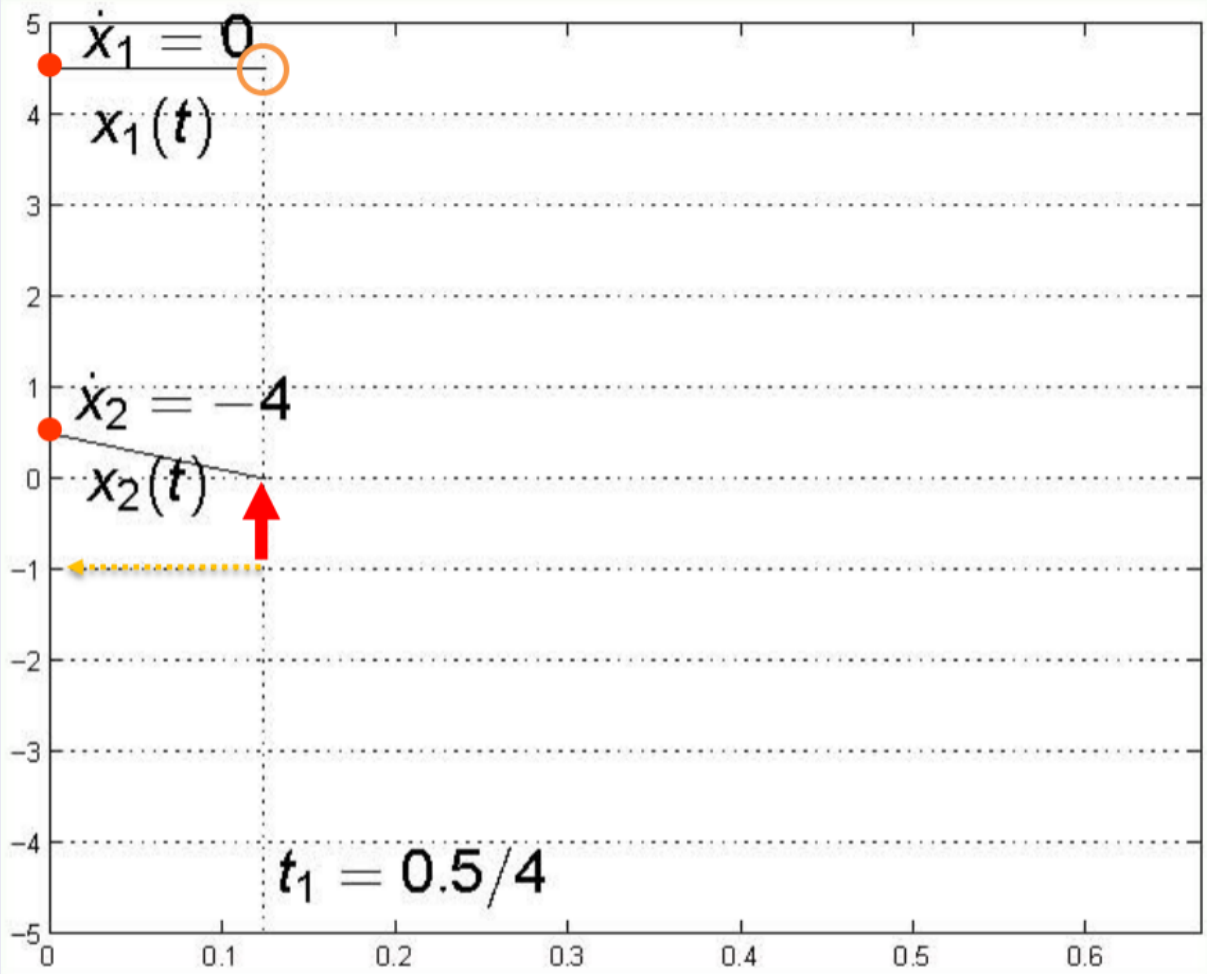
- $x_1(t)$ and $x_2(t)$ correspond to the original state variables, whereas $q_1(t)$ and $q_2(t)$ correspond to the quantized state variables.

Equation

$$\dot{x}_1(t) = \lfloor x_2(t) \rfloor = q_2(t)$$
$$\dot{x}_2(t) = -\lfloor x_1(t) \rfloor = -q_1(t)$$

Initial Conditions

$$x_1(0) = 4.5$$
$$x_2(0) = 0.5$$



Equation

$$\dot{x}_1(t) = \lfloor x_2(t) \rfloor = q_2(t)$$
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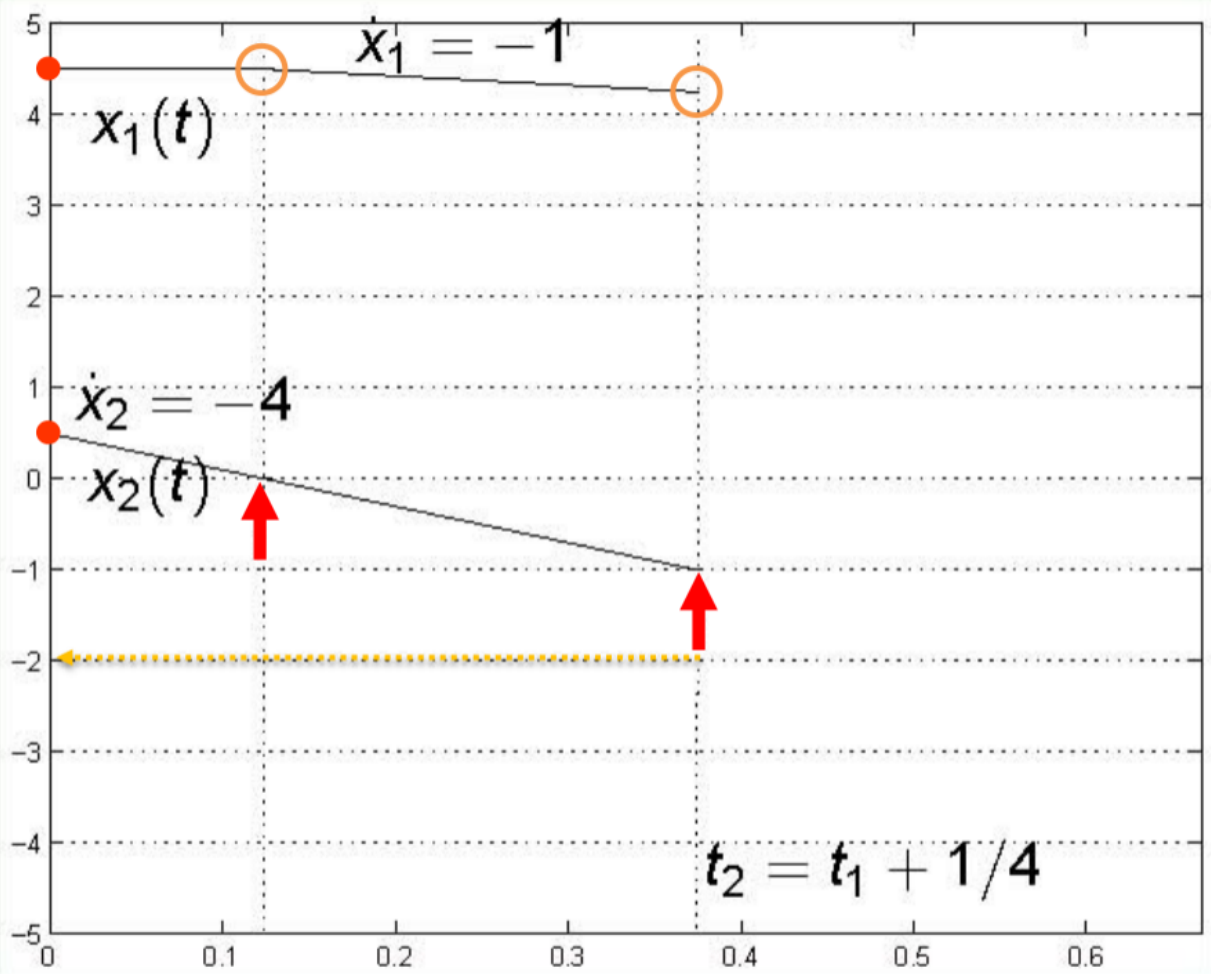

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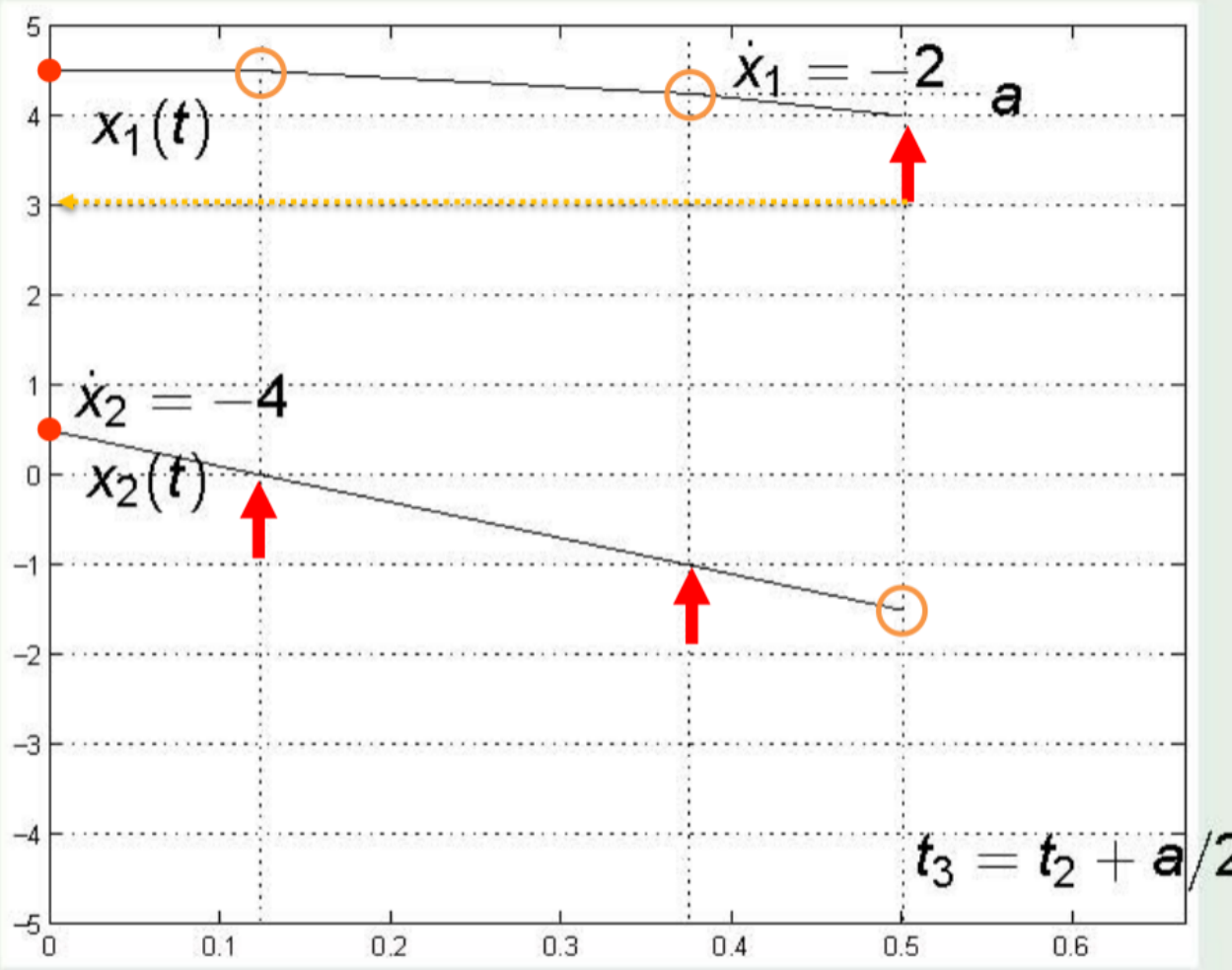

Equation

$$\dot{x}_1(t) = \lfloor x_2(t) \rfloor = q_2(t)$$
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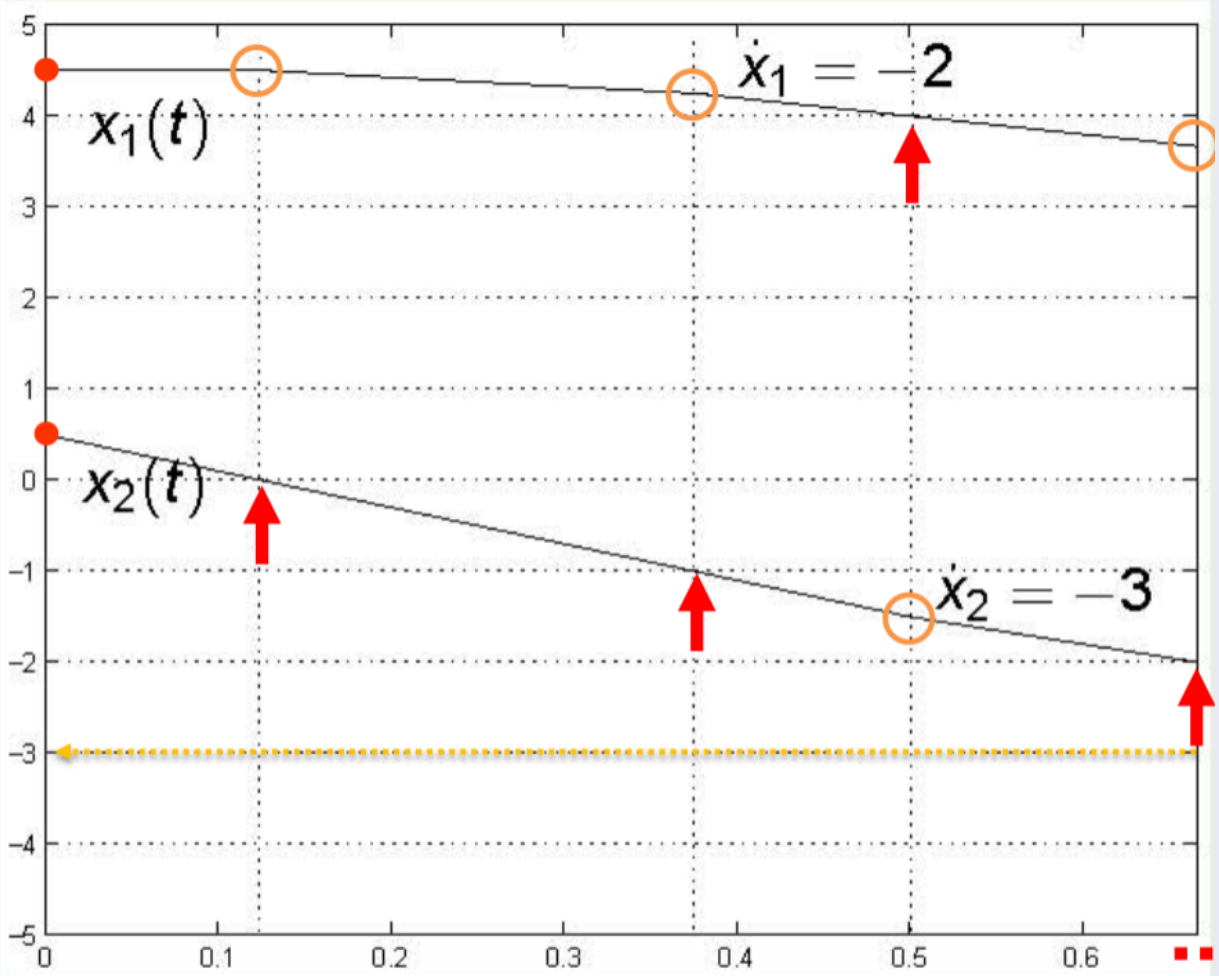
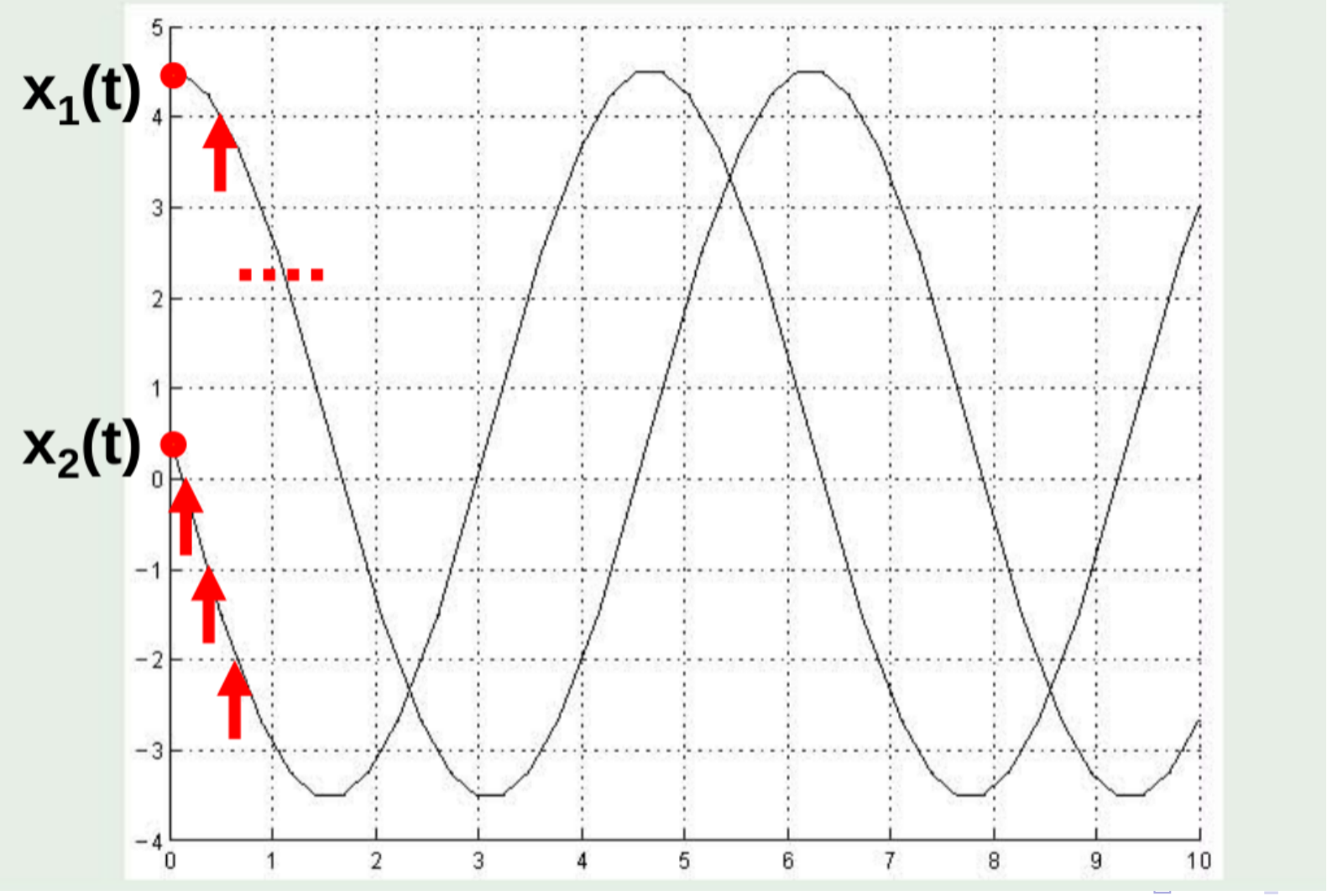


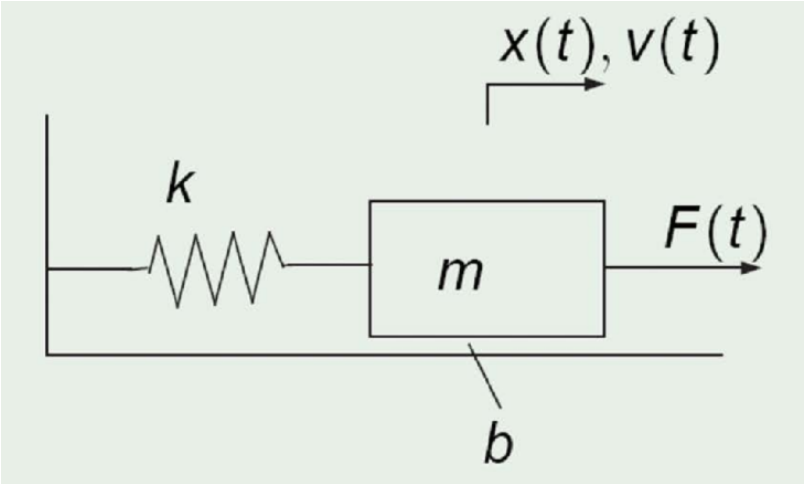
- Solution for the Quantized System



QSS Explained

State Quantization

- Quantized State System (QSS) (Kofman E., 2001)
  - Family of numerical methods based on the principle of state quantization.
  - Quantize the state variables with discrete quanta in place of partitioning time in discrete steps.
  - Implemented in several general purpose M&S tools (most advanced: PowerDEVS).
  - Recently also as a stand-alone QSS numerical solver (which we have already started using!).
  - Step is now a misleading term: QSS are inherently asynchronous and step-less methods.



ODE

$$\dot{x}(t) = v(t)$$
$$\dot{v}(t) = -\frac{k}{m}x(t) - \frac{b}{m}v(t) + \frac{1}{m}F(t)$$

QSS

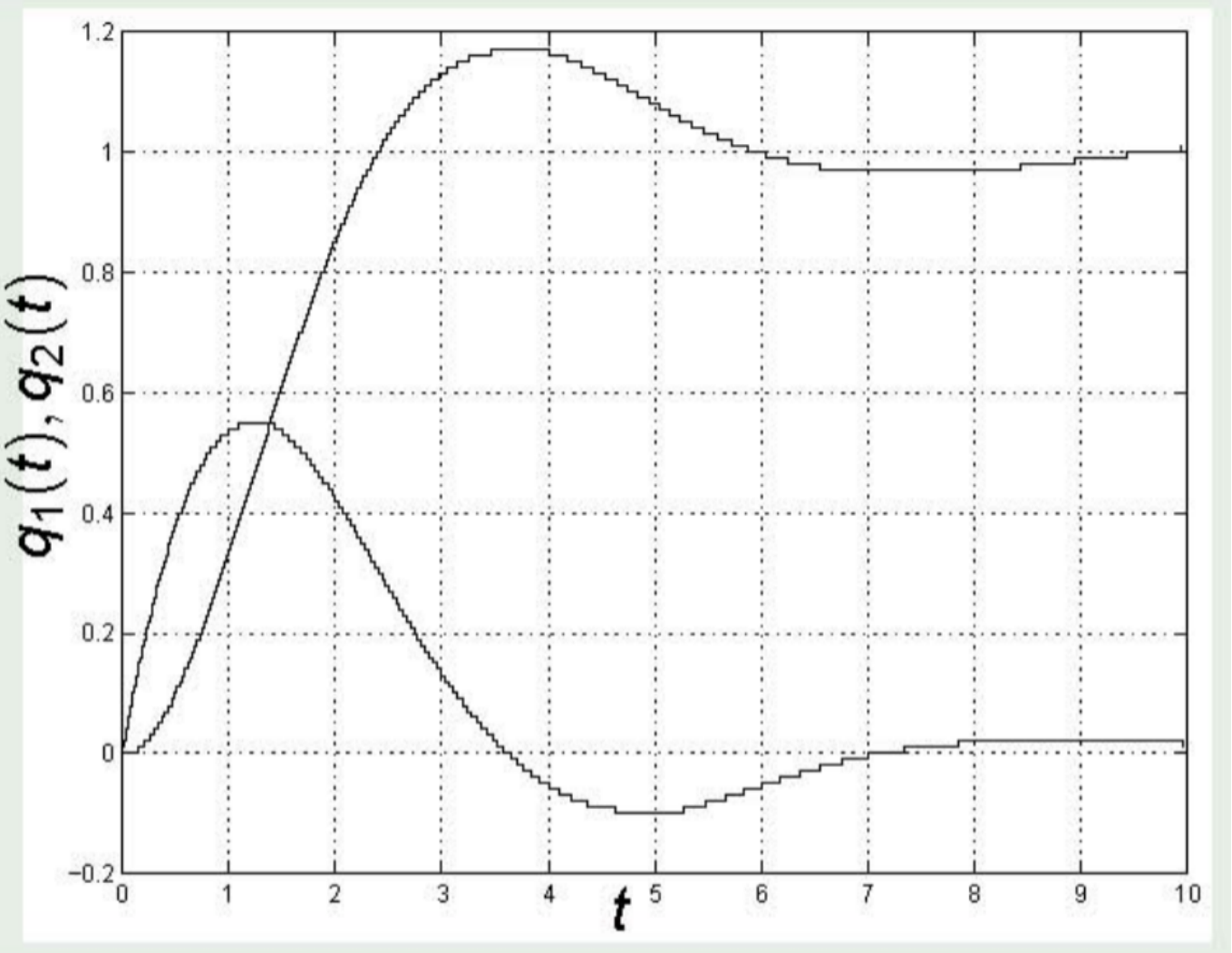
$$\dot{x}_1(t) = q_2(t)$$
$$\dot{x}_2(t) = -\frac{k}{m}q_1(t) - \frac{b}{m}q_2(t) + \frac{1}{m}F(t)$$

For the simulation, we take $m = b = k = 1$.

QSS Explained

More Complex Example

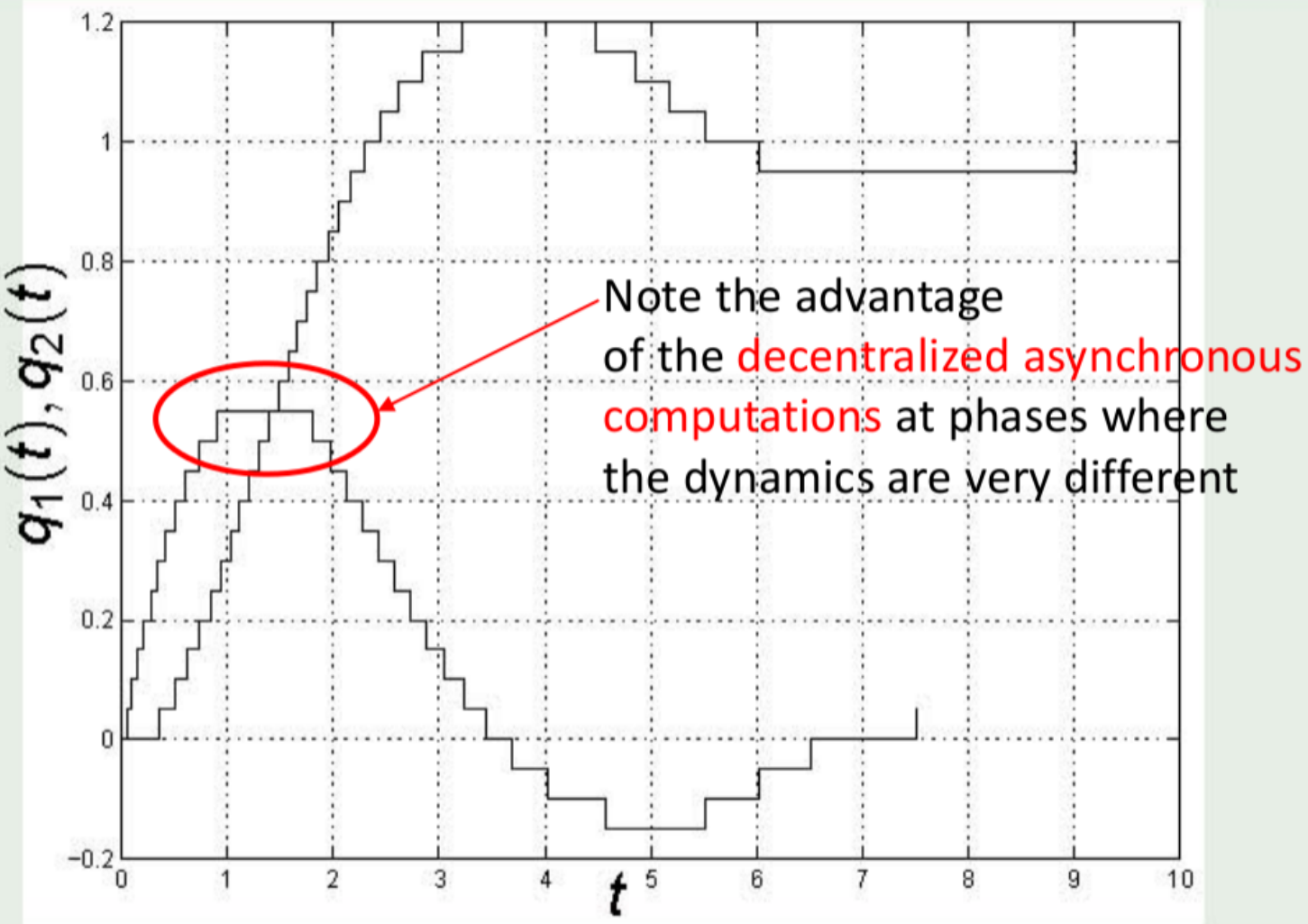
- QSS1 Solution with quantum size $\Delta Q = 0.01$



QSS Explained

More Complex Example

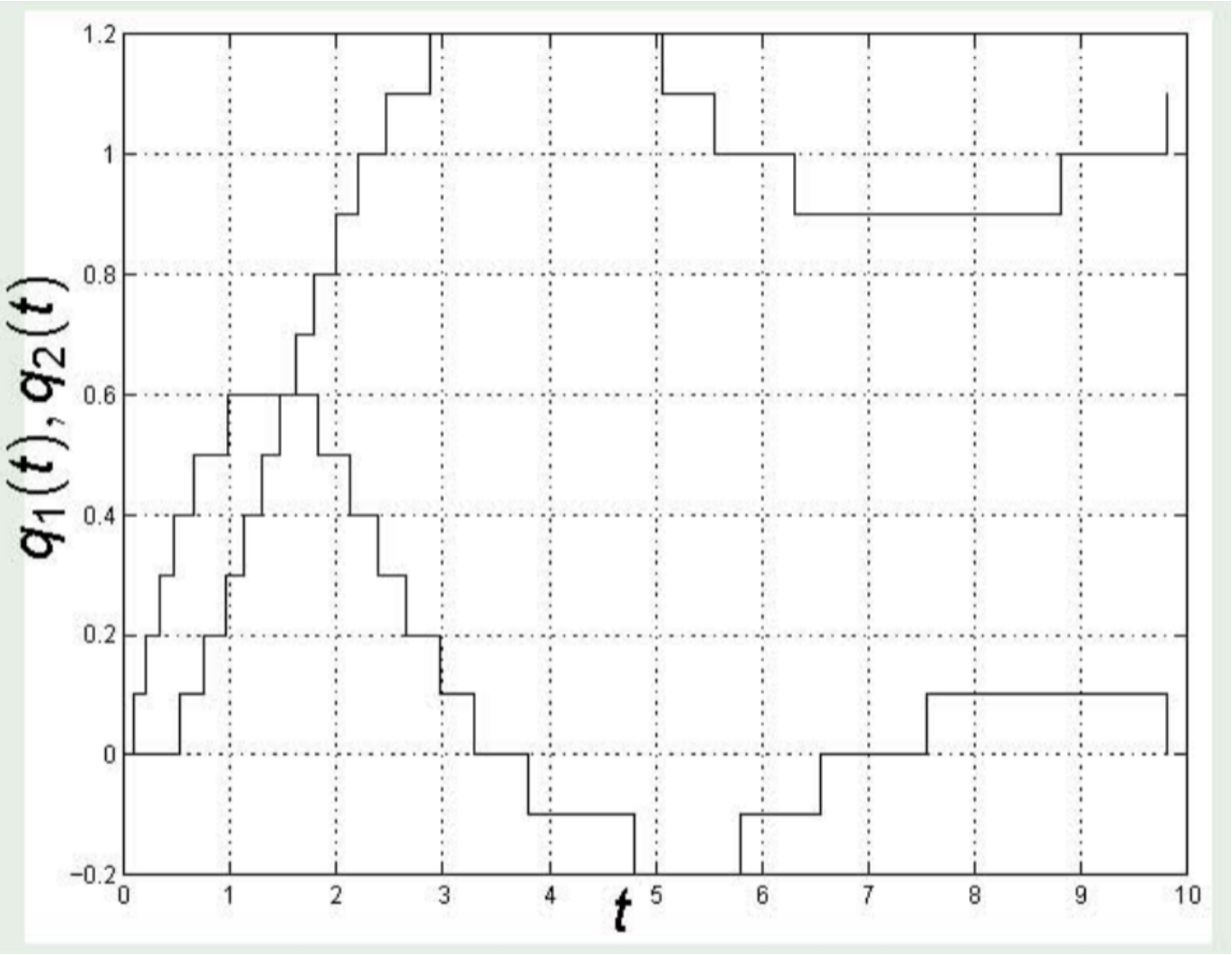
- QSS1 Solution with quantum size $\Delta Q = 0.05$



QSS Explained

More Complex Example

- QSS1 Solution with quantum size $\Delta Q = 0.1$



QSS Explained

Advantages and Disadvantages

- We have presented the first order accurate QSS (QSS1)
- Advantages:
  - Stability and Global Error Bound (at least for linear systems)
  - Decentralized dynamics (decoupled, independent computation of changes in state variables) which makes it naturally asynchronous.
  - Efficiently simulates heavily discontinuous systems
  - Dense polynomial output, with trivial detection and handling of discontinuities.
- Disadvantages
  - Oscillations appear. Problems with stiff systems
    Solution: Linearly Implicit LIQSS family methods
  - The Quantum must be chosen
    Solution: Logarithmic (adaptive) Quantum controls the relative error automatically
  - The # of computational steps grows linearly with precision
    Solution: Higher order methods QSS2, QSS3, QSS4

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Exploring Geant4 Parameters

Simple Example for Exploration Purposes

A charged particle in a static, homogeneus magnetic field pointing in $\hat{z}$.
Equation of motion: $m\frac{d}{dt}(\gamma\frac{dx}{dt}) = q(v \times B)$
This system has an analytical solution which is a circle in the x-y plane.
$R = 38.085mm$
$T = 0.799s$

We identified and focused on a set of Geant4 parameters which can be controlled and should impact the simulation time and numerical error.

Fixed Parameters

- $deltaOneStep = 1.0E\text{-}2mm$
- $deltaInt = 1.0E\text{-}5mm$

Experiments Varying Parameters

- Vary epsilon
- Vary stepMax
- Vary deltaChord

Vary epsilon

Fixed Parameters

- $deltaChord = 0.25mm$
- $stepMax = 20mm$
- $epsilonMin = epsilonMax = epsilon$
- $r_RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(G4x_i\text{-}ANx_i)^2 + (G4y_i\text{-}ANy_i)^2}$

Experiment

- Vary *epsilon* from $1E$-3 to $1E$-12 and measure the impact on the simulation time and simulation error.
- We expect the simulation time to increase when *epsilon* becomes smaller (searching for more accuracy), whereas the error should decrease.

Vary epsilon - Plots

TODO: Show plots:

- *MaxXError* vs distance
- $MaxV_xError$ vs distance + scatter plot + histogram

Vary epsilon - Results and Conclusions

- The simulation time increases when *epsilon* becomes smaller, as expected.
- The error when compared to the analytical solution is not affected considerable by the variation of *epsilon*
- The tiny variation observed is counterintuitive: for smaller values of *epsilon* the error increases.
- We made several experiments to try to explain this behavior, but didn't succeed.
- Runge-Kutta may be too accurate for this simple example, so that epsilon may not be controlling the steps at all.
- TODO: measure the accuracy of the individual Runge-Kutta steps to validate the previous hypothesis.

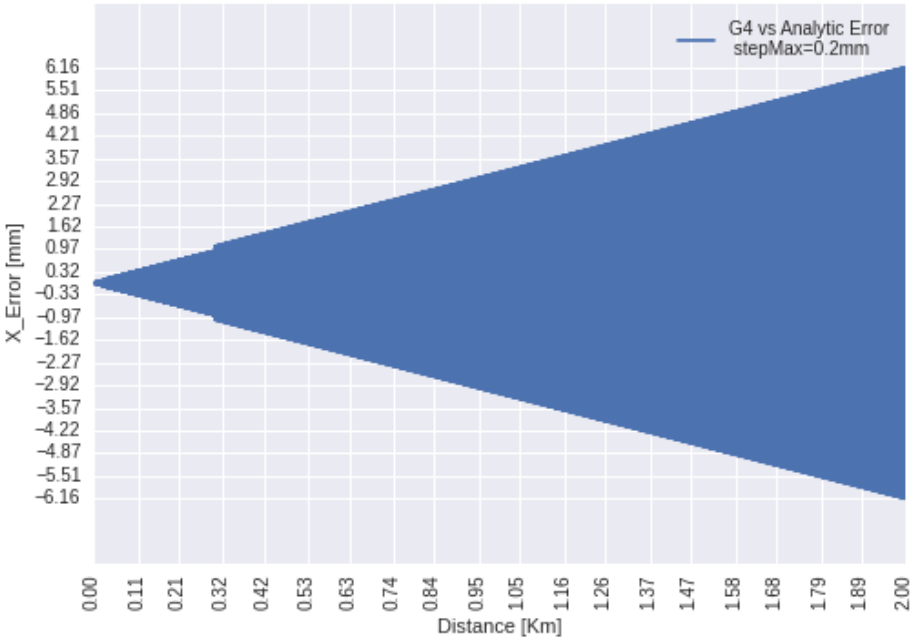
Experiment 2 - Vary stepMax

Fixed Parameters

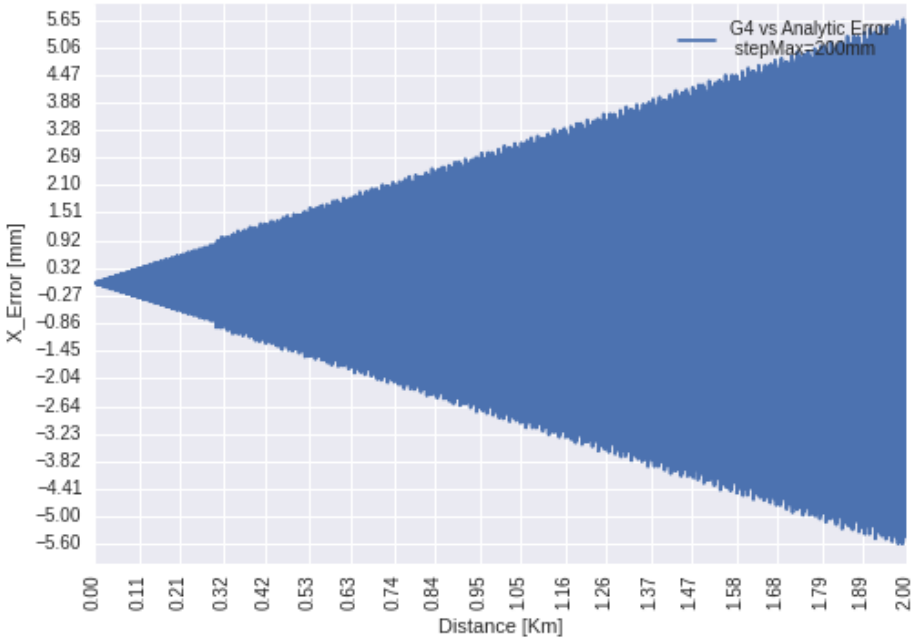
- $deltaChord = 0.25mm$
- $epsilonMin = epsilonMax = 1.0E\text{-}3$

					r_error[mm]				
stepMax	Simulation Time [s]	RHS evaluation steps	Output Steps	Ratio	1 km	100 m	10 m	1 m	100 mm
0.2	814.81	5.50e8	?	?	1.74E+0	1.74E-1	1.74E-2	1.76E-3	1.67E-4
1	171.02	1.10e8	1000000	111	1.74E+0	1.74E-1	1.74E-2	1.76E-3	1.66E-4
2	88.19	5.50e7	500000	11	1.74E+0	1.74E-1	1.74E-2	1.76E-3	1.64E-4
5	33.12	2.20e7	200000	11	1.74E+0	1.74E-1	1.74E-2	1.75E-3	1.58E-4
10	21.90	2.20e7	100000	22	1.74E+0	1.74E-1	1.74E-2	1.74E-3	1.45E-4
20	13.79	1.65e7	500001	33	1.73E+0	1.73E-1	1.73E-2	1.72E-3	1.26E-4
50	8.31	1.32e7	200001	66	1.71E+0	1.71E-1	1.71E-2	1.66E-3	6.91E-5
100	7.17	1.32e7	100001	132	1.68+0	1.68E-1	1.67E-2	1.56E-3	
150	6.84	1.32e7	66668	198	1.64E+0	1.64E-1	1.64E-2	1.58E-3	
200	6.38	1.26e7	50001	252	1.61E+0	1.61E-1	1.59E-2	1.36E-3	

Experiment 2 - Vary stepMax



: (a) stepMax=0.2mm



: (b) stepMax=200mm

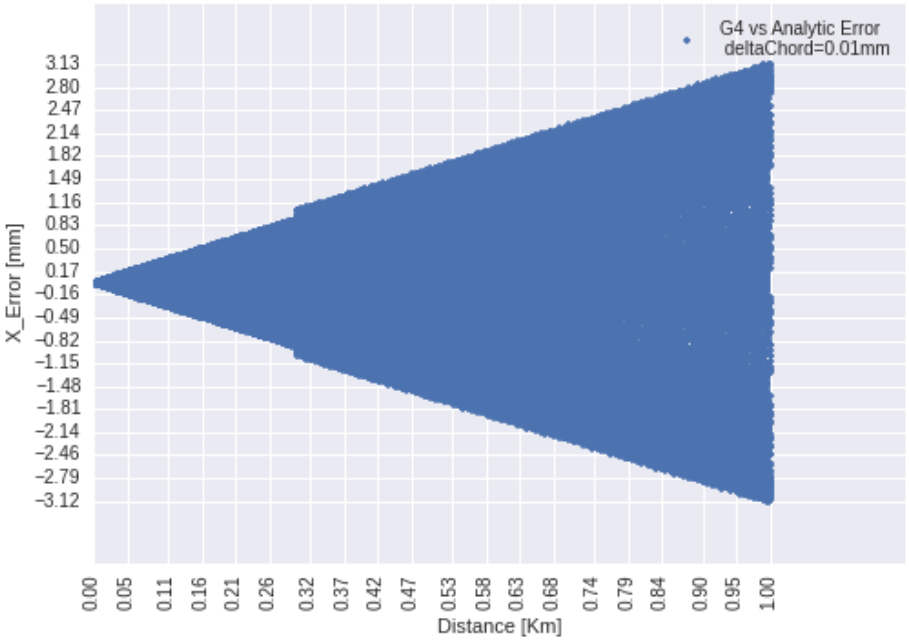
Experiment 4 - Vary deltaChord

Fixed Parameters

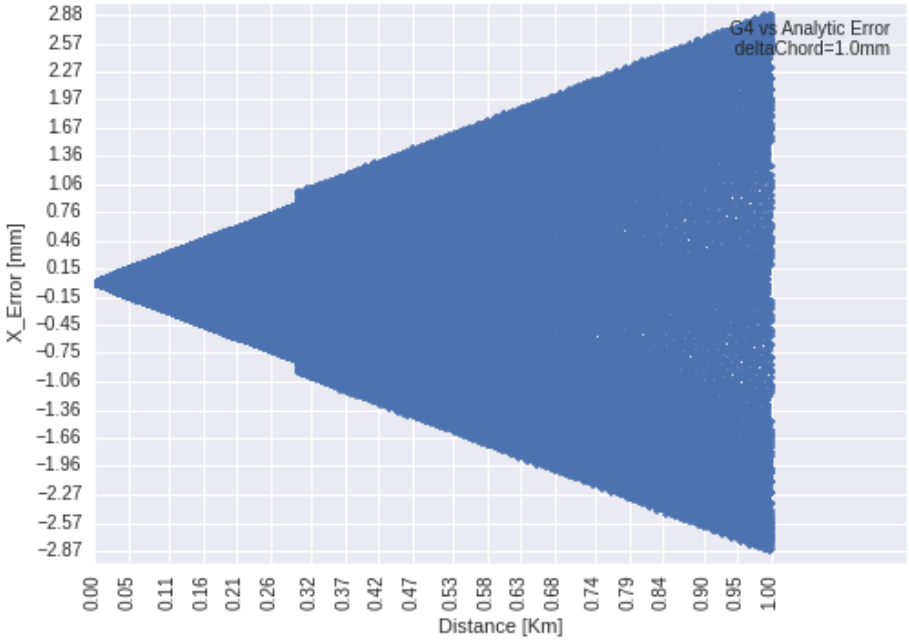
- $stepMax = 20mm$
- $epsilonMin = epsilonMax = 1.0E\text{-}3$

					r_error[mm]				
deltaChord	Simulation Time [s]	RHS evaluation steps	Output Steps	Ratio	1 km	100 m	10 m	1 m	100 mm
0.01	3.9	6.60e6	? 50001	132	1.74E+0	1.74E-1	1.74E-2	1.74E-3	1.30E-4
0.05	2.3	3.30e6	50001	66	1.74E+0	1.74E-1	1.74E-2	1.74E-3	1.30E-4
0.25	1.5	1.65e6	50001	33	1.73E+0	1.73E-1	1.73E-2	1.72E-3	1.26E-4
0.5	1.3	1.10e6	50001	22	1.70E+0	1.70E-1	1.70E-2	1.68E-3	1.14E-4
1.0	1.3	1.10e6	50001	22	1.60E+0	1.60E-1	1.59E-2	1.52E-3	5.27E-5

Experiment 4 - Vary deltaChord



: (a) deltaChord=0.01mm



: (b) deltaChord=1.0mm

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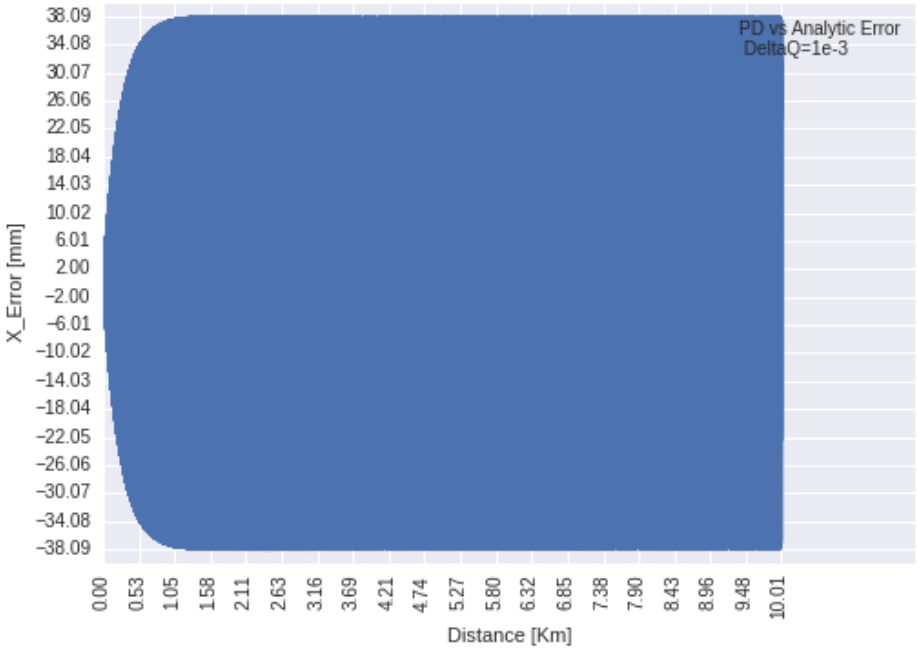
Experiment 3 - Vary deltaQ

Settings

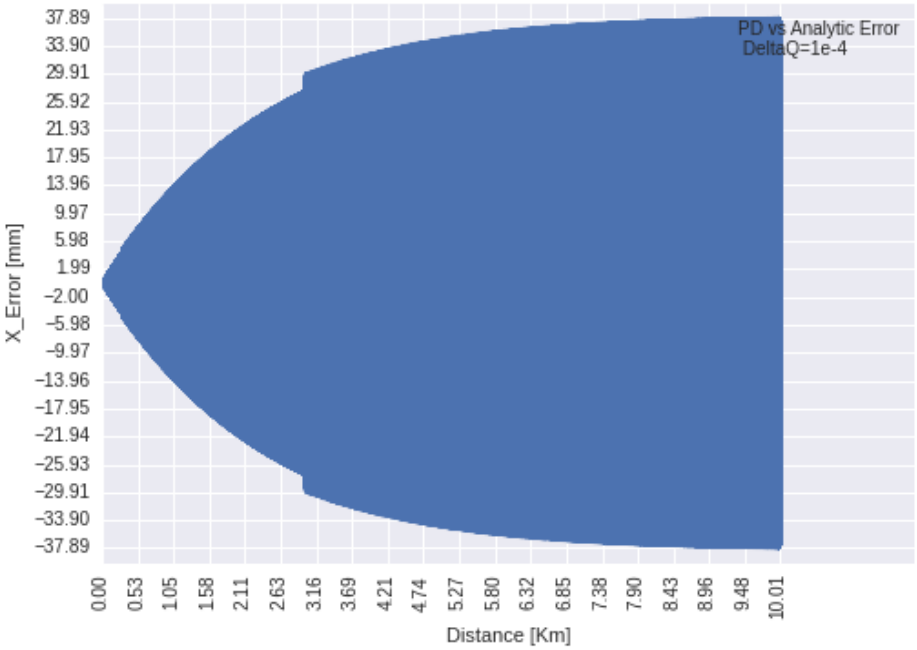
- The simulation was done with the QSS3 method.
- $DeltaQmin = DeltaQ * 1E\text{-}3$

			r_error[mm]				
DeltaQ	Simulation Time [s]	PD evaluation steps	1 km	100 m	10 m	1 m	100 mm
1.0E-3	1.33	2.40e6	2.17E+1	6.11E+0	7.48E-1	8.17E-2	7.27E-3
1.0E-4	8.89	1.42e7	6.44E+0	7.89E-1	8.28E-2	8.65E-3	8.32E-4
1.0E-5	16.3	3.08e7	1.09E+0	1.13E-1	1.14E-2	1.18E-3	1.09E-4
1.0E-6	35.6	6.64e7	7.68E-1	7.69E-2	7.71E-3	7.64E-4	8.00E-5
1.0E-7	77.6	1.43e8	7.64E-1	7.65E-2	7.62E-3	7.67E-4	7.64E-5

Experiment 3 - Vary DeltaQ

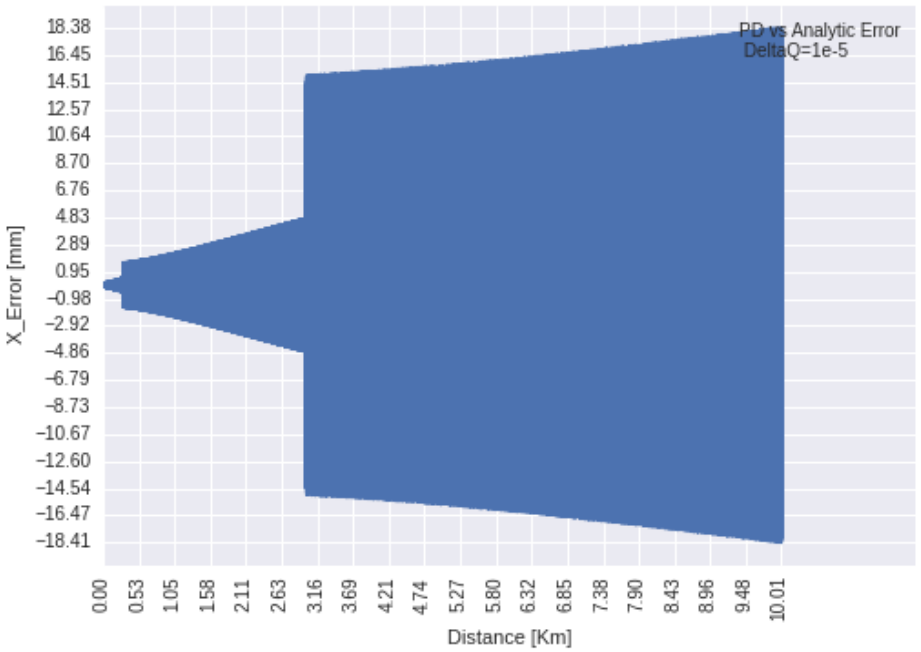


: (a) DeltaQ=1E-3

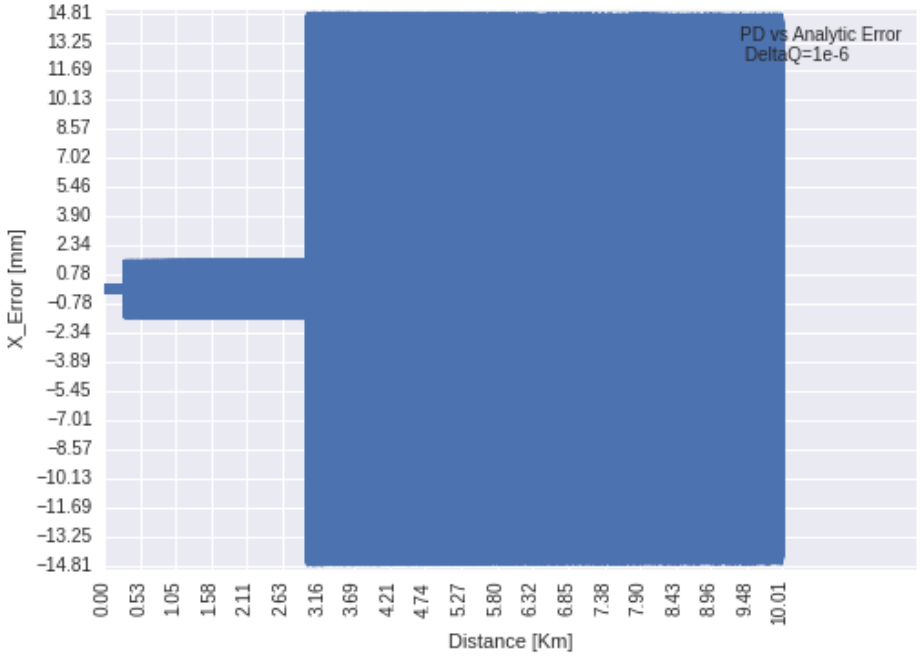


: (b) DeltaQ=1E-4

Experiment 3 - Vary DeltaQ



: (c) DeltaQ=1E-5



: (d) DeltaQ=1E-6

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Experiment 5 - Vary number of Planes in $\hat{x}$

Settings

- We set rectangles larger than the trajectory in the y-z plane.
- Planes are equispaced.
- We used the G4VPReplica method.

# Planes	Simulation Time [s]	RHS evaluation steps	r_error [mm]	Output Steps	Steps Ratio
0	1.4	1.65E6	1.73	50001	33.00
5	3.8	2.94E6	1.74	58507	50.25
10	6.6	5.14E6	1.74	91937	55.91
20	12.3	9.65E6	1.74	167157	57.73
40	23.8	1.90E7	1.74	317596	59.88
80	50.2	3.90E7	1.74	643548	60.60
100	59.7	4.58E7	1.74	793987	57.68
150	88.2	6.80E7	1.74	1195158	56.90
200	114.9	8.70E6	1.74	1579614	55.08

Questions?