Particle Tracking in Geant4

A very brief introduction to Runge-Kutta-Nystrom methods

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Outline

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3. Runge-Kutta (RK) solvers for first order systems of ODE's
4. Runge-Kutta-Nystrom solvers for 2nd order systems
5. Challenges and other desirable's
    - Integrating solutions w.r.t. Arc Length
    - Dense output (Polynomial interpolation)
    - Trigonometrically fitted Runge-Kutta methods

About Me

I am a PhD student in Mathematics at George Washington University in Washington DC (USA, if you didn't know already). My thesis topic is in Topological Graph Theory, specifically bijective methods in cellular map enumeration – which is completely different from what I will be doing with CERN through GSoC 2015.

I like all areas of math however, including numerical analysis. Ultimately I would like to go into modern Quantum Physics, or low-dimensional topology (such as 4-manifold theory).

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I am very grateful for the opportunity to work with CERN this Summer on this project.

Detector Geometry and Particle Trajectory

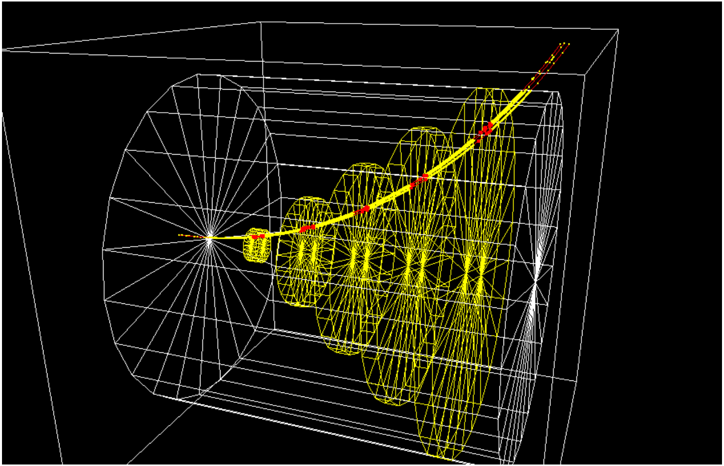

Figure : An example due to John Apostolakis

Summary of Physics for Particles in a Magnetic Field

We have from Electrodynamics the equations

$$\frac{dx}{dt} = \frac{p}{m} \qquad \text{and} \qquad \frac{dp}{dt} = q\left(v \times B_x\right)$$

where

- x is position
- v is velocity
- m is mass of the particle
- $p = mv$ is momentum
- B_x is the magnetic field at x.
- q is charge of the particle

RK method of s stages (with coefficients a_{ij}, b_i, and c_i)

We want to numerically solve the system $y'(t) = F(t, y)$:

$$\text{Input } y_n \approx y(t_n) \xrightarrow{\text{RK (one step)}} \text{Output } y_{n+1} \approx y(t_n + h).$$

Procedure: First caculate

$$\begin{aligned}
K_1 &= F(t_n, y_n), \\
K_2 &= F(t_n + c_2 h, y_n + h(a_{21} K_1)), \\
K_3 &= F(t_n + c_3 h, y_n + h(a_{31} K_1 + a_{32} K_2)) \\
&\ \ \vdots \\
K_s &= F(t_n + c_s h, y_n + h(a_{s1} K_1 + a_{s2} K_2 + \cdots + a_{s,s-1} K_{s-1})).
\end{aligned}$$

and then (finally):

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i K_i,$$

The Attraction of Runge-Kutta-*Nystrom* solvers

This is all good, but we can do better. Our system

$$\frac{dx}{dt} = \frac{p}{m}, \frac{dp}{dt} = q(v \times B_x) \iff \begin{pmatrix} x \\ p \end{pmatrix}' = \begin{pmatrix} p/m \\ \frac{q}{m}(p \times B_x) \end{pmatrix}$$

Is almost in the form

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}' = \begin{pmatrix} u_2 \\ F(u_1, u_2) \end{pmatrix}$$

which is a first order formulation of the 2nd order ODE

$$y''(t) = F(t, y, y')$$

For reasons of computational efficiency we want to exploit this. Runge-Kutta-Nystrom methods are designed specifically for this type of problem.

An RKN method example: 3 stage Charwa/Sharma

For the second order problem

$$y'' = f(t, y, y'), \qquad y(t_0) = y_0, \quad y'(t_0) = y'_0$$

Starting with an approximate (y_k, y'_k) we first calculate the following quantities

$$\begin{aligned}
K_1 =& f(t_k + 0h, y_k + 0hy'_k, y'_k) \\
K_2 =& f(t_k + 2/3h, y_k + 2/3hy'_k + h^2(-1/9)K_1, y'_k + 2/3h) \\
K_3 =& f(t_k + 2/3h, y_k + 2/3hy'_k + h^2(2/9K_1 + 0K_2), \\
& \quad y'_k + h(1/3K_1 + 1/3K_2))
\end{aligned}$$

and finally construct the next approximating point

$$\begin{aligned}
y_{k+1} &= y_k + hy'_k + h^2(1/4K_1 + 0K_2 + 1/4K_3) \\
y'_{k+1} &= y'_k + h(1/4K_1 + 0K_2 + 3/4K_3)
\end{aligned}$$

The Challenge

Not only do we want to be able to implement Nystrom methods, we also want these extra features:

- Trajectories paramterized with respect to arc length s (this gives us more control over how far the particle travels in a single step)

$$x(t(s)) \qquad \text{and} \qquad \left\| \frac{dx}{ds} \right\| = 1$$

- Dense interpolation to detect when a particle trajectory passes through a volume. For each step, a polynomial

$$P_n(t) \text{ s.t. } P_n(t_n + \sigma h) \approx y(t_n + \sigma h) \text{ for } \sigma \in [0, 1]$$

- Trigonometrically fitted RKN methods for when the trajectory of the particle is known to be an approximate to a helical path.

Thank you!