The Cockcroft Institute of Accelerator Science and Technology

UNIVERSITY OF LIVERPOOL

Nonlinear Single-Particle Dynamics in High Energy Accelerators

Part 5: Integrators II

This course consists of eight lectures:

1. Introduction – some examples of nonlinear dynamics
2. Basic mathematical tools and concepts
3. Representations of dynamical maps
4. Integrators I
5. Integrators II
6. Phase space portraits and "phenomenology"
7. Normal form analysis
8. Some numerical techniques

We have seen how nonlinear dynamics can play an important role in some diverse and common accelerator systems. Nonlinear effects have to be taken into account when designing such systems.

A number of powerful tools for analysis of nonlinear systems are developed from Hamiltonian mechanics. Using these tools, the solutions to the equations of motion for a particle moving through a component in an accelerator beamline may be represented in various ways, including: (truncated) power series; Lie transform; (implicit) generating function.

In the case that the Hamiltonian can be written as a sum of integrable terms, the algebra associated with Lie transforms allows construction of an explicit symplectic integrator that is accurate to some specified order.

In particular, we can use the BCH formula to construct a symmetric or Yoshida factorisation of the Lie transform. For example, if:

$$H = H_d + H_k \tag{1}$$

then:

$$e^{-\frac{1}{2}L:H_d:} e^{-L:H_k:} e^{-\frac{1}{2}L:H_d:} = e^{-L:H+O(L^2):}. \tag{2}$$

If H_d and H_k are each integrable, then the above expression gives us a second-order explicit symplectic integrator.

Symmetric factorisation is straightforward to implement for a rectangular multipole. In that case, we can write the accelerator hamiltonian in the form:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - p_x^2 - p_y^2 - \frac{1}{\beta_0^2\gamma_0^2}} - a_s + \frac{\delta}{\beta_0}. \qquad (3)$$

where

$$a_s = \frac{qA_s}{P_0}, \qquad (4)$$

and A_s is the longitudinal component of the vector potential.

For a rectangular multipole, the field can be derived from a vector potential with *only* a longitudinal component; but not all magnetic fields in accelerators can be derived in this way. What happens in the more general case?

Our main goal in this lecture will be to derive an explicit symplectic integrator that can be applied to a general static magnetic field for which the vector potential is known analytically.

We shall follow the technique proposed by Y. Wu, E. Forest and D. Robin:

> "Explicit symplectic integrator for s-dependent static magnetic field," Phys. Rev. E 68, 046502 (2003).

The symplectic integrator will be expressed as a product of Lie transforms.

We shall then briefly discuss the related problem of expressing a magnetic field that may be known numerically (e.g. from a magnetic modelling code, such as Opera) in an analytical form.

Hamiltonian for a general (s-dependent) static magnetic field

If the Hamiltonian is independent of the distance s along the reference trajectory, we can express the map for some function f of the dynamical variables as:

$$f(s) = e^{-s:H:} f(0). \tag{5}$$

Recall the Hamiltonian for a general magnetic field with a straight (i.e. zero curvature) reference trajectory:

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2\gamma_0^2}} - a_s + \frac{\delta}{\beta_0} \tag{6}$$

where the normalised vector potential $\vec{a} = (a_x, a_y, a_s)$ is a function of the coordinates:

$$\vec{a} = \vec{a}(x, y, s). \tag{7}$$

If the Hamiltonian depends on s, the mapping (5) is no longer valid. However, we can recover the use of Lie transformations for evolving functions by extending phase space...

Extended phase space

We can extend phase space by introducing an additional dynamical variables (s, p_s), where s was previously the independent variable, and p_s is a momentum conjugate to s.

We now need a new independent variable: let us call this σ. The independent variable σ represents an integration step. To evolve a system from $s = 0$ to $s = L$, we integrate the equations of motion with respect to σ, until the dynamical variable s is equal to L.

To take account of the evolution of s, we add an additional term, p_s to the Hamiltonian (6):

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2\gamma_0^2}} - a_s + \frac{\delta}{\beta_0} + p_s. \tag{8}$$

Since the Hamiltonian is independent of σ, we can now write:

$$f(\sigma) = e^{-\sigma :H:} f(0). \tag{9}$$

The evolution of s is given by:

$$\frac{ds}{d\sigma} = \frac{\partial H}{\partial p_s} = 1. \tag{10}$$

In effect, $s = \sigma$ (assuming $s = 0$ at $\sigma = 0$).

However, treating s as a dynamical variable, with evolution given by a term p_s in the Hamiltonian will affect *where* we evaluate the vector potential at each step through the field. This can have a significant effect on the results.

We now need to split the Hamiltonian (8):

$$H = -\sqrt{\left(\frac{1}{\beta_0} + \delta\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2 \gamma_0^2}} - a_s + \frac{\delta}{\beta_0} + p_s.$$

into integrable terms.

If the only non-zero component of the vector potential is a_s, the Hamiltonian can be split into two separately integrable terms. However, if we also need a component a_x or a_y to describe the field, then the coordinates and the momenta now both appear within the square root: this means that we cannot then express the Hamiltonian simply as a sum of integrable terms.

To proceed, we make the paraxial approximation, in which we express the square root as a Taylor series. To second order in the transverse dynamical variables (and to second order also in γ_0), this gives:

$$H = H_1 + H_2 + H_3 + O(3) \tag{11}$$

where:

$$H_1 = -\left(\frac{1}{\beta_0} + \delta\right) + \frac{1}{2\beta_0^2\gamma_0^2}\left(\frac{1}{\beta_0} + \delta\right)^{-1} + \frac{\delta}{\beta_0} + \frac{(p_x - a_x)^2}{2\left(\frac{1}{\beta_0} + \delta\right)} + p_s \tag{12}$$

$$H_2 = \frac{(p_y - a_y)^2}{2\left(\frac{1}{\beta_0} + \delta\right)} \tag{13}$$

$$H_3 = -a_s. \tag{14}$$

Separating the Hamiltonian into integrable terms

This appears to be a strange way to split the Hamiltonian: H_3 depends only on the coordinates, so is integrable; but H_1 and H_2 still depend on the coordinates and the momenta.

However, we now note that in general, we can make a gauge transformation to make one component of the vector potential vanish. That is, if we define:

$$\psi = \int_0^x A_x(x', y, s)\, dx', \tag{15}$$

then the field derived from the vector potential:

$$\vec{A}' = \vec{A} - \nabla\psi \tag{16}$$

is the same as the field derived from $\vec{A}$, that is:

$$\vec{B} = \nabla \times \vec{A} = \nabla \times \vec{A}'. \tag{17}$$

But the x component of $\vec{A}'$ vanishes.

Therefore, we can, without loss of generality, work in a gauge where $a_x = 0$. In that case, H_1 becomes:

$$H_1 = -\left(\frac{1}{\beta_0} + \delta\right) + \frac{1}{2\beta_0^2\gamma_0^2}\left(\frac{1}{\beta_0} + \delta\right)^{-1} + \frac{\delta}{\beta_0} + \frac{p_x^2}{2\left(\frac{1}{\beta_0} + \delta\right)} + p_s. \quad (18)$$

In an appropriate gauge, H_1 depends only on the momenta, and is therefore integrable.

That only leaves us with H_2 that we do not (yet) know how to integrate. What can we do for that term?

At this stage, we write the map generated by H_2 as a Lie transform:

$$\mathcal{M}_2(\Delta\sigma) = e^{-\Delta\sigma :H_2:} = \exp\left(-\Delta\sigma : \frac{(p_y - a_y)^2}{2\left(\frac{1}{\beta_0} + \delta\right)} :\right). \quad (19)$$

Now we use Rule 5 for the algebra of Lie transforms:

$$e^{:f:}e^{:g:}e^{-:f:} = \exp :e^{:f:}g:, \quad (20)$$

and Rule 3:

$$e^{:f:}g(h) = g\left(e^{:f:}h\right). \quad (21)$$

Using these rules, we observe that if:

$$e^{:I_y:} \; : \; p_y \mapsto p_y - a_y, \quad (22)$$

then we can write:

$$\mathcal{M}_2(\Delta\sigma) = e^{:I_y:} \exp\left(-\Delta\sigma : \frac{p_y^2}{2\left(\frac{1}{\beta_0} + \delta\right)} :\right) e^{-:I_y:}. \quad (23)$$

Finally, it turns out to be rather straightforward to write down a generator I_y for the map that satisfies (22). The required generator is:

$$I_y = \int_0^y a_y(x, y', s)\, dy'. \tag{24}$$

Since I_y is independent of the momenta, it leaves the coordinates unchanged:

$$e^{:I_y:} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{25}$$

The effect of the map generated by I_y on the momenta can be found by treating I_y as a Hamiltonian, and solving Hamilton's equations for unit step in the independent variable. (In fact, what we are doing is making a canonical transformation). We find:

$$e^{:I_y:}\, p_x = p_x - \int_0^y \frac{\partial}{\partial x} a_y(x, y', s)\, dy', \tag{26}$$

$$e^{:I_y:}\, p_y = p_y - a_y, \tag{27}$$

$$e^{:I_y:}\, \delta = \delta. \tag{28}$$

The effect of the inverse map (i.e. the map generated by $-I_y$) is simply found by replacing the minus signs in the above equations by plus signs.

Now we are in a position to write down an explicit symplectic integrator for a particle moving through a general static magnetic field. The second-order (in $\Delta\sigma$) integrator may be written:

$$\begin{aligned} \mathcal{M}(\Delta\sigma) &= e^{-\Delta\sigma :H_1+H_2+H_3:} \\ &\approx e^{-\frac{\Delta\sigma}{2}:H_1+H_3:} e^{-\Delta\sigma :H_2:} e^{-\frac{\Delta\sigma}{2}:H_1+H_3:} \\ &\approx e^{-\frac{\Delta\sigma}{4}:H_1:} e^{-\frac{\Delta\sigma}{2}:H_3:} e^{-\frac{\Delta\sigma}{4}:H_1:} e^{-\Delta\sigma :H_2:} e^{-\frac{\Delta\sigma}{4}:H_1:} e^{-\frac{\Delta\sigma}{2}:H_3:} e^{-\frac{\Delta\sigma}{4}:H_1:} \end{aligned} \tag{29}$$

where:

$$e^{-\Delta\sigma :H_2:} = e^{:I_y:} e^{-\Delta\sigma :\tilde{H}_2:} e^{-:I_y:}, \tag{30}$$

and from (24):

$$I_y = \int_0^y a_y(x, y', s)\, dy', \qquad \tilde{H}_2 = \frac{p_y^2}{2\left(\frac{1}{\beta_0} + \delta\right)}. \tag{31}$$

Each factor in the map given (jointly) by (29) and (30) can be written explicitly in closed form: we have constructed an explicit second-order integrator for a general static magnetic field.

Since each factor is itself a symplectic map, the overall map must be symplectic.

The "drift" maps $e^{-\frac{\Delta\sigma}{4}:H_1:}$ and $e^{-\Delta\sigma :\tilde{H}_2:}$ are actually independent of the vector potential (i.e. they are independent of the field). However, to write explicitly the "kick" maps $e^{:I_y:}$ and $e^{-\frac{\Delta\sigma}{2}:H_3:}$, we need to know the vector potential.

To see how the explicit second-order integrator works in practice, let us look at a specific example: the field in a wiggler. A simple representation of a wiggler field is given by:

$$B_x = -B_0 \frac{k_x}{k_y} \sin k_x x \sinh k_y y \cos k_s s, \tag{32}$$

$$B_y = B_0 \cos k_x x \cosh k_y y \cos k_s s, \tag{33}$$

$$B_s = -B_0 \frac{k_s}{k_y} \cos k_x x \sinh k_y y \sin k_s s. \tag{34}$$

The field amplitude is B_0, and the period of the wiggler is λ_w, given by:

$$\lambda_w = \frac{2\pi}{k_s}. \tag{35}$$

The value of k_x determines the transverse "roll-off" of the field. Maxwell's equations $\nabla \cdot \vec{B} = \nabla \times \vec{B} = 0$ are satisfied if:

$$k_y = \sqrt{k_x^2 + k_s^2}. \tag{36}$$

The vector potential in a suitable gauge (i.e. with $A_x = 0$) is:

$$A_x = 0, \tag{37}$$

$$A_y = -B_0 \frac{k_s}{k_x k_y} \sin k_x x \sinh k_y y \sin k_s s, \tag{38}$$

$$A_s = -B_0 \frac{1}{k_x} \sin k_x x \cosh k_y y \cos k_s s. \tag{39}$$

It is now possible to write down in explicit closed form each factor in the second-order symplectic integrator, (29) and (30): this is left as an exercise for the student!

If we select some specific values for the various parameters, we can make some numerical comparisons between our second-order integrator, and other integration methods.

Peak magnetic field	B_0	1.7 T
Wiggler period	λ_w	0.1 m
Field roll-off	k_x	400 m^{-1}
Reference energy	E_0	511 MeV
Relativistic factor	γ_0	1000

Note that the reference trajectory is a straight line along the axis of the wiggler: this defines the coordinate system used to describe the magnetic field. The fact that this is not a physical trajectory for a charged particle moving through the wiggler does not matter.

The following plots compare the trajectory of a particle computed in two different ways:

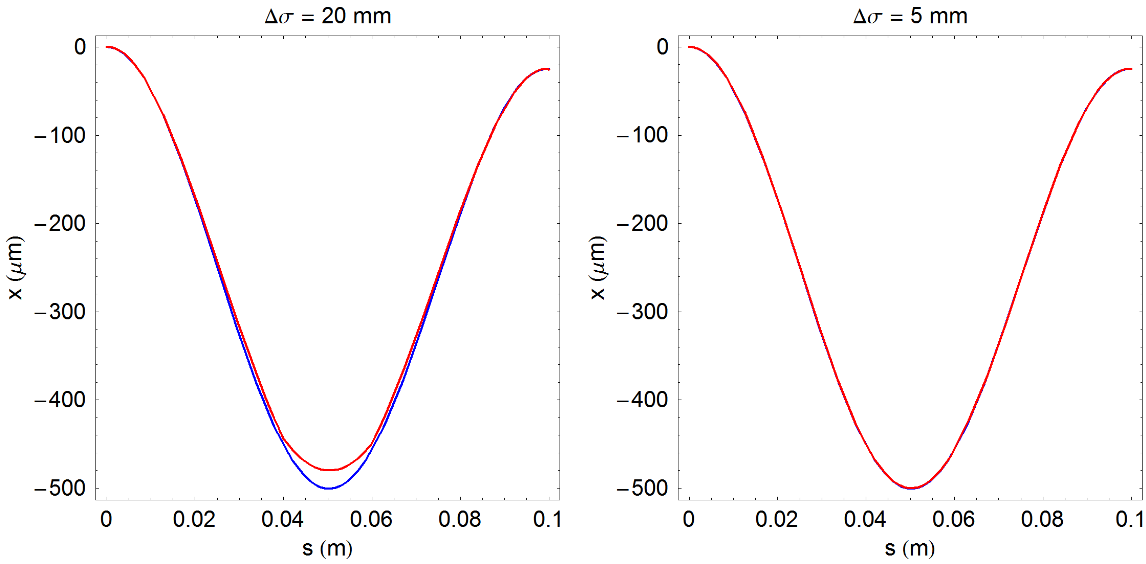
Blue: integration of the equations of motion based on the exact Hamiltonian (8), i.e. without any paraxial approximation, using an adaptive high-order Runge-Kutta algorithm in Mathematica.

Red: computation of the trajectory using the second-order explicit symplectic integrator (29), (30).

Note that we launch a particle at $s = \sigma = 0$, with $x = p_x = p_y = z = \delta = 0$, and $y = 1\,\mathrm{mm}$.

Since the field varies continuously with σ, we expect that the accuracy of our second-order integrator will improve as we reduce the step size $\Delta\sigma$.

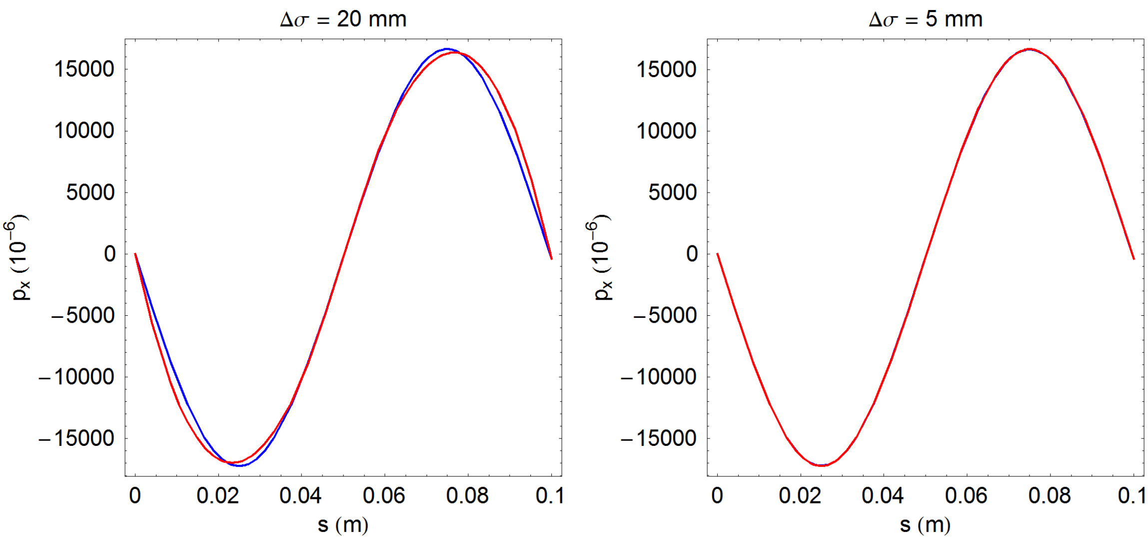
Explicit symplectic integrator: example



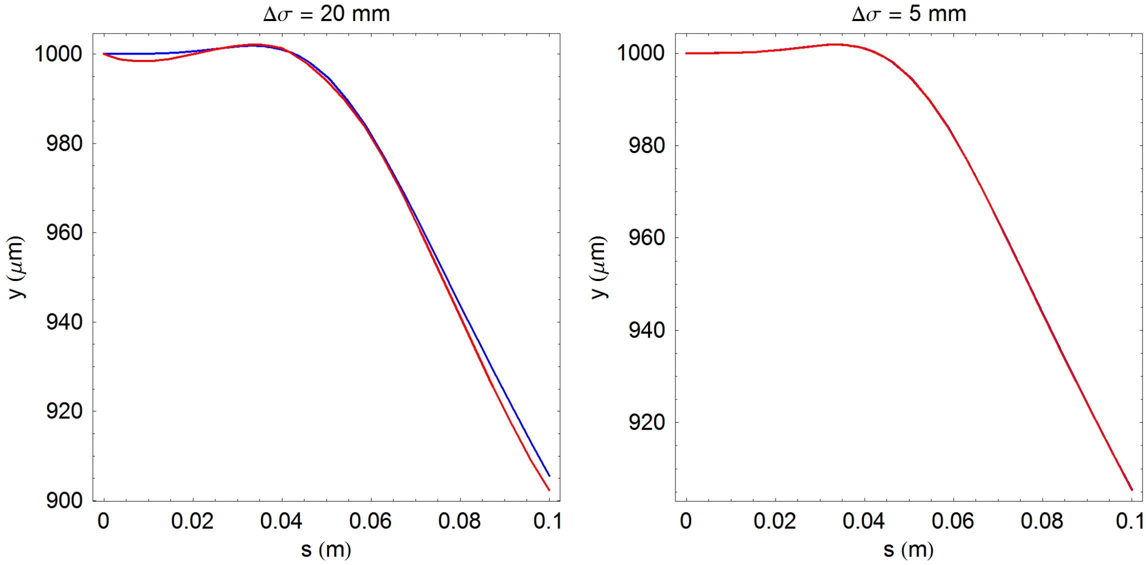
Blue line: integration using adaptive Runge-Kutta in Mathematica.

Red line: second-order explicit symplectic integrator.

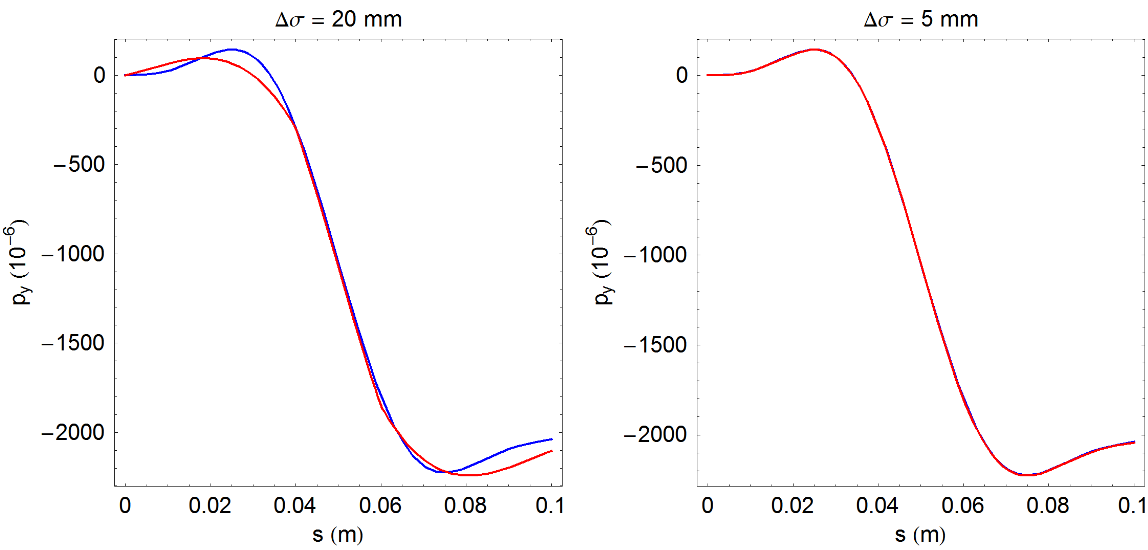
Explicit symplectic integrator: example



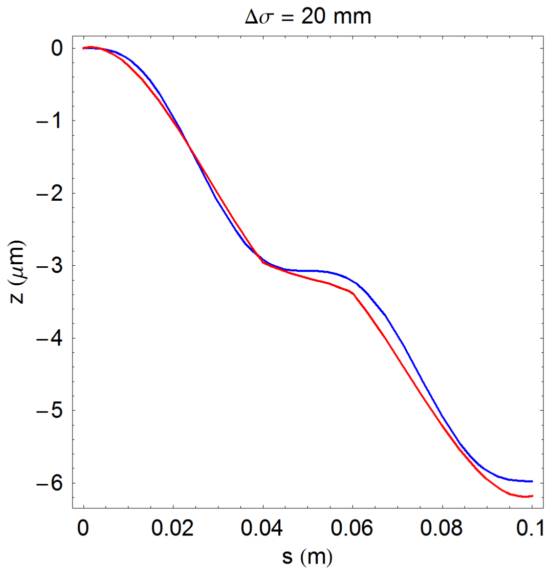
Explicit symplectic integrator: example

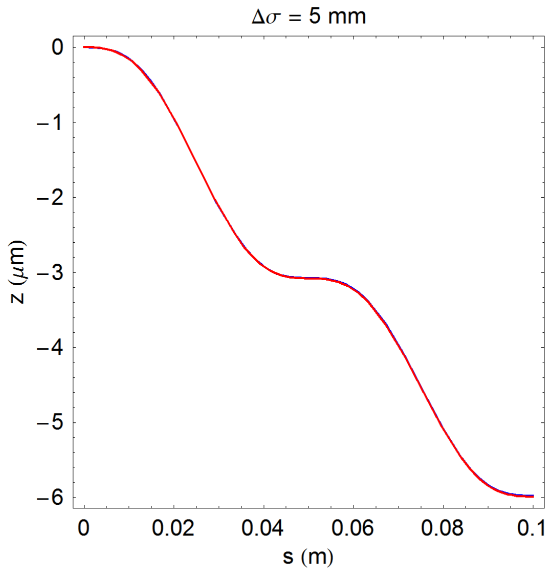


Explicit symplectic integrator: example



Explicit symplectic integrator: example





Symplecticity

We see that there is good agreement between the Runge-Kutta and the symplectic integration, if the step size for the symplectic integration is small enough.

The "advantage" of the symplectic integration is that, even if the step size is large so that the result is not accurate, it is at least symplectic.

A non-symplectic integration algorithm, such as Runge-Kutta, must approach symplecticity as a limit; but with an algorithm of this type, the symplecticity depends on the accuracy with which the results match the true dynamics.

In the above example, we wrote down an analytical representation of the field. This was necessary in order to apply our explicit symplectic integrator.

But it happens more commonly that we have a numerical field map, for example the values of the field components B_x, B_y and B_z on a grid of points over some region within the field. This is not convenient for applying our symplectic integrator.

However, there are techniques that will allow construction of an analytical representation of the field from numerical data. Such a process is commonly called "field fitting". Generally, field fitting requires some care to achieve reasonably accurate and reliable results. Here, we outline one technique that has some practical advantages.

We begin by recalling the field we wrote down for a wiggler, (32), (33), (34):

$$\begin{aligned} B_x &= -B_0 \frac{k_x}{k_y} \sin k_x x \, \sinh k_y y \, \cos k_s s, \\ B_y &= B_0 \cos k_x x \, \cosh k_y y \, \cos k_s s, \\ B_s &= -B_0 \frac{k_s}{k_y} \cos k_x x \, \sinh k_y y \, \sin k_s s. \end{aligned}$$

Maxwell's equations (zero divergence and curl) are satisfied if:

$$k_y = \sqrt{k_x^2 + k_s^2}, \qquad (40)$$

so k_y is determined by the values of k_x and k_s. However, k_x, k_s and B_0 are "free" parameters.

We see that it is possible to construct a more general field by superposing fields with a range of values for the free parameters:

$$B_x = -\int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \frac{k_x}{k_y} \sin k_x x \, \sinh k_y y \, \cos k_s s, \quad (41)$$

$$B_y = \int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \cos k_x x \, \cosh k_y y \, \cos k_s s, \quad (42)$$

$$B_s = -\int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \frac{k_s}{k_y} \cos k_x x \, \sinh k_y y \, \sin k_s s. \quad (43)$$

For $y = 0$, we see that (42) has the form of a 2-D Fourier transform of $\tilde{B}(k_x, k_s)$. Therefore, we can obtain $\tilde{B}(k_x, k_s)$ from an inverse Fourier transform of $B_y(x, y = 0, s)$. If B_y is known on a set of grid points, then we perform a discrete inverse Fourier transform, to determine a finite set of coefficients $\tilde{B}(k_x, k_s)$.

Constructing an analytical field representation

The corresponding potential can be obtained from a generalisation of (37), (38) and (39):

$$A_x = 0, \quad (44)$$

$$A_y = -\int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \frac{k_s}{k_x k_y} \sin k_x x \, \sinh k_y y \, \sin k_s s, \quad (45)$$

$$A_s = -\int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \frac{1}{k_x} \sin k_x x \, \cosh k_y y \, \cos k_s s. \quad (46)$$

Of course, in general, we will need to include terms with different phases in x and s; but this is a straightforward generalisation. We therefore have, in principle, the tools we need to implement our explicit symplectic integrator for an (initially) numerical field map.

There are, however, two significant complications to implementing this technique directly.

First, we note that the field has a hyperbolic dependence on y (42):

$$B_y = \int dk_x \int dk_s \, \tilde{B}(k_x, k_s) \cos k_x x \, \cosh k_y y \, \cos k_s s.$$

This means that any small error in $\tilde{B}(k_x, k_s)$ arising will be amplified exponentially as we move away from $y = 0$.

This is unpleasant, but we can in fact get around it fairly easily, simply by performing the inverse Fourier transform of $B_y(x, y, s)$ on a plane $y = y_0$ (after scaling the field values by $\cosh k_y y_0$). Any error in $\tilde{B}(k_x, k_s)$ will then be damped exponentially as we move towards $y = 0$. If we choose y_0 at the boundary of the region within which we are interested in the dynamics, then we should be able to calculate the dynamics accurately.

A more serious difficulty arises from the dependence of our basis functions on x. For a finite range of k_x, the only fields we can accurately describe by our mode decomposition are those that are periodic in x. This does not describe very well the fields that tend to occur in accelerators. The consequence is that it is generally rather difficult to get an accurate description of the field, at least without using a very large number of modes.

We would do better to choose a set of basis functions that reflects more closely the geometry with which we are dealing. For example, we can work in cylindrical polar coordinates, with the axis of the cylinder defining the reference trajectory. In that case, there is always a real periodicity in the azimuthal angle ϕ.

In cylindrical polar coordinates, a field satisfying Maxwell's equations can be represented by:

$$B_\rho = \int dk_s \sum_m \tilde{B}_m(k_s) I'_m(k_s\rho) \sin m\phi \cos k_s s, \tag{47}$$

$$B_\phi = \int dk_s \sum_m \tilde{B}_m(k_s) \frac{m}{k_s\rho} I_m(k_s\rho) \cos m\phi \cos k_s s, \tag{48}$$

$$B_s = -\int dk_s \sum_m \tilde{B}_m(k_s) I_m(k_s\rho) \sin m\phi \sin k_s s. \tag{49}$$

Here, the functions $I_m(r)$ are modified Bessel functions: broadly speaking, they are to regular Bessel functions as hyperbolic trigonometric functions are to regular trigonometric functions.

Note that in this decomposition, the index m has a nice interpretation: $m = 1$ gives the (normal) dipole component, $m = 2$ the (normal) quadrupole component, and so on. Skew fields are obtained simply by a change of phase of the trig functions (in the azimuthal coordinate).

If we look at the radial component of the field (47):

$$B_\rho = \int dk_s \sum_m \tilde{B}_m(k_s) I'_m(k_s\rho) \sin m\phi \cos k_s s,$$

then we see that we can obtain the functions $\tilde{B}_m(k_s)$ from a 2-D inverse Fourier transform of the field component B_ρ on the surface of a cylinder of given radius ρ_0. This is sufficient to determine all field components everywhere.

Note that the behaviour of the modified Bessel function is such that small errors are exponentially damped within the cylinder of radius ρ_0, and grow exponentially outside this cylinder.

To construct an integrator using Hamiltonian methods, we need an expression for the vector potential (ideally, with one component equal to zero). The field (47), (48) and (49) can be obtained from the vector potential:

$$A_\rho = -\int dk_s \sum_m \tilde{B}_m(k_s) \frac{\rho}{m} I_m(k_s \rho) \cos m\phi \sin k_s s, \qquad (50)$$

$$A_\phi = 0, \qquad (51)$$

$$A_s = -\int dk_s \sum_m \tilde{B}_m(k_s) \frac{\rho}{m} I'_m(k_s \rho) \cos m\phi \cos k_s s. \qquad (52)$$

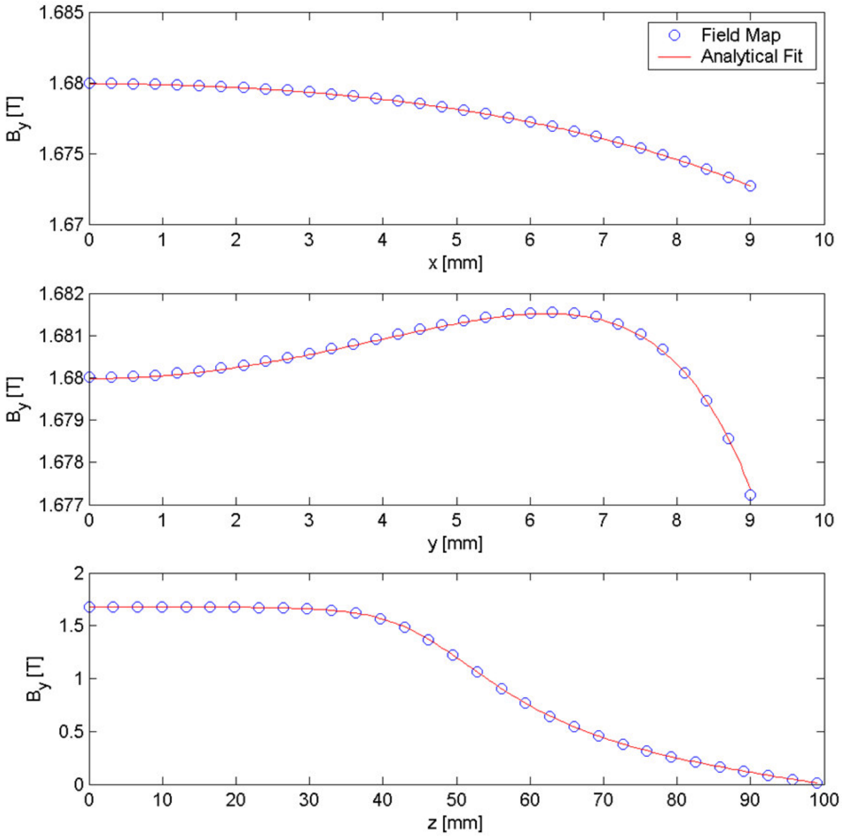
Of course, to complete the construction of an integrator, we need to either: convert the cylindrical representation of the vector potential to cartesian coordinates; or, convert the accelerator Hamiltonian from cartesian to cylindrical coordinates. Both approaches present certain challenges, and we do not develop them further in these lectures.

To finish this lecture, we give an illustration of the quality of the field fit that can be achieved using the cylindrical basis. As an example, we use a numerical field map generated for a design for a permanent magnet wiggler for the TESLA damping ring.

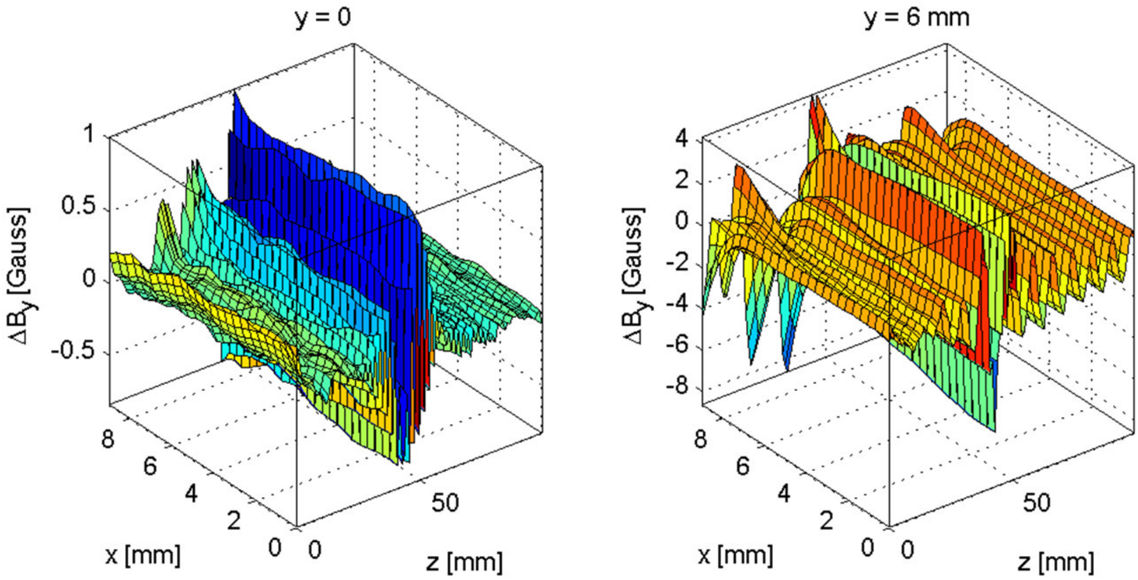
The (nominal) peak field of the wiggler is 1.7 T, and the period is 0.4 m.

The fits shown on the following slides were obtained using 18 azimuthal and 100 longitudinal modes, and fitting on a cylinder of radius 9 mm.

Field fit to TESLA damping wiggler



Field fit to TESLA damping wiggler: residuals



Summary

We have seen how to construct an explicit symplectic integrator for a general static magnetic field, in the case that the vector potential is known analytically.

The accuracy of the integrator improves as the step size through the field is made smaller. However, for any step size, the integrator provides symplectic integration. This is in contrast to some other integration techniques (e.g. Runge-Kutta) that are only symplectic to the extent that they are accurate.

To apply the explicit symplectic integrator, we need an analytical expression for the vector potential. There are techniques available that can be used to construct appropriate expressions from numerical field data.

Further reading

I am indebted to Alex Dragt for much of the material on field fitting in this lecture. The topic can be developed much further, to include such topics as generalised gradients, and basis functions for elliptical geometries.

For further reading, I would strongly recommend Alex's book:

> "Lie methods for nonlinear dynamics with applications to accelerator physics"
> http://www.physics.umd.edu/dsat/dsatliemethods.html

Coming next...

We are now able to track particles through a wide variety of nonlinear accelerator components.

In the final three lectures, we shall explore the global dynamics of an accelerator, and try to understand the features of the dynamics that results from particles passing repeatedly through nonlinear beamlines, for example in a storage ring.

Exercises

1. Using the vector potential (37), (38), (39), write down in explicit closed form each factor in the second-order symplectic integrator (29) and (30). Show that each of these maps is symplectic.