Numerical computations in an accelerating gap or in a cavity

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1. Introduction:

1-1 For the numerical computation in an accelerating field in DYNAC (see CAVNUM in the DYNAC User Guide), one focuses on a numerical step-by-step method based on the 5 points Boole's method (sometimes also referred to as Bode's method) [1]. The step of size h in the azimuthally direction z is divided in 4 parts of equivalent lengths. Let us the azimuthally positions z_0, z_1, z_2, z_3, z_4 such that:

$$z_1 - z_0 = h/4\,,\; z_2 - z_0 = h/2\,,\; z_3 - z_0 = 3h/4,\; z_4 - z_0 = h \tag{1}$$

The 5 points Bode's rule is as follow:

$$\int_{z_0}^{z_4 = z_0 + h} f(z)dz = \frac{h}{90}\left[7f(z_0) + 32f(z_1) + 12f(z_2) + 32f(z_3) + 7f(z_4)\right] \tag{1-a}$$

Such a process is very convenient when the shape of the electric field $E(z)$ becomes complex, since one has 4 parts of $E(z)$ for each step size h.

1-2 The electric field $E(z)$ being given along the axis of the structure, the current electric field $E(z,0,t)$ takes on the form:

$$E(z,0,t) = E(z)\cos(\omega t + \varphi_i) \tag{2}$$

φ_i : Phase at the entrance of the electric field $E(z)$.

1-3 The transverse motion can be derived from an integration of the equation of the type:

$$\frac{d(mv_r)}{dt} = q\left(E_r - v_z B_\theta\right)$$

After integration over the step size h, the transverse momentum is changed by the amount $\Delta(mv_r)$ and the variation in slope r' becomes:

$$\Delta r' = \frac{\Delta(mv_r)}{mv_z} - \frac{mv_r}{mv_z}\Delta(mv_z) + \ldots..$$

The extra-terms are due to the fact that r and r' are not canonically conjugates, the conjugate of r is mv_r. As a consequence, computations are complicated and developing second order corrections to improve the accuracy of the transverse motion is hardly possible. This problem can be resolved in using the following Picht transformations:

$$R = r\sqrt{\beta\gamma}\,,\quad R' = dR/dz \tag{3}$$

The quantities R, R' are referred to as the 'reduced coordinates'. The advantage of the Picht transformation results from the facts that R, R' are canonically conjugates.

In the terms of Cartesian coordinates $r \equiv (x, y)$ and $r' \equiv (x', y')$, the 'reduced coordinates' $R \equiv (X, Y)$ and $R' \equiv (X', Y')$ are given by:

$$R = r\left(\gamma^2 - 1\right)^{0.25}\,,\quad R' = r'\left(\gamma^2 - 1\right)^{0.25} + 0.5R\gamma\left(\gamma^2 - 1\right)^{-1} \tag{4}$$

The coordinate $R(z)$ can be expanded on the general form as:

$$R(z) = a + b(z - z_0) + c(z - z_0)^2 + \ldots\ldots \quad \text{, with} \quad z_0 \le z \le z_4$$

The step size h being taken sufficiently small, this development may be limited as:

$$R(z) = R_0 + R_0^{'}(z - z_0) \tag{5}$$

2. Dynamics in the longitudinal direction.

2-1 Energy gain

When crossing the step of size h, the energy $W = m_0 c^2 \gamma$ is changed by the amount $\Delta\gamma$:

$$\Delta\gamma = \frac{q}{m_0 c^2} \int_{z_0}^{z_4} E_z(z,0,t)\left[1 + K_1\left(R^2 + RR^{'}(z - z_0)\right)\right] dz \tag{6}$$

With: $$K_1(\beta,\gamma) = \frac{\omega^2}{4c^2\beta^3\gamma^3}$$

Pertaining to the transverse coupling terms in eq.6 (these are of second order and the step size h being taken sufficiently small), one can assume that the velocity β and the reduced coordinates $R, R^{'}$ remain constant over this step size h and are equal to the values $\beta_0, R_0, R_0^{'}$ at the entrance z_0 .

In this case:

$$K_1(\beta,\gamma) = \frac{\omega^2}{4c^2 {\beta_0}^3 {\gamma_0}^3} \quad , \quad R = R_0, R^{'} = R_0^{'} \tag{7}$$

Let t_0, t_1, t_2, t_3, t_4 be the times at the positions z_0, z_1, z_2, z_3, z_4, respectively one has (see also remark1):

$$t_1 = t_0 + \frac{h}{4\beta_0 c} \;,\; t_2 = t_0 + \frac{h}{2\beta_0 c} \;,\; t_3 = t_0 + \frac{3h}{4\beta_0 c} \;,\; t_4 = t_0 + \frac{h}{\beta_0 c} \tag{8}$$

Two different types of integrals appear in eq.6:

$$I_1 = \int_{z_0}^{z_4} E_z(z,0,t)dz \;,\; I_2 = \int_{z_0}^{z_4} E_z(z,0,t)(z - z_0)dz \tag{9}$$

Rewriting I_1 and I_2 with the 5 points Bode's rule, one obtains:

$$I_1 = \frac{h}{90}\left[7E(z_0,0,t_0) + 32E(z_1,0,t_1) + 12E(z_2,0,t_2) + 32E(z_3,0,t_3) + 7E(z_4,0,t_4)\right] \tag{10}$$

$$I_2 = \frac{h^2}{90}\left[8E(z_1,0,t_1) + 6E(z_2,0,t_2) + 24E(z_3,0,t_3) + 7E(z_4,0,t_4)\right] \tag{11}$$

Therefore, eq.6 can be rewritten as:

$$\Delta\gamma = \frac{q}{m_0 c^2}\left[\left(1 + R_0^2 K_1(\beta_0,\gamma_0)\right)I_1 + R_0 R_0^{'} K_1(\beta_0,\gamma_0) I_2\right] \tag{12}$$

At the end of the step of length h, one will have:

$$\gamma_4 = \gamma_0 + \Delta\gamma \tag{13}$$

REMARK 1: It could be necessary to improve the computations above, particularly for low energy particles.

For this, consider the series expansion of γ_4 with respect to γ_0 :

$$\gamma_4 = \gamma_0 + h\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} + \frac{h^2}{2}\left(\frac{\partial^2 \gamma}{\partial z^2}\right)_{z_0} \tag{14}$$

With:

$$\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} = \frac{q}{m_0 c^2} E(z_0, 0, t_0) \tag{15}$$

From eq.14, one obtains:

$$\left(\frac{\partial^2 \gamma}{\partial z^2}\right)_{z_0} = \frac{2\Delta\gamma}{h^2} - 2\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} \frac{1}{h} \tag{16}$$

Therefore, one can write:

$$\gamma_1 = \gamma_0 + \frac{h}{4}\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} + \frac{h^2}{32}\left(\frac{\partial^2 \gamma}{\partial z^2}\right)_{z_0} \tag{17}$$

$$\gamma_2 = \gamma_0 + \frac{h}{2}\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} + \frac{h^2}{8}\left(\frac{\partial^2 \gamma}{\partial z^2}\right)_{z_0} \tag{18}$$

$$\gamma_3 = \gamma_0 + \frac{3h}{4}\left(\frac{\partial \gamma}{\partial z}\right)_{z_0} + \frac{9h^2}{32}\left(\frac{\partial^2 \gamma}{\partial z^2}\right)_{z_0} \tag{19}$$

From eq.17 to eq.19, one can rewrite eq.6 as follow:

$$t_1 = t_0 + \frac{h}{4\beta_0 c}\ ,\ t_2 = t_1 + \frac{h}{4\beta_1 c}\ ,\ t_3 = t_2 + \frac{h}{4\beta_2 c}\ ,\ t_4 = t_3 + \frac{h}{4\beta_3 c} \tag{20}$$

In this case, the strategy to be applied is as follow:

a) Assuming that $\beta = \beta_0$ all over the step, one computes the predictor $\Delta\gamma$ as above.

b) From this predictor $\Delta\gamma$ and by using eq.17 to eq.19, one obtains the velocities $\beta_1, \beta_2, \beta_3$. This will allow computing the corrected value $\Delta\gamma$.

2-2 Phase jump

The time t is changed by the amount Δt [2] such that:

$$\Delta t = \frac{q}{m_0 c^3} \int_{z_0}^{z_4} \frac{1}{\beta^3 \gamma^3} E_z(z,0,t)\left[1 + K_1\left(R^2 + RR^{'}(z - z_0)\right)\right](z - z_0)dz \tag{21}$$

One will also assume that:

$$K_1(\beta,\gamma) = \frac{\omega^2}{4c^2\beta_0^{\ 3}\gamma_0^{\ 3}} \quad , \quad R = R_0, R^{'} = R_0^{'}$$

At the end of the step h, one has:

$$t_4 = t_0 + \Delta t + \frac{h}{\beta_0 c} \tag{22}$$

Two different types of integrals appear in eq.21:

$$I_3 = \int_{z_0}^{z_4} \frac{1}{\beta^3\gamma^3} E_z(z,0,t)(z - z_0)dz \ , \quad I_4 = \int_{z_0}^{z_4} \frac{1}{\beta^3\gamma^3} E_z(z,0,t)(z - z_0)^2 dz \tag{23}$$

Rewriting the integral I_3 , I_4 with the 5 points Bode's rule, one obtains:

$$I_3 = \frac{h^2}{90}\left[\frac{8}{\beta_1^3\gamma_1^3}E(z_1,0,t_1) + \frac{6}{\beta_2^3\gamma_2^3}E(z_2,0,t_2) + \frac{24}{\beta_3^3\gamma_3^3}E(z_3,0,t_3) + \frac{7}{\beta_4^3\gamma_4^3}E(z_4,0,t_4)\right] \tag{24}$$

$$I_4 = \frac{h^3}{90}\left[\frac{2}{\beta_1^3\gamma_1^3}E(z_1,0,t_1) + \frac{3}{\beta_2^3\gamma_2^3}E(z_2,0,t_2) + \frac{18}{\beta_3^3\gamma_3^3}E(z_3,0,t_3) + \frac{7}{\beta_4^3\gamma_4^3}E(z_4,0,t_4)\right] \tag{25}$$

Therefore, eq.21 can be rewritten as:

$$\Delta t = \frac{q}{m_0 c^3}\left[\left(1 + R_0^2 K_1\right)I_3 + R_0 R_0^{'} K_1 I_4\right] \tag{26}$$

3. The dynamics in the transverse directions.

With the reduced coordinates given in eq.6, the transverse motion is controlled by the following relation (see eq.10, ref [2] p. 218):

$$\frac{d^2R}{dz^2} - R(z)G_1(\gamma)\frac{\partial E_z}{\partial t} + R(z)\,G_2(\gamma)\,E_z^2 = 0 \tag{27}$$

With:

$$G_1(\gamma) = \left(\frac{q}{2m_0c^3}\right)\left(\gamma^2 - 1\right)^{-3/2}$$

$$G_2(\gamma) = \left(\frac{q}{2m_0c^2}\right)^2 \frac{\gamma^2 + 2}{\left(\gamma^2 - 1\right)^2}$$

REMARK 2: Pertaining to low energy electrons, the second term on the right hand side of eq.27 becomes predominant.
For protons or heavy ions, this term becomes insignificant and can be omitted.

Therefore, here one will consider eq.27 of the form:

$$\frac{d^2R}{dz^2} - R(z)G_1(\gamma)\frac{\partial E_z}{\partial t} = 0 \tag{28}$$

With:

$$\frac{\partial E_z}{\partial t} \equiv E^{'}(z,0,t) = -\omega E(z)\sin(\omega t + \varphi_i) \tag{29}$$

The coordinate $R(z)$ may be limited as:

$$R(z) = R_0 + R_0^{'}(z - z_0)$$

In which R_0 , $R_0^{'}$ represent the ‘reduced coordinates’ at the entrance of the step.

Over the step of size h , the slope $R^{'}$ is changed by the amount $\Delta R^{'}$ [2]:

$$\Delta R^{'} = \int_{z_0}^{z_4} \frac{d^2 R}{du^2}\, du = \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t)\left(R_0 + R_0^{'}(z - z_0)\right) dz \tag{30}$$

Using the 5 points Bode’s rule, one obtains:

$$J_1 \equiv \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t)\, dz = \tag{31}$$

$$\frac{h}{90}\left[7G_1(\gamma_0)E^{'}(z_0,0,t_0) + 32G_1(\gamma_1)E^{'}(z_1,0,t_1) + 12G_1(\gamma_2)E^{'}(z_2,0,t_2) + 32G_1(\gamma_3)E^{'}(z_3,0,t_3) + 7G_1(\gamma_4)E^{'}(z_4,0,t_4)\right]$$

And:

$$J_2 \equiv \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t_0)(z - z_0)\, dz = \tag{32}$$

$$= \frac{h^2}{90}\left[8G_1(\gamma_1)E^{'}(z_1,0,t_1) + 6G_1(\gamma_2)E^{'}(z_2,0,t_2) + 24G_1(\gamma_3)E^{'}(z_3,0,t_3) + 7G_1(\gamma_4)E^{'}(z_4,0,t_4)\right]$$

One can write eq.30 as:

$$\Delta R^{'} = R_0 J_1 + R_0^{'} J_2 \tag{33}$$

At the exit of the step h , the slope $R_4^{'}$ is given by:

$$R_4^{'} = R_0^{'} + \Delta R^{'} \tag{34}$$

Let ΔR be the jump of the reduced coordinate R over the step h :

$$\Delta R = \int_{z_0}^{z_4} \Delta R^{'}(z)\, dz \tag{35}$$

From eq.30, one can write:

$$\Delta R = R_0 \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t)(z - z_0)\, dz + R_0^{'} \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t)(z - z_0)^2\, dz \tag{36}$$

The first integral in the right hand side of eq.36 has been given in eq.32 (see the integral J_2)

By using the 5 points Bode's rule, the second integral in eq.36 gives way to:

$$J_3 \equiv \int_{z_0}^{z_4} G_1(\gamma) E^{'}(z,0,t_0)\,(z-z_0)^2\,dz = \tag{37}$$

$$= \frac{h^3}{90}\left[2G_1(\gamma_1)E^{'}(z_1,0,t_1) + 3G_1(\gamma_2)E^{'}(z_2,0,t_2) + 18G_1(\gamma_3)E^{'}(z_3,0,t_3) + 7G_1(\gamma_4)E^{'}(z_4,0,t_4)\right]$$

Therefore, one can rewrite eq.36 as:

$$\Delta R = R_0 J_2 + R_0^{'} J_3 \tag{38}$$

At the end of the step of size h , one will have:

$$R_4 = R_0 + \Delta R + hR_0^{'} \tag{39}$$

Given R_4 , $R_4^{'}$, it is a simple matter returning to the Cartesian coordinates r_4 , $r_4^{'}$ from eq.4.

4 Search for the phase $\hat{\varphi}$ giving the maximum energy gain in the structure.

Only the principle of the method is given in this section. The concept of transit time factors is used (it is based on a Fourier analysis of the axial field $E(z)$).

From the entrance as origin, one can compute over the length L (of the structure):

$$T(k) = \int_0^L E(z)\cos(kz)dz \quad , \quad S(k) = \int_0^L E(z)\sin(kz)dz \tag{40}$$

With: $k = \dfrac{\omega}{\beta c}$

Let us consider a particle traveling at a constant velocity with a phase of the form:

$$\varphi = kz + \varphi_0 \tag{41}$$

From a Fourier expansion of the field distribution with T and S coefficients and according to the derivation used in [2], one has for the energy gain:

$$\Delta W(k,\varphi_0) = q\left[T(k)\cos\varphi_0 - S(k)\sin\varphi_0\right] \tag{42}$$

It has a maximum for the phase $\varphi_0 = \hat{\varphi}$ with:

$$\tan\hat{\varphi} = -\,S(k)/T(k) \tag{43}$$

The crucial point is that one doesn't know the suitable value k to be applied in eq.40. A specific strategy will be required for this:

a) We start from $k = k_1$, with $k_1 = \omega/(\beta_0 c)$ where β_0 is the velocity at the entrance of the structure. This will allow computing the coefficients $T(k_1)$, $S(k_1)$ from which are obtained $\hat{\varphi}$ and $\Delta W(k_1, \hat{\varphi})$ (this allows computing the relativistic β_2).

b) Let $k_2 = \omega/(\beta_2 c)$ be the k value at the end L of the structure. Assuming a zero phase at the entrance, at the exit one will have the phase φ_2 [2] such that:

$$\varphi_2 = \Delta\varphi + k_2 L \tag{44}$$

With:

$$\Delta\varphi = \frac{\omega\, q}{m_0 c^3} \int_0^L \frac{1}{\beta_2^3 \gamma_2^3} E_z(z,0,t)(z - z_0) dz \tag{45}$$

The suitable value $\hat{k}$ to be used in eq.40 is taken in such a way that over the length we have:

$$L\hat{k} = \varphi_2$$

Then, from eq.44:

$$\hat{k} = k_2 + \frac{\Delta\varphi}{L} \tag{46}$$

REFERENCES

[1] M. Abramowith and I.A. Stegun: *Handbook of Mathematical functions,* Dover Publications, Inc., N.Y.
[2] P.Lapostolle, E. Tanke and S.Valero: *A New Method in Beam Dynamics Computations for Electrons and Ions in Complex Accelerating Element,* Particle Accelerators, 1994, vol. 44., pp. 215-255