



Numerical Methods I

Kevin Li

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Outline



Introduction to macroparticle models – implementations, applications and examples

- Part 1 numerical modelling
 - Initialisation
 - Simple tracking
 - Chromaticity and detuning
 - Wakefields with examples
 - Constant wakes
 - Dipole wakes
 - TMCI & headtail modes

- Part 2 electron cloud
 - Modelling of e-cloud interactions
 - PIC solvers
 - Application for e-cloud instabilities



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Why numerical methods?



 Computational physics is somewhere between experimental and theoretical physics



Macroparticle models



- Macroparticle models are used to study the dynamics of multi-particle systems, i.e. plasmas or beams
- Macroparticle models permit a seamless mapping of realistic systems into a computational environment – they are fairly easy to implement





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Macroparticle models



- Macroparticle models are used to study the dynamics of multi-particle systems, i.e. plasmas or beams
- Macroparticle models permit a seamless mapping of realistic systems into a computational environment – they are fairly easy to implement
- A macroparticle is a numerical representation of a clustered collection of physical particles → this increases the granularity of the numerical system (i.e. one must beware of numerical noise issues) but allows to treat large systems within the given limitations of computational resources





Accelerator-beam system – modelling







Accelerator-beam system - modelling



• Possible program layout

By closing the loop, we introduce collective effects which can act as a feedback mechanism:

- New equilibrium solutions
- Damping or growth of the stationary solutions \rightarrow instabilities



coordinates and momenta



Numerical representation of the beam





Beam:

$$\begin{pmatrix} x_{i} \\ x'_{i} \end{pmatrix} \\ \begin{pmatrix} y_{i} \\ y'_{i} \end{pmatrix}$$

 $\begin{pmatrix} z_i \\ \delta_i \end{pmatrix}$

$$\begin{pmatrix} q_i \\ m_i \end{pmatrix}, \quad i = 1, \dots, N$$
 Macroparticle
number

Can. conjugate coordinates and momenta

Memory (assume q, m are identical):

	array	array	array	array	array	array
count	х	x'	у	y'	Z	delta
0						
1						
2						
3						
4						
5						
6						
7						
8						
9						

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Numerical representation of the beam

Initial conditions of the beam/particles

Profile	Size	Matching
Gaussian	Emittance	Optics
Parabolic		
Flat		

- We use random number generators to obtain random distributions of coordinates and momenta
- Example transverse Gaussian beam in the SPS with normalized emittance of 2 um (0.35 eVs longitudinal)

$$\begin{split} \varepsilon_{\perp} &= \beta \gamma \sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle xx' \rangle^2} \\ &= \beta \gamma \sigma_x \sigma_{x'} \\ \varepsilon_{\parallel} &= 4\pi \sigma_z \sigma_\delta \frac{p_0}{e} \end{split}$$

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- We have identified with the beam and allocated a field of memory and filled this with the can. conjugate coordinates and momenta in accordance with our specifications for beam profile and emittance and machine optics.
- We are now ready to investigate how to implement the beam dynamics

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Numerical representation of the linear lattice

p0

p1

- Quadrupoles \rightarrow focusing
- Particle dynamics along the linear periodic lattice is described by Hill's equation

$$x'' + K(s)x = 0$$
, $K(s) = K(s + L)$

• Hill's equation can be solved to obtain the linear transfer map from one point to another along the ring:

$$\mathcal{M} = \begin{pmatrix} \sqrt{\beta_1} & 0\\ -\frac{\alpha_1}{\sqrt{\beta_1}} & \frac{1}{\sqrt{\beta_1}} \end{pmatrix} \begin{pmatrix} \cos(\Delta\mu_{0\to1}) & \sin(\Delta\mu_{0\to1})\\ -\sin(\Delta\mu_{0\to1}) & \cos(\Delta\mu_{0\to1}) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\beta_0}} & 0\\ \frac{\alpha_0}{\sqrt{\beta_0}} & \sqrt{\beta_0} \end{pmatrix}$$
$$Q_x = \oint \frac{\Delta\mu}{2\pi}$$

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E. D. Courant and H. S. Snyder, Theory of the Alternating-Gradient Synchrotron, Annals of Physics 3 (1958)

Numerical representation of the linear lattice

- 1. The optics functions can be obtained from a Twiss file (e.g. MAD-X)
- 2. We can make the smooth approximation

$$\beta_x = \text{constant}$$

$$Q_x = \frac{C}{2\pi\beta_x}, \left(Q_s = \frac{\eta C}{2\pi\beta_z}\right)$$
$$\Delta\mu_x = Q_x \frac{L}{\alpha}$$

C: Ring circumference

$$\mathcal{M} = \begin{pmatrix} \sqrt{\beta_1} & 0\\ -\frac{\alpha_1}{\sqrt{\beta_1}} & \frac{1}{\sqrt{\beta_1}} \end{pmatrix} \begin{pmatrix} \cos(\Delta\mu_{0\to1}) & \sin(\Delta\mu_{0\to1})\\ -\sin(\Delta\mu_{0\to1}) & \cos(\Delta\mu_{0\to1}) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\beta_0}} & 0\\ \frac{\alpha_0}{\sqrt{\beta_0}} & \sqrt{\beta_0} \end{pmatrix}$$

 $\begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_1 = \mathcal{M} \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_0$ $i = 1, \dots, N$

• The numerical implementation is then simply the matrix product applied to all macroparticles in all panes

All matrix elements are constant

E. D. Courant and H. S. Snyder, Theory of the Alternating-Gradient Synchrotron, Annals of Physics 3 (1958)

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Numerical representation of the long. motion

p0 y x z p1

$$z_{i,k+1/2} = z_{i,k} - \frac{\eta C}{2} \delta_{i,k}$$

$$\delta_{i,k+1} = \delta_{i,k} + \frac{e V_{\text{RF}}}{m\gamma\beta^2 c^2} \sin\left(\frac{2\pi h}{C} z_{i,k+1/2}\right)$$

$$z_{i,k+1} = z_{i,k+1/2} - \frac{\eta C}{2} \delta_{i,k+1}$$

$$i = 1, \dots, N$$

k: iteration/turn

 Particle dynamics in the longitudinal plane are described by the longitudinal equations of motion

$$z' = -\eta \,\delta$$
$$\delta' = \frac{e \, V_{\rm RF}}{m\gamma\beta^2 c^2 \, C} \sin\left(\frac{2\pi h}{C} \, z\right)$$

- $V_{\rm RF}$: RF voltage
- $h = \frac{\omega_{\rm RF}}{\omega_0}$: harmonic number
- ω_0 : Revolution frequency
- C: circumference
- These can be solved numerically via a symplectic integration scheme – iterative turn-by-turn advancement of the coordinates and momenta

W. Herr, *Tools for Non Linear Dynamics*, CAS Poland 2015

E. Forest, Beam Dynamics: A New Attitude and Framwork, 1998

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Example: SPS – transverse and longitudinal

• We can now input the optics functions along with the RF parameters and observe the oscillations

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Example: PS Booster hollow bunches

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- Generation of 'hollow' bunches for mitigation of transverse space charge
- Modulation of the reference phase at 490 Hz with an amplitude of 18 deg (reconstructed from 3.4 mm amplitude and the waterfall plot) for 4 synchrotron periods
- Simulations are capable of reproducing as well as predicting

- We have implemented a beam to initializing a field of memory with the beam's can. conjugate coordinates and momenta.
- We have implemented linear transverse tracking as a 2D matrix multiplication looped over the set of macroparticles in the beam.
- We have implemented longitudinal tracking as a second order symplectic integration scheme looped over the set of macroparticles in the beam.
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What else do we need?

- We have learned or we may know from operational experience that there are a set of crucial machine parameters to influence beam stability – among them chromaticity and amplitude detuning
- Chromaticity
 - Controlled with sextupoles provides chromatic shift of bunch spectrum wrt. impedance
 - \circ Changes interaction of beam with impedance
 - Damping or excitation of headtail modes
- Amplitude detuning
 - Controlled with octupoles provides (incoherent) tune spread
 - Leads to absorption of coherent power into the incoherent spectrum → Landau damping
- Of course, to study intensity effects, these need to be included in our model – fortunately, this is pretty simple!

Chromaticity and amplitude detuning

$$\mathcal{M} = \begin{pmatrix} \sqrt{\beta_1} & 0\\ -\frac{\alpha_1}{\sqrt{\beta_1}} & \frac{1}{\sqrt{\beta_1}} \end{pmatrix} \begin{pmatrix} \cos(\Delta\mu) & \sin(\Delta\mu) \\ -\sin(\Delta\mu) & \cos(\Delta\mu) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\beta_0}} & 0\\ \frac{\alpha_0}{\sqrt{\beta_0}} & \sqrt{\beta_0} \end{pmatrix}$$

$$\begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_1 = \mathcal{M} \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_0$$
$$i = 1, \dots, N$$

• The numerical implementation is then simply the matrix product applied to all macroparticles in all panes

All matrix elements are constant

Chromaticity and amplitude detuning

- $\begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_1 = \underbrace{\mathcal{M}_i}_{i} \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_0$ $i = 1, \dots, N$
 - The numerical implementation is then simply the matrix product applied to all macroparticles in all panes

All matrix elements are macroparticle dependent

Example: filamentation as result of detuning

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Example: filamentation as result of detuning

- We have added chromaticity and detuning with amplitude to our transverse tracking.
- We now have all the necessary single-particle dynamics implemented to serve as platform onto which we now will add collective effects interactions.

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Accelerator beam system - wakefields

• Our first 'real' collective interaction from impedances

When the loop closes, either the beam will find a new stable equilibrium configuration ...

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... or it might develop an instability along the bunch train ...

Numerical implementation of wakefields

 We have learned how to track a macroparticle beam through a linear periodic lattice and how to include chromaticity and detuning with amplitude p0 Chromaticity: Detuning with amplitude: continuous detuning coupling to longitudinal $\Delta \mu_{i} \sim \Delta \mu_{0,i} + \left[\xi \, \delta_{i} \right] + \alpha_{xx} \, J_{x,i} + \alpha_{xy} \, J_{y,i}$ p1 \mathcal{Z} $\mathcal{M}_{i} = \begin{pmatrix} \sqrt{\beta_{1}} & 0\\ -\frac{\alpha_{1}}{\sqrt{\beta_{1}}} & \frac{1}{\sqrt{\beta_{1}}} \end{pmatrix} \begin{pmatrix} \cos(\Delta\mu_{i}) & \sin(\Delta\mu_{i})\\ -\sin(\Delta\mu_{i}) & \cos(\Delta\mu_{i}) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\beta_{0}}} & 0\\ \frac{\alpha_{0}}{\sqrt{\beta_{0}}} & \sqrt{\beta_{0}} \end{pmatrix}$ $\begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_1 = \mathcal{M}_i \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \Big|_0$ $i = 1, \ldots, N$

Numerical implementation of wakefields



- To be numerically more efficient, the beam is longitudinally sliced into a set of slices
- Provided the slices are thin enough to sample the wake fields, the wakes can be assumed constant within a single slice
- The kick on to the set of macroparticles in slice 'i' generated by the set of macroparticles in slice 'j' via the wake fields now becomes:

- The wake functions are obtained externally from electromagnetic codes such as ACE3P, CST, GdfidL, HFSS...
- In the tracking code, the wake fields at p1 need to update the macroparticle momenta (i.e. they provide a kick)
- The kick on to a macroparticle 'i' generated by all macroparticles 'j' via the wake fields is:

$$\begin{split} & {}'[i] = -\frac{e^2}{m\gamma\beta^2c^2} & \Delta x'_i = -\frac{e^2}{m\gamma\beta^2c^2} \\ & \times \sum_{j=0}^{n_slices} \begin{cases} N[j] \cdot W_{Cx}[i-j] \\ N[j]\langle x \rangle[j] \cdot W_{Dx}[i-j] \\ N[j] \cdot W_{Qx}[i-j] \Delta x[i] \end{cases} & \times \sum_{j=0}^{n_macroparticles} \begin{cases} W_{Cx}(z_i - z_j) \\ \Delta x_j \cdot W_{Dx}(z_i - z_j) \\ W_{Qx}(z_i - z_j) \Delta x_i \end{cases}$$



 Δx



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- Provided the slices are thin enough to sample the wake fields, the wakes can be assumed constant within a single slice
- The kick on to the set of macroparticles in slice 'i' generated by the set of macroparticles in slice 'j' via the wake fields now becomes

$$\Delta x'[i] = -\frac{e^2}{m\gamma\beta^2 c^2}$$

$$\times \sum_{j=0}^{n_slices} \begin{cases} N[j] \cdot W_{Cx}[i-j] \\ N[j]\langle x \rangle [j] \cdot W_{Dx}[i-j] \\ N[j] \cdot W_{Qx}[i-j] \Delta x[i] \end{cases}$$

- N[i]: number of macroparticles in slice 'i'
 → can be pre-computed and stored in memory
- W[i]: wake function pre-computed and stored in memory for all differences i-j

Count	0	1	2	3	4	5	6
N[i]							
W[i]						•••	



Relativistic vs. non-relativistic wakes



- Relativistic wakes only affect trailing particles following the source particle
- Finite values range for negative distances, i.e. (-L, 0) or "tail head"
 - L: bunch length

- Nonrelativistic wakes can also affect particles ahead of the source particle
- Finite values extend from (-L, L) or "tail –head" & "head – tail"
 - L: bunch length













 Bin particles into slices (apply after each update of longitudinal coordinates) – binning needs to be fine enough as to sample the wake function







- Bin particles into slices (apply after each update of longitudinal coordinates) – binning needs to be fine enough as to sample the wake function
- 2. Perform convolution to obtain wake kicks



$$\Delta x'[i] = -\frac{e^2}{m\gamma\beta^2 c^2} \sum_{j=0}^{i} N[j] \cdot W_{Cx}[i-j]$$





- Bin particles into 1. slices (apply after each update of longitudinal coordinates) binning needs to be fine enough as to sample the wake function
- 2. Perform convolution to obtain wake kicks
- 3. Apply wake kicks (momentum update)

Bunch & slices Wake field $W_{Cx}[i]$ Wake kicks $\Delta x'[i]$ Macroparticles per slice N[i] Slice index n 0 $\Delta x'[i] = -\frac{e^2}{m\gamma\beta^2c^2} \sum_{i=0}^{r} N[j] \cdot W_{Cx}[i-j], \quad x'[i] \to x'[i] + \Delta x'[i], \quad i = 1, \dots, \text{n_slices}$



Summary – where are we?



• We are now ready to track a full turn including the interaction with wake fields



$$\left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_{k+1} = \mathcal{M}_i \left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_k$$

- 1. Initialise a macroparticle distribution with a given emittance
- 2. Update transverse coordinates and momenta according to the linear periodic transfer map – adjust the individual phase advance according to chromaticity and detuning with amplitude
- 3. Update the longitudinal coordinates and momenta according to the leapfrog integration scheme
- Update momenta only (apply kicks) according to wake field generated kicks
- 5. Repeat turn-by-turn...



5























Examples – dipole wakes





• Without synchrotron motion:

kicks accumulate turn after turn – the beam is unstable \rightarrow beam break-up in linacs





- Without synchrotron motion: kicks accumulate turn after turn – the beam is unstable → beam break-up in linacs
- With synchrotron motion:
 - Chromaticity = 0
 - Synchrotron sidebands are well separated \rightarrow beam is stable
 - Synchrotron sidebands couple \rightarrow (transverse) mode coupling instability
 - Chromaticity $\neq 0$
 - Headtail modes \rightarrow beam is unstable (can be very weak and often damped by non-linearities)



Dipole wakes – beam break-up





Dipole wakes - beam break-up







Dipole wakes – TMCI below threshold







Dipole wakes – TMCI below threshold





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Dipole wakes – TMCI above threshold



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Dipole wakes – TMCI above threshold





Raising the TMCI threshold – SPS Q20 optics



- In simulations we have the possibility to perform scans of variables, e.g. we can run 100 simulations in parallel changing the beam intensity
- We can then perform a spectral analysis of each simulation...
- ... and stack all obtained plot behind one another to obtain...
- ... the typical visualization plots of TMCI



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The mode number is given as

$$m = \frac{Q_x - Q_{x0}}{Q_s}$$

The modes are separated by the synchrotron tune.

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Example non-relativistic wakes





Example non-relativistic wakes





Dipole wakes – headtail modes





Dipole wakes – headtail modes





Example: Headtail modes in the LHC







End of part I



- Numerical methods allow us
 - to study conditions not realizable in a machine
 - to disentangle effects
 - to use unprecedented analysis tools
- Macroparticle models closely resemble real systems and are relatively easy to implement
- We have learned how to model and implement macroparticle simulations to study intensity effects in circular accelerators





Backup



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Wakefields – rough formalism



$$H = \frac{1}{2}p_x^2 + \frac{1}{2}K(s)x^2 + \sum_k \frac{e^2}{m\gamma\beta^2 c^2 C} \iiint \rho(x_s, z_s) w(x, x_s, z - z_s - kC) \, dx_s \, dz_s \, dx$$



Wakefields – rough formalism



$$H = \frac{1}{2}p_x^2 + \frac{1}{2}K(s)x^2 + \sum_k \frac{e^2}{m\gamma\beta^2c^2C} \iiint \rho(x_s, z_s) w(x, x_s, z - z_s - kC) dx_s dz_s dx$$
$$= \dots + \sum_k \frac{e^2}{m\gamma\beta^2c^2C} \iiint \rho(x_s, z_s) \sum_{mn} x^n x_s^m W_{mn}(z - z_s - kC) dx_s dz_s dx$$
$$= \dots + \sum_k \frac{e^2}{m\gamma\beta^2c^2C} \sum_{mn} \int x^n \int \lambda_m(z_s) W_{mn}(z - z_s - kC) dz_s dx$$
$$\lambda_m(z_s) = \int \rho(x_s, z_s) x_s^m dx_s$$

• Expansion



Wakefields – rough formalism



$$H = \frac{1}{2}p_x^2 + \frac{1}{2}K(s)x^2 + \sum_k \frac{e^2}{m\gamma\beta^2 c^2 C} \sum_{mn} \int x^n \int \lambda_m(z_s) W_{mn}(z - z_s - kC) dz_s dx$$
$$\lambda_m(z_s) = \int \rho(x_s, z_s) x_s^m dx_s$$



n	m	type
0	0, 1	
1	0	

Constant transverse wake (n=0, m=0) Dipole transverse wake (n=0, m=1) Quadrupole transverse wake (n=1, m=0)













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Examples – quadrupole wakes








Examples – quadrupole wakes





Examples – quadrupole wakes





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Examples – dipole wakes $H = \frac{1}{2}p_x^2 + \frac{1}{2}K(s)x^2 + \frac{e^2}{m\gamma\beta^2c^2C} \int_{j=0}^{n} \sum_{j=0}^{\text{slices-1}} \lambda(z_j) \langle x \rangle|_j W_{11}(z-z_j) \Delta z_j$ Dipolar term \Rightarrow orbit kick Offset dependent orbit kick \Rightarrow kicks can accumulate

 Without synchrotron motion: kicks accumulate turn after turn – the beam is unstable → beam break-up in linacs





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