

Numerical Methods II

Kevin Li

With acknowledgements to:

H. Bartosik, X. Buffat, L.R. Carver, S. Hegglin, G. Iadarola, L. Mether,
E. Metral, N. Mounet, A. Oeftiger, A. Romano, G. Rumolo, B. Salvant,
M. Schenk

Introduction to macroparticle models – implementations, applications and examples

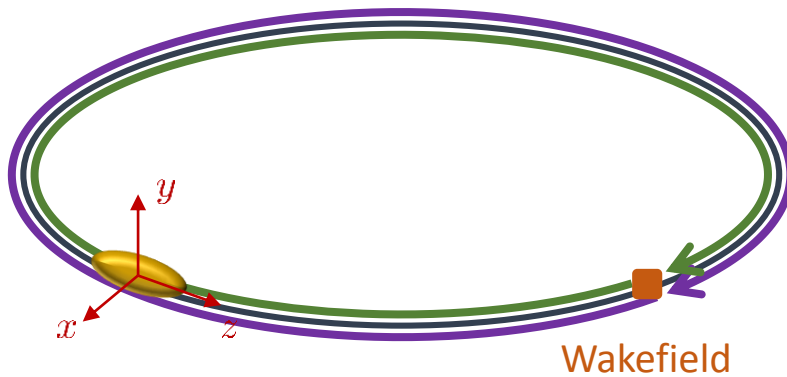
- Part 1 – numerical modelling
 - Initialisation
 - Simple tracking
 - Chromaticity and detuning
 - Wakefields with examples
 - Constant wakes
 - Dipole wakes
 - TMCI & headtail modes
- Part 2 – electron cloud
 - Modelling of e-cloud interactions
 - PIC solvers
 - Application for e-cloud instabilities

Introduction to macroparticle models – implementations, applications and examples

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Summary – where are we?

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



$$\begin{array}{l} \left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_{k+1} = \mathcal{M}_i \left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_k \\ \left. \begin{pmatrix} z_i \\ \delta_i \end{pmatrix} \right|_{k+1} = \mathcal{I} \left[\left. \begin{pmatrix} z_i \\ \delta_i \end{pmatrix} \right|_k \right] \\ \left. x'_i \right|_{k+1} = \left. x'_i \right|_k + \mathcal{W}\mathcal{K} \end{array}$$

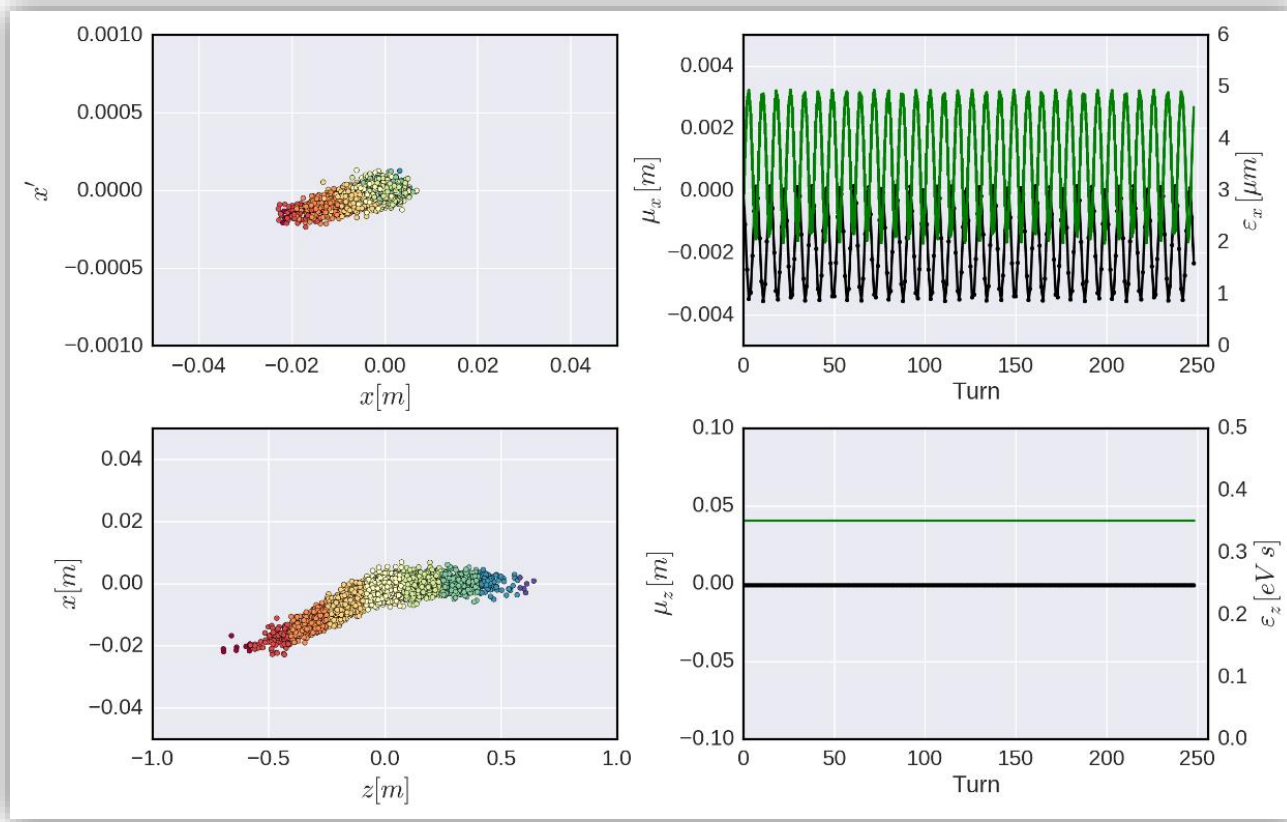
1. Initialise a macroparticle distribution with a given emittance
2. Update transverse coordinates and momenta according to the linear periodic transfer map – adjust the individual phase advance according to chromaticity and detuning with amplitude
3. Update the longitudinal coordinates and momenta according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

Examples – constant wakes

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

Dipolar term \rightarrow orbit kick

Slice dependent change of closed orbit
(if line density does not change)



Examples – dipole wakes

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

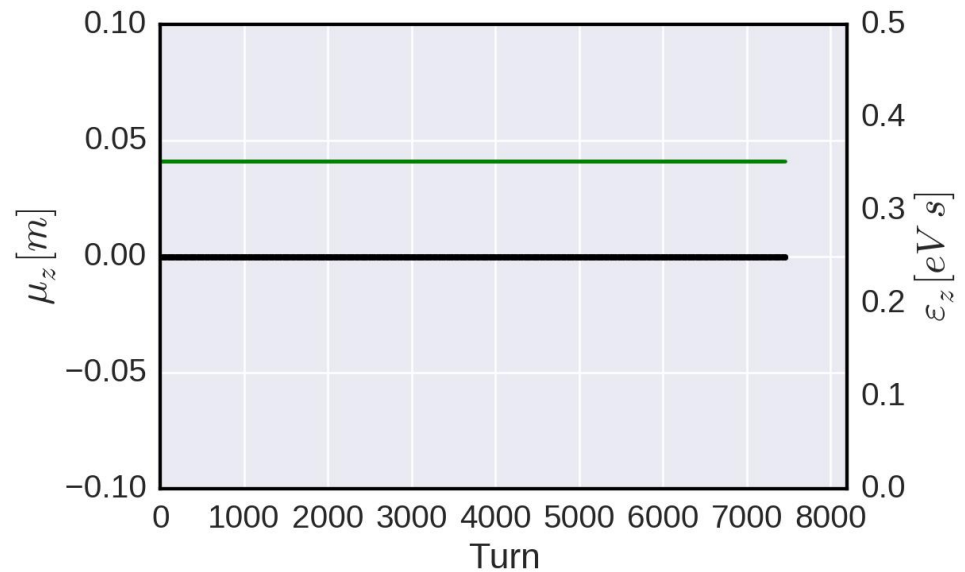
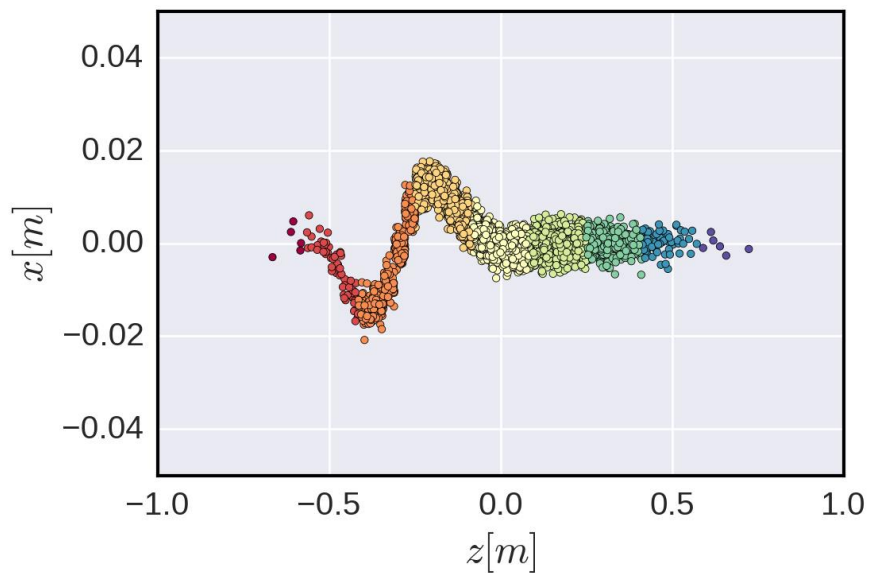
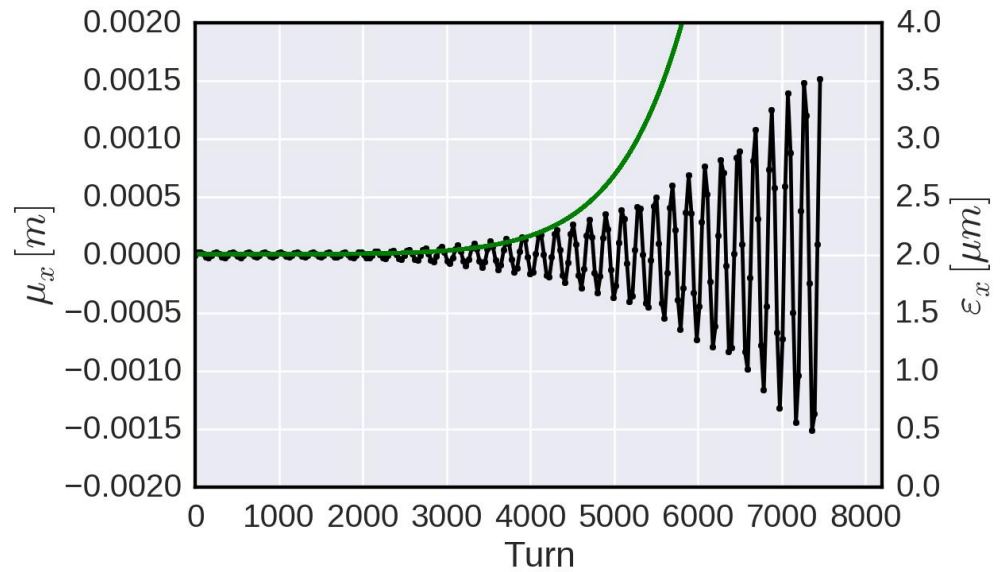
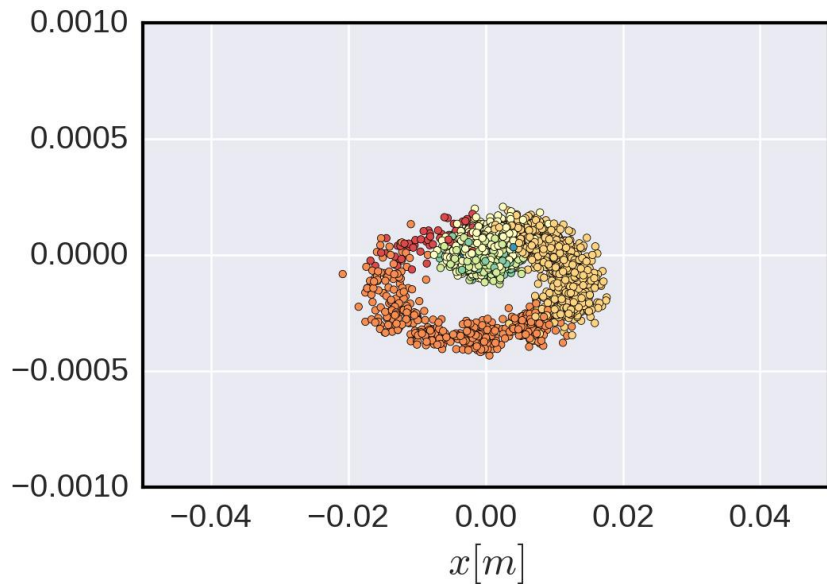
Dipolar term → orbit kick

Offset dependent orbit kick → kicks can accumulate

With synchrotron motion we can get into a feedback loop

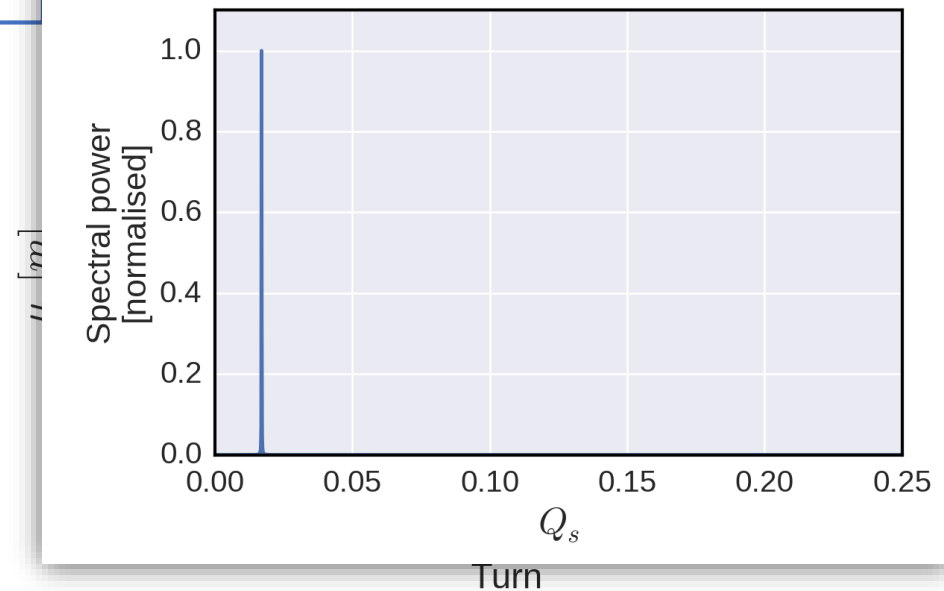
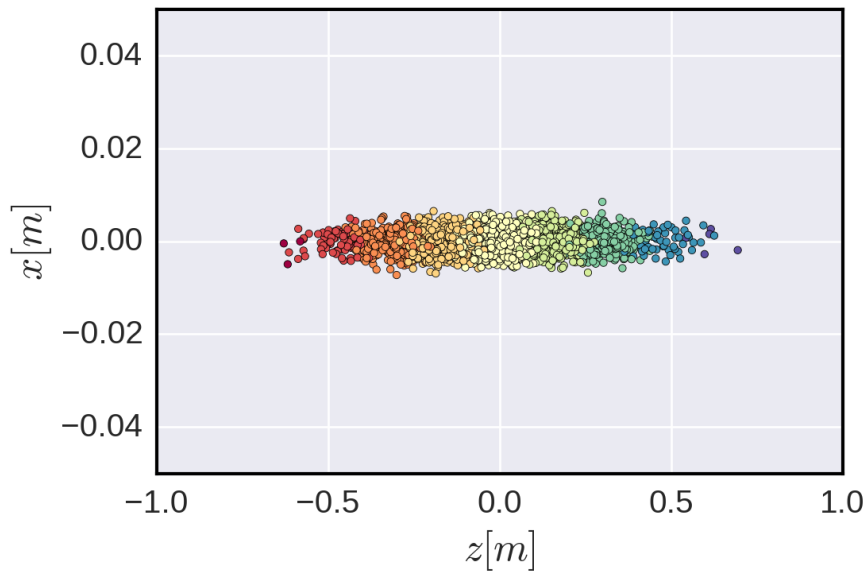
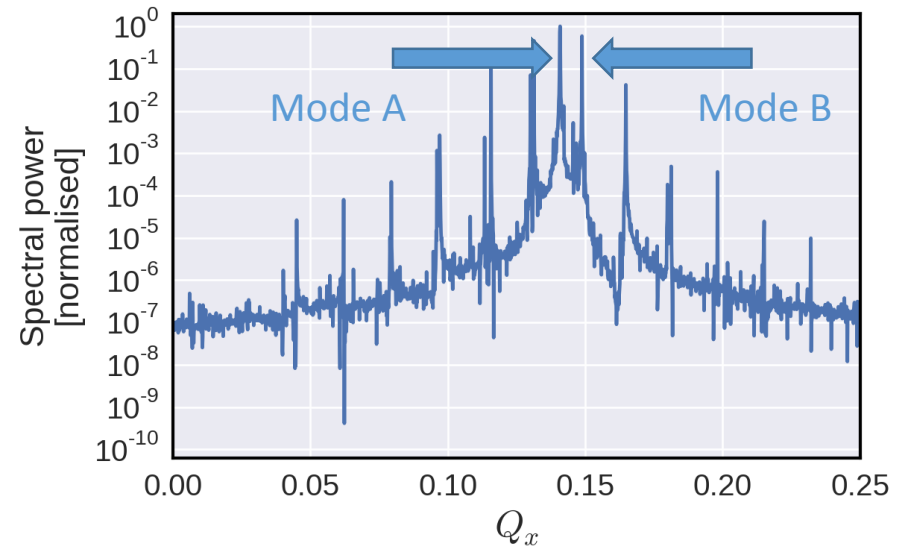
- Without synchrotron motion:
kicks accumulate turn after turn – the **beam is unstable** → beam break-up in linacs
- With synchrotron motion:
 - Chromaticity = 0
 - Synchrotron sidebands are well separated → **beam is stable**
 - Synchrotron sidebands couple → **(transverse) mode coupling instability**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

Dipole wakes – beam break-up



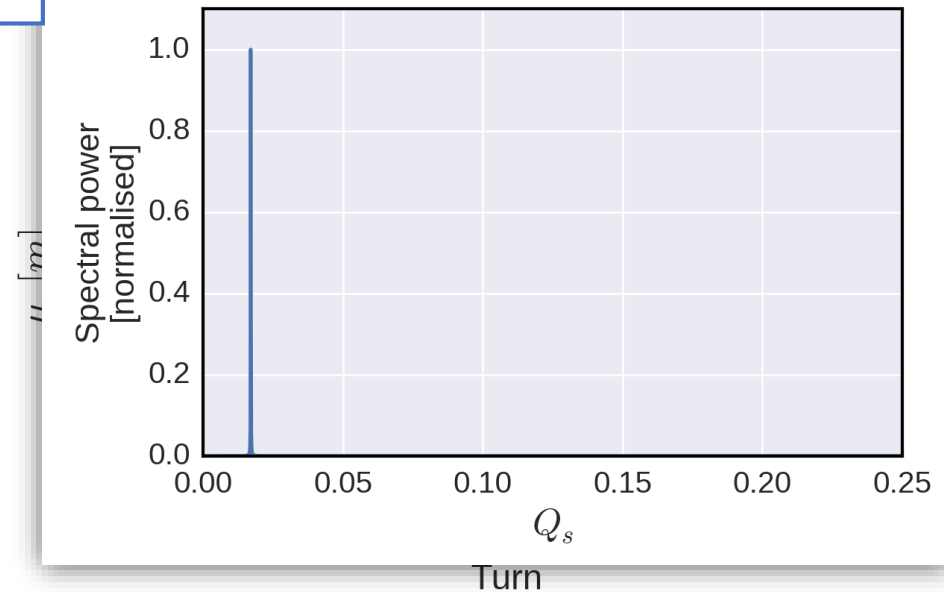
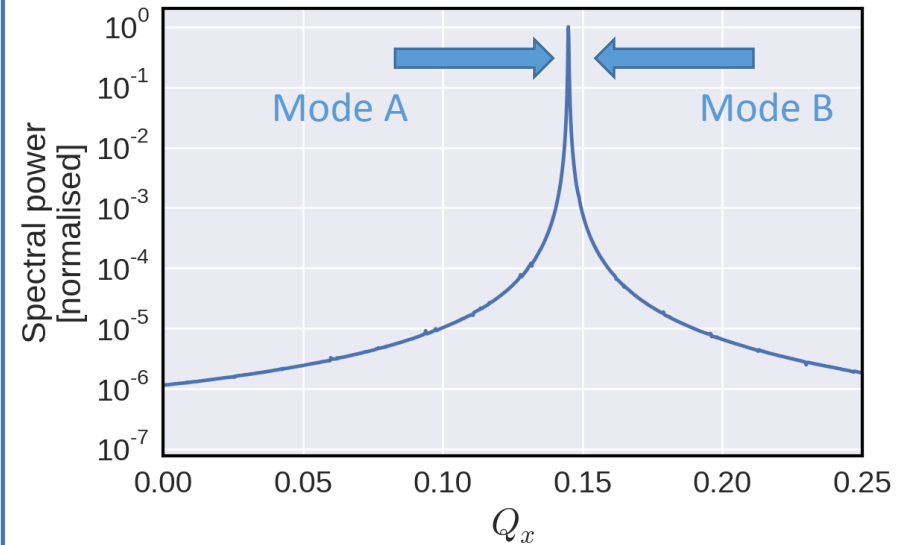
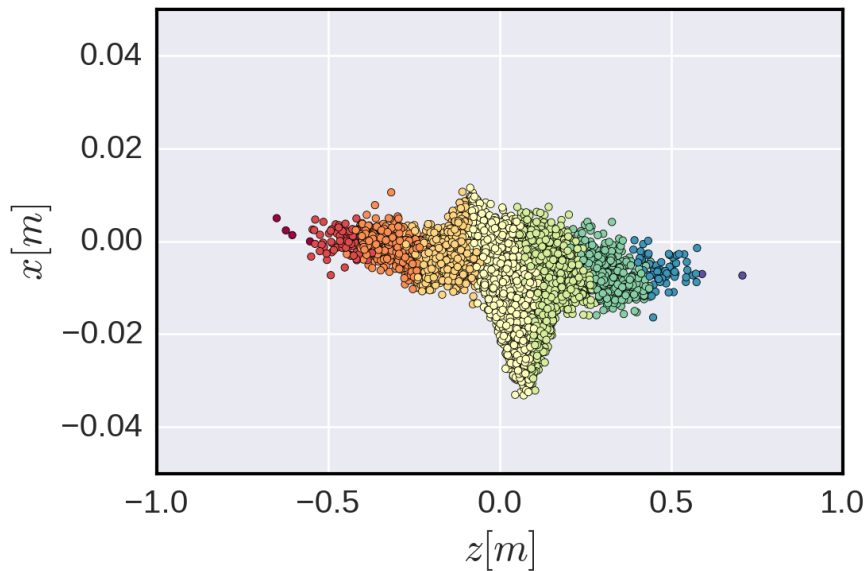
Dipole wakes – TMCI below threshold

As the intensity increases the coherent modes shift – here, modes A and B are approaching each other



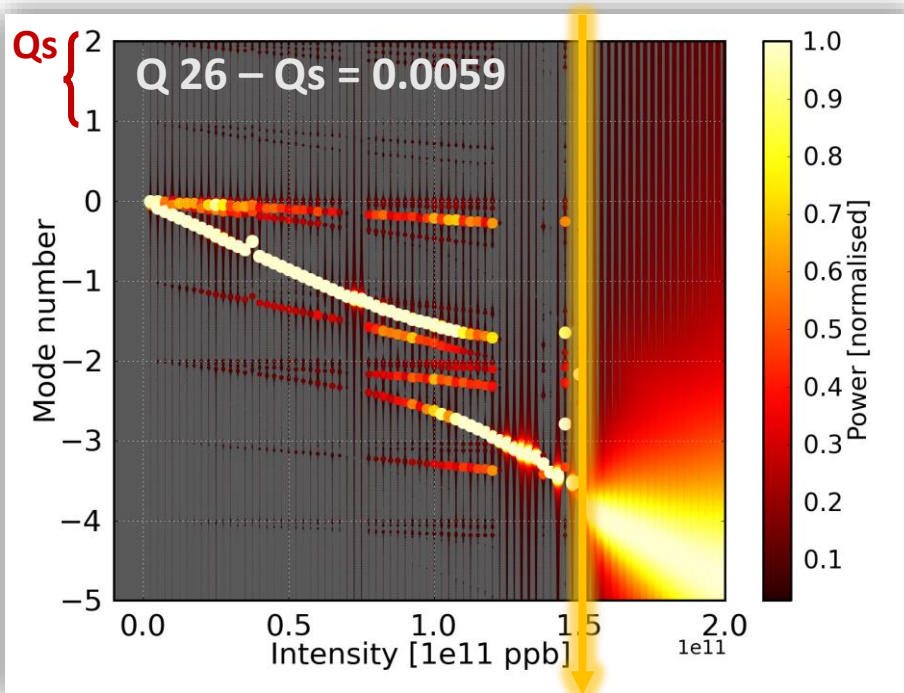
Dipole wakes – TMCI above threshold

When the two modes merge a fast coherent instability arises – the transverse mode coupling instability (TMCI) which often is a hard intensity limit in many machines

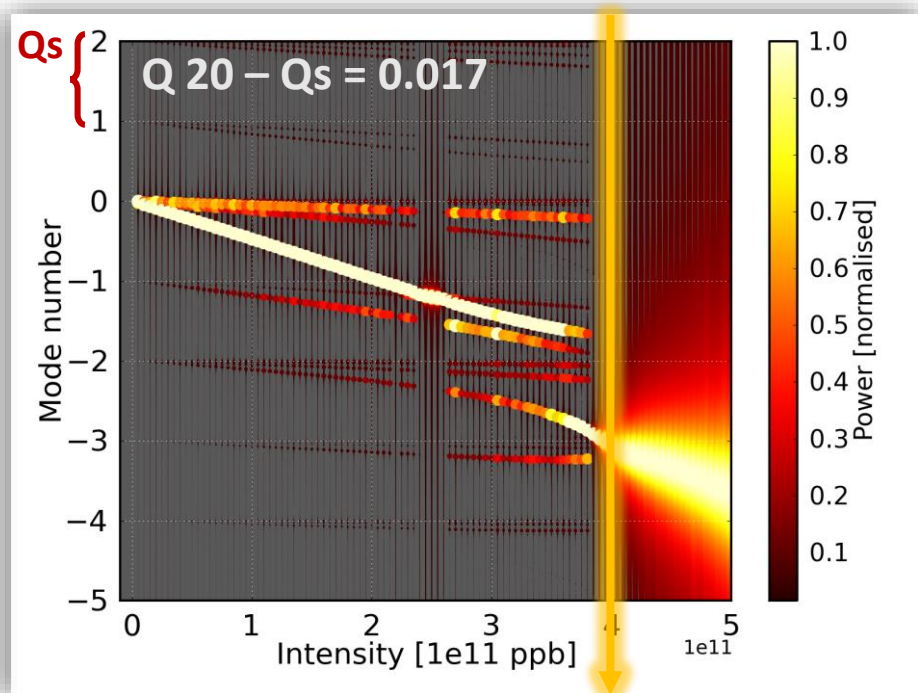


Raising the TMCI threshold – SPS Q20 optics

- 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



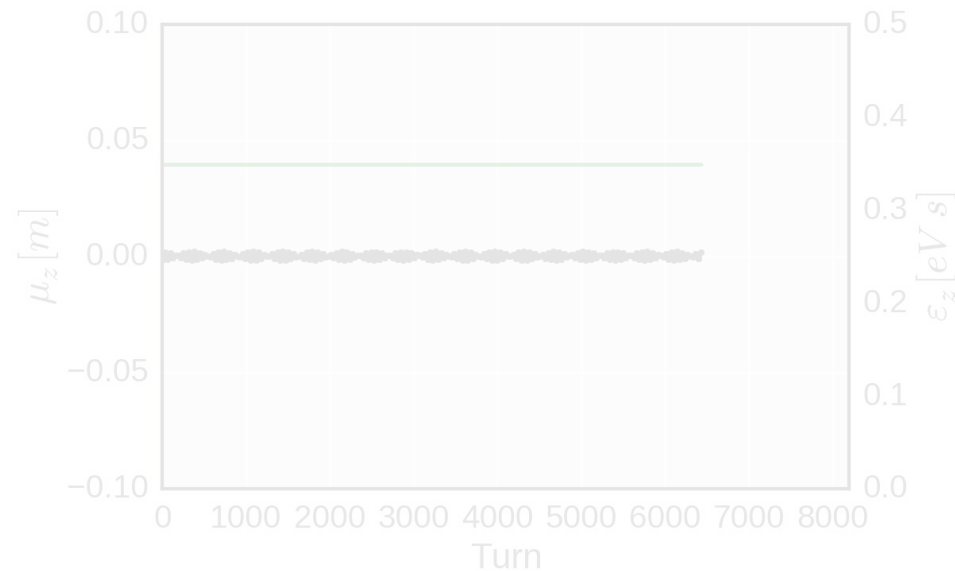
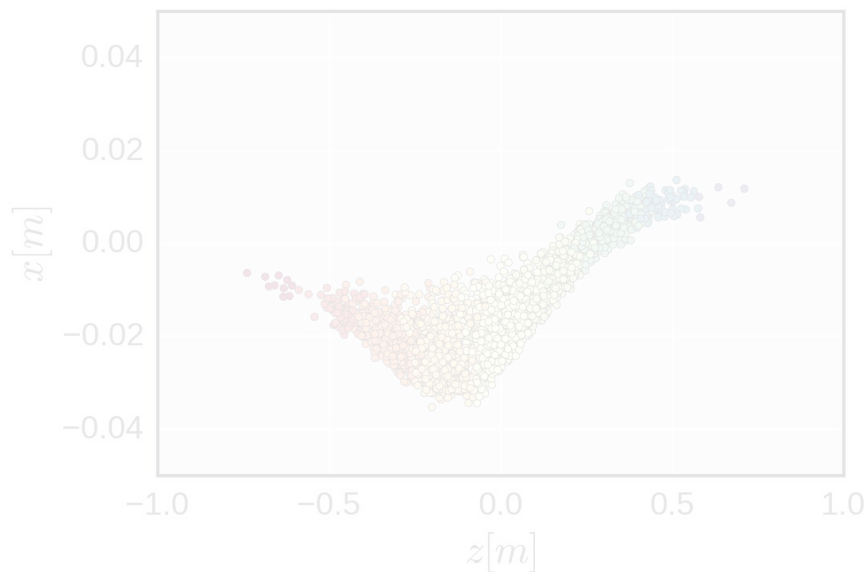
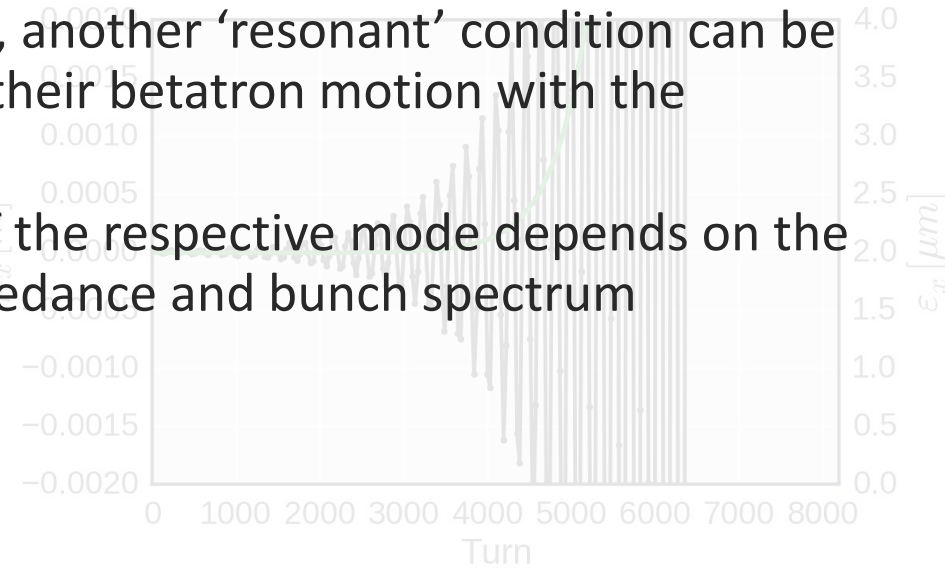
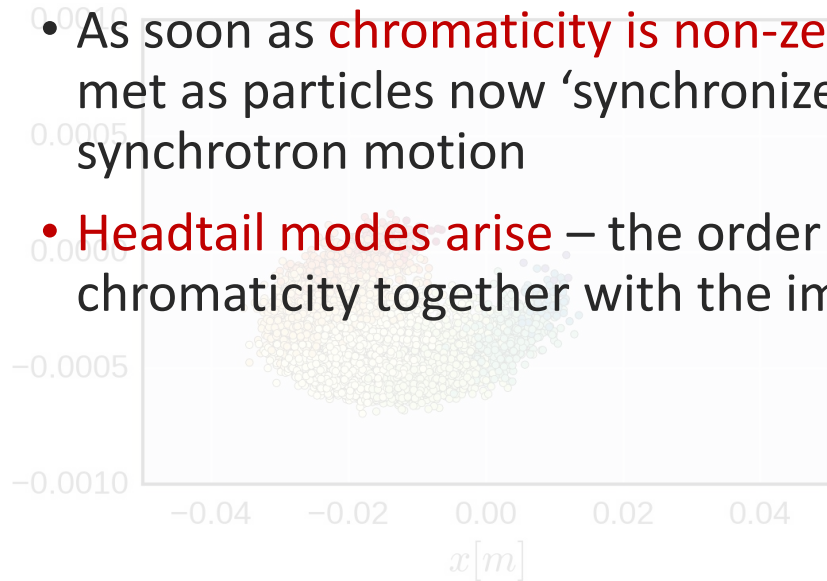
TMCI threshold



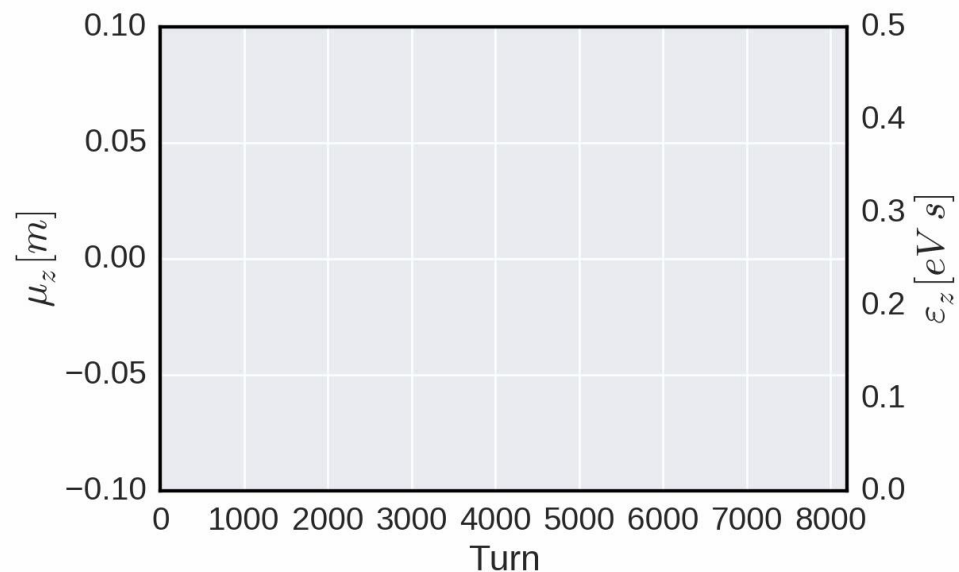
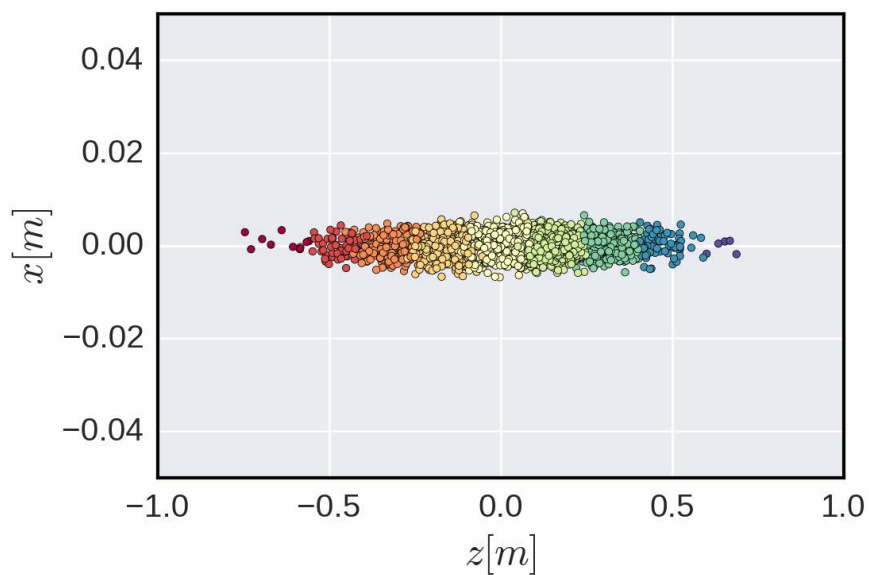
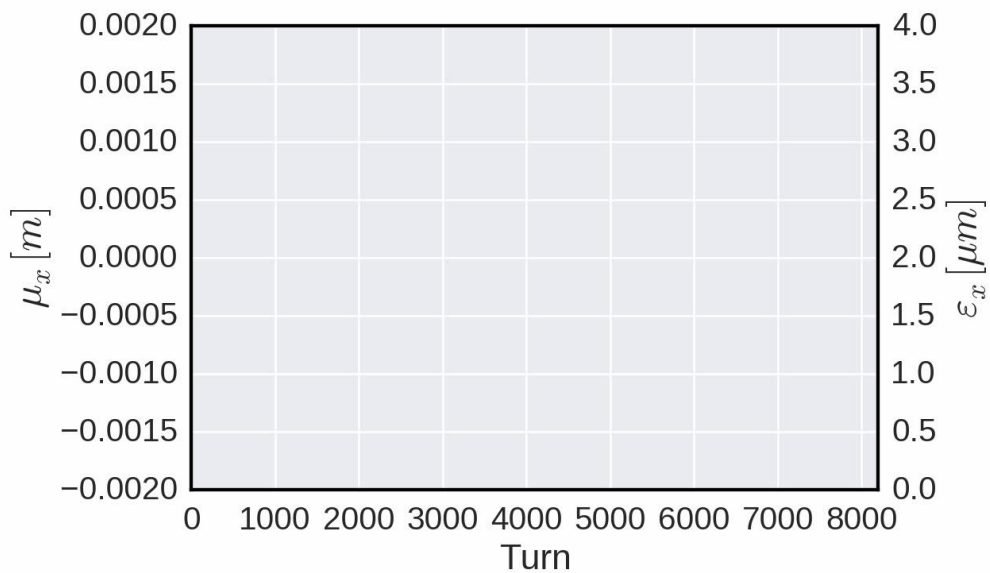
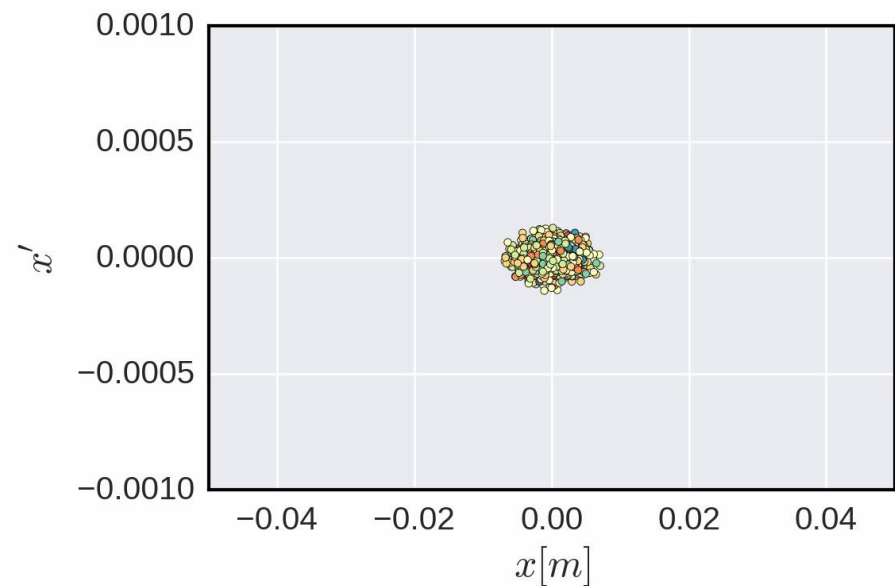
TMCI threshold

Dipole wakes – headtail modes

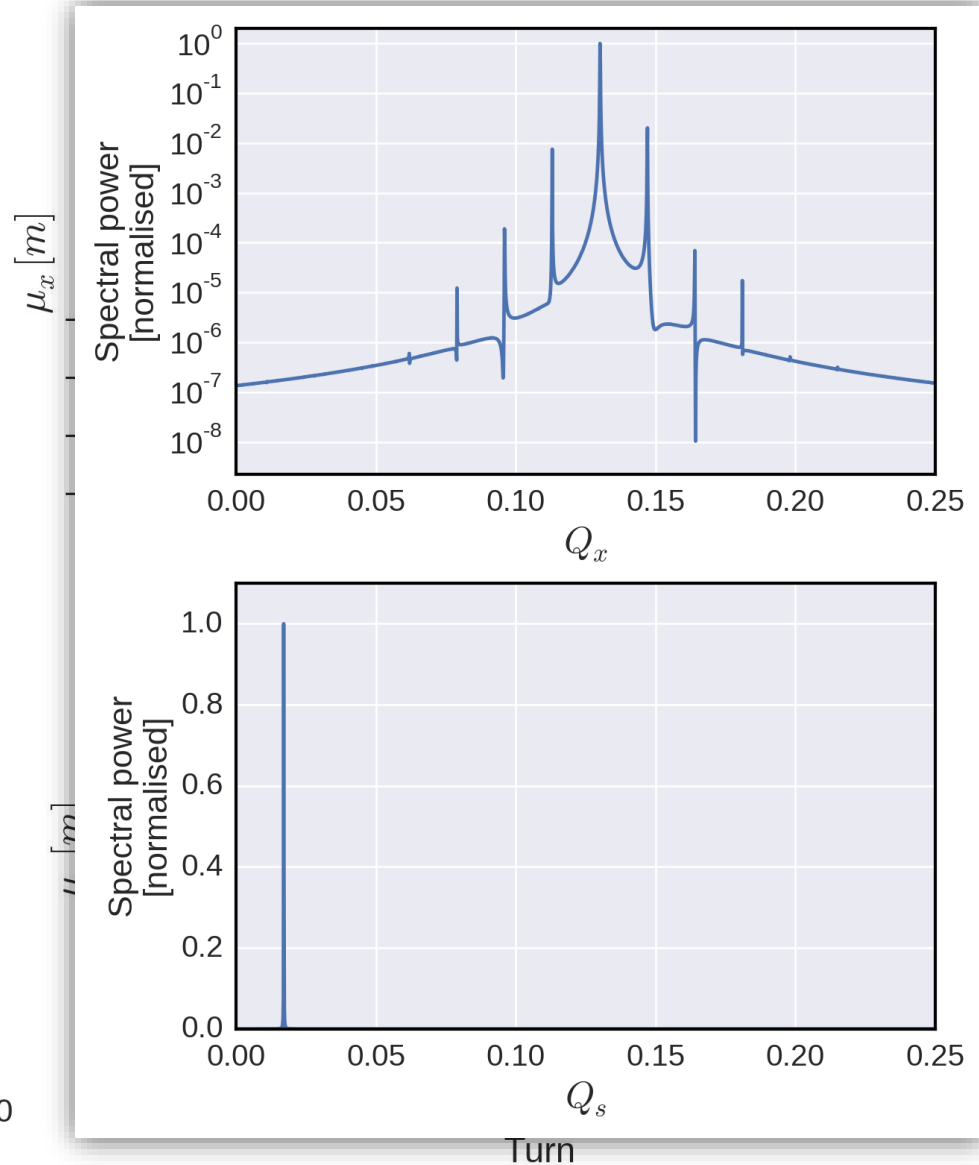
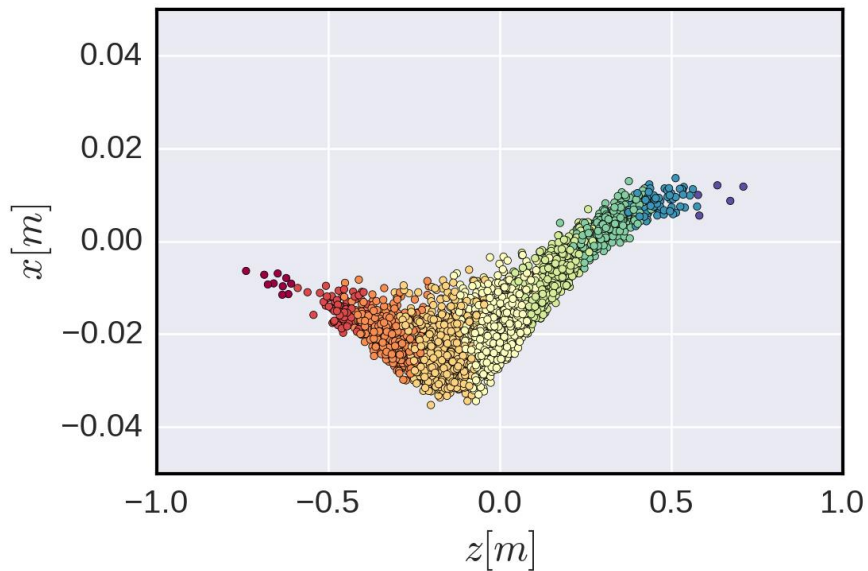
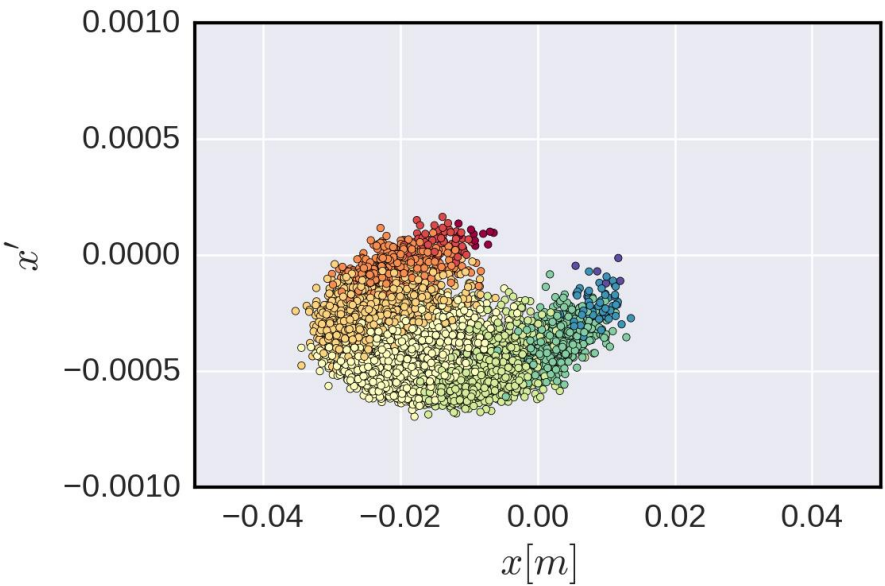
- As soon as **chromaticity is non-zero**, another ‘resonant’ condition can be met as particles now ‘synchronize’ their betatron motion with the synchrotron motion
- **Headtail modes arise** – the order of the respective mode depends on the chromaticity together with the impedance and bunch spectrum



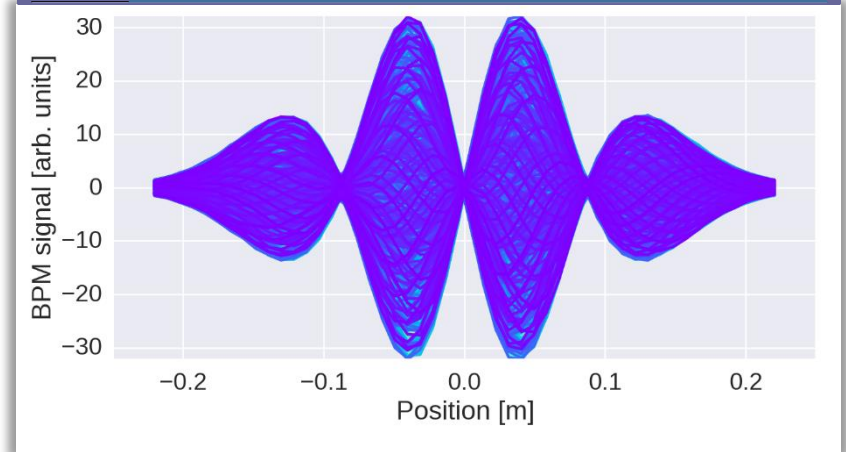
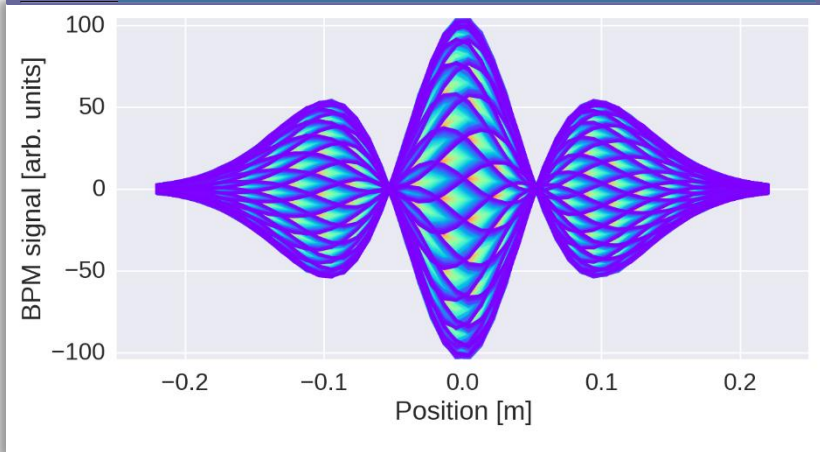
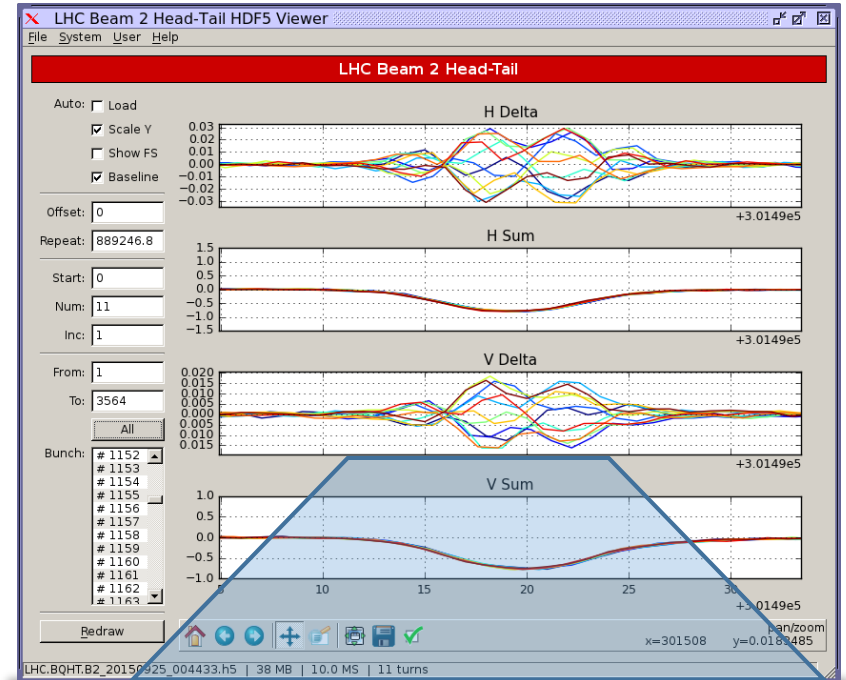
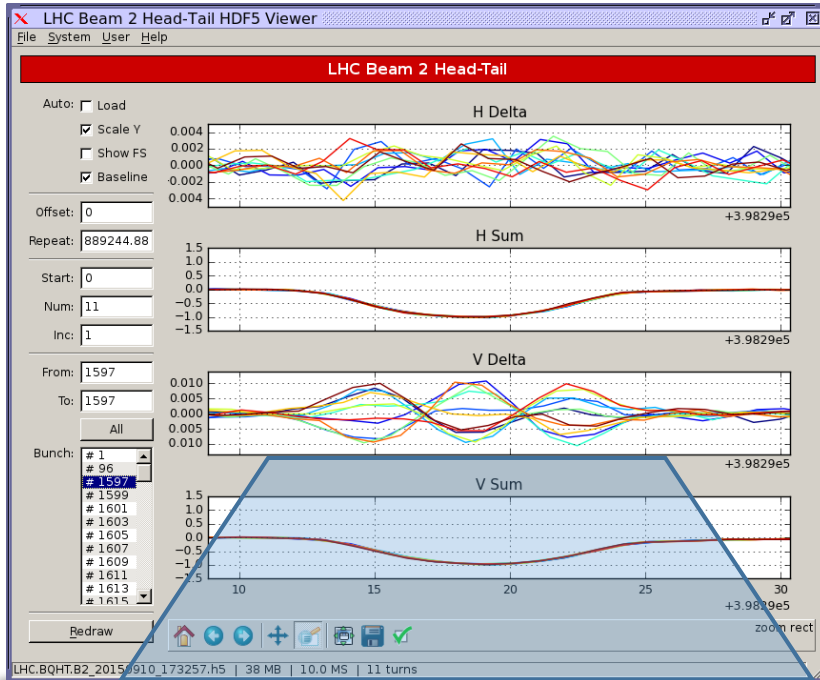
Dipole wakes – headtail modes



Dipole wakes – headtail modes



Example: Headtail modes in the LHC



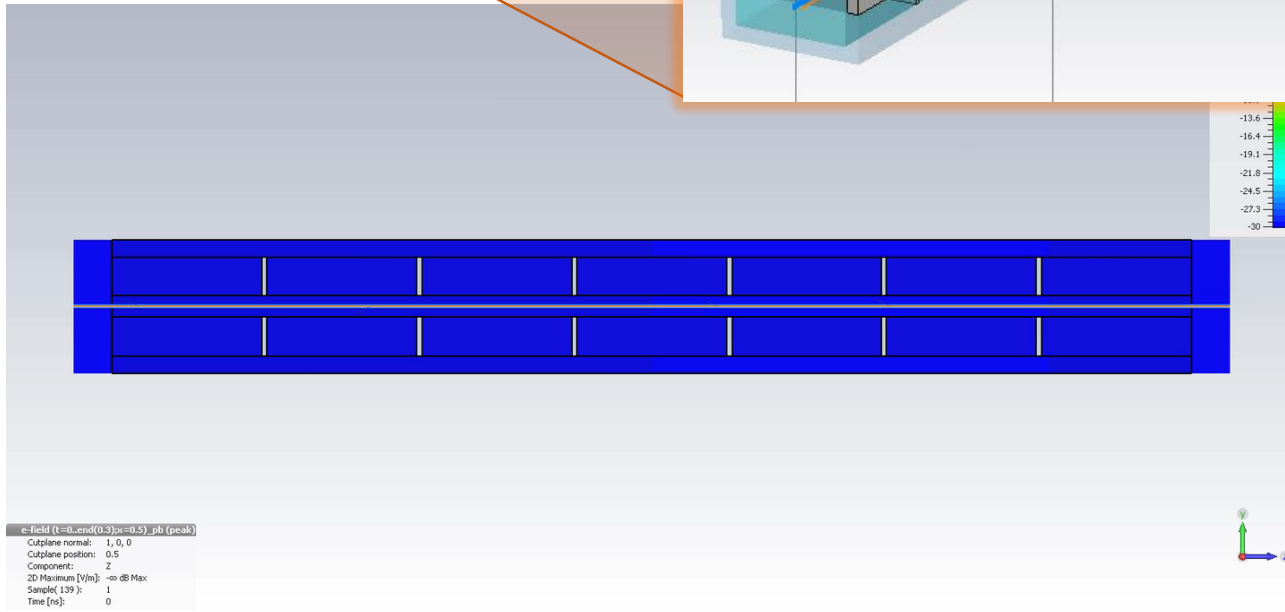
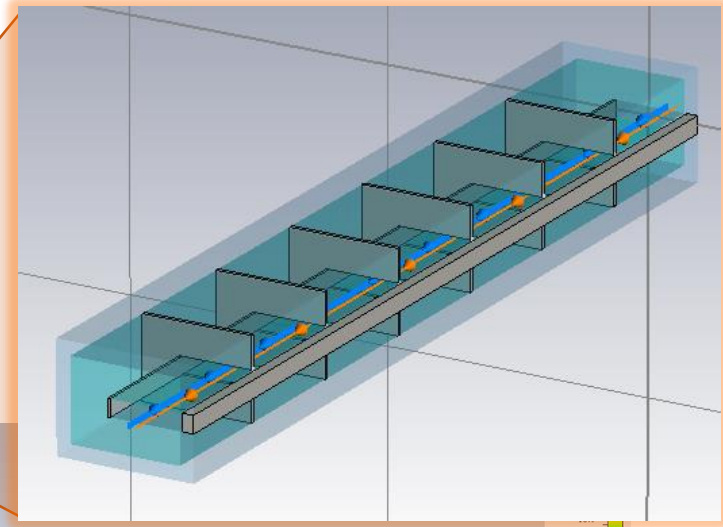
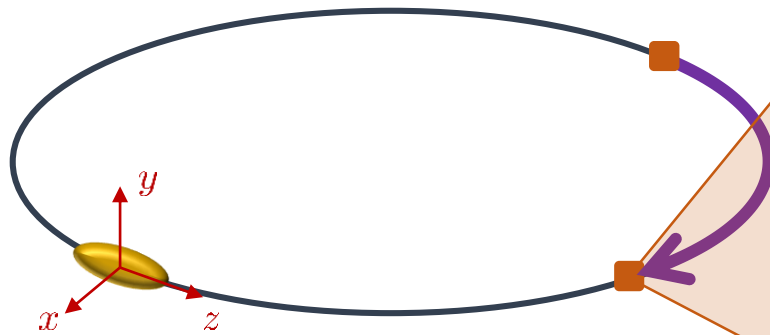
- Numerical methods allow us
 - to study conditions not realizable in a machine
 - to disentangle effects
 - to use unprecedented analysis tools
- Macroparticle models **closely resemble real systems** and are relatively **easy to implement**
- We have learned how to **model and implement macroparticle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

Introduction to macroparticle models – implementations, applications and examples

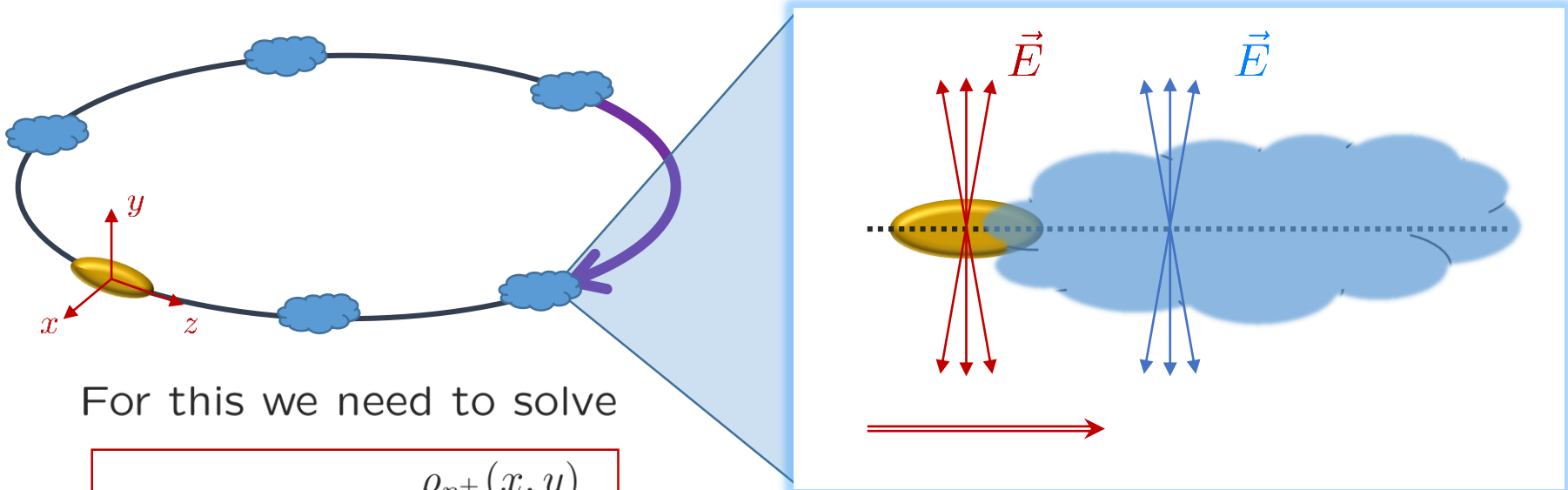
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 - **Modelling of e-cloud interactions**
 - PIC solvers
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Accelerator beam system - wakefields

- Our first 'real' collective interaction from impedances



- Two stream collective interaction – much more involved



For this we need to solve

$$\Delta \phi(x, y)_{p^+} = -\frac{\rho_{p^+}(x, y)}{\epsilon_0}$$

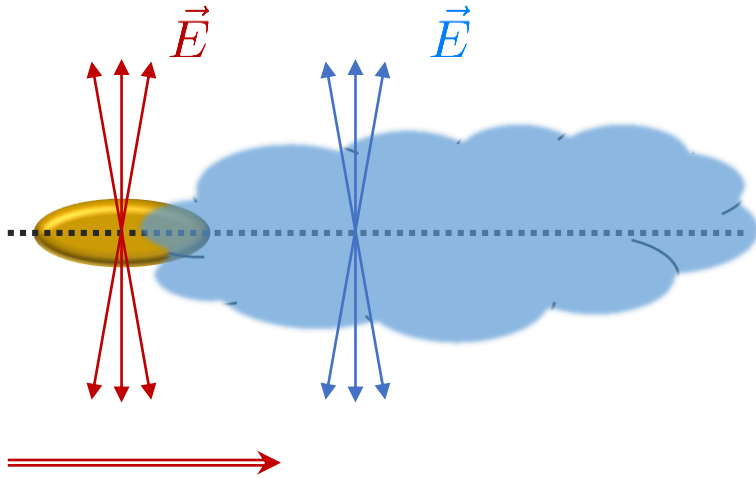
$$\Delta \phi(x, y)_{e^-} = -\frac{\rho_{e^-}(x, y)}{\epsilon_0}$$

and apply the corresponding kicks to the cloud and the beam

Approximations here:

- The beam is **ultra-relativistic**
- The electron velocity is **well below c**
- The electron cloud has a **low aspect ratio**

Accelerator beam system – electron clouds



count	x	x'	y	y'
0
1
2
3
4

count	x	y	phi
0
1
2
3
4

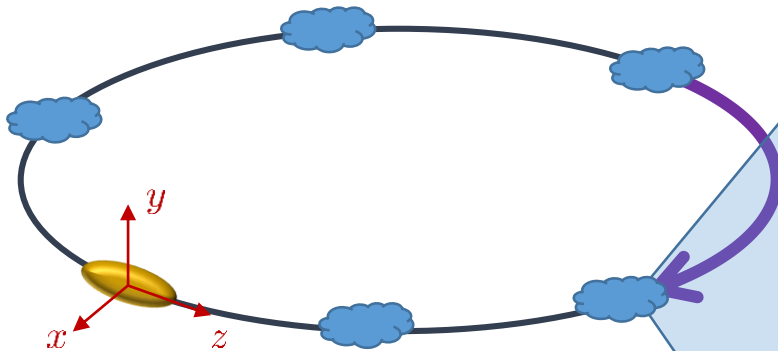
More memory, more computation steps
– overall more challenging

- **Two macroparticle systems** now need to be solved simultaneously
- The electric field evaluation usually is the **most time-consuming** step and should be done **efficiently**
- Keep track of macroparticle systems and fields

count	x	y	phi
0	...	4...	...
1	...	5...	...
2

count	x	x'	y	y'	z	delta
0	...	4...
1	...	5...
2
3
4
5
6

Electron clouds in a drift section



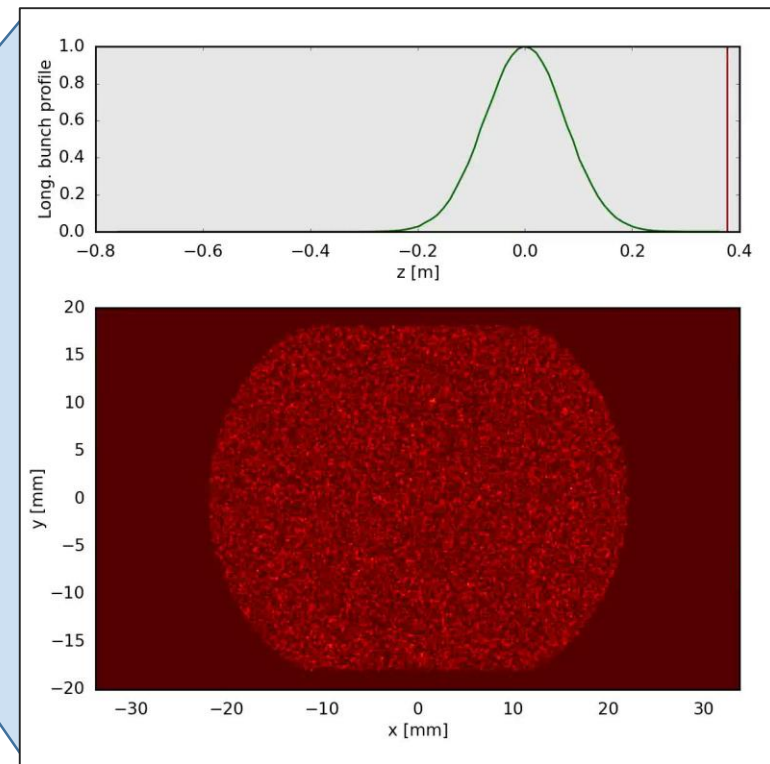
For this we need to solve

$$\Delta \phi(x, y)_{p^+} = -\frac{\rho_{p^+}(x, y)}{\epsilon_0}$$

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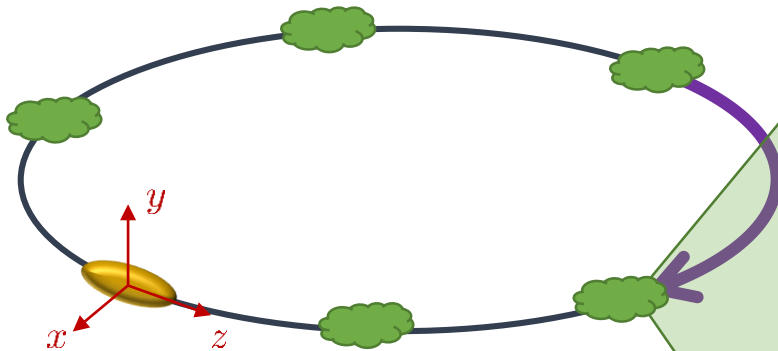
and apply the corresponding kicks to the cloud and the beam

- Two stream collective interaction – much more involved



- Beam passage leads to a **pinch of the cloud** which in turn acts back on the beam – differently each turn

Electron clouds in a bending magnet



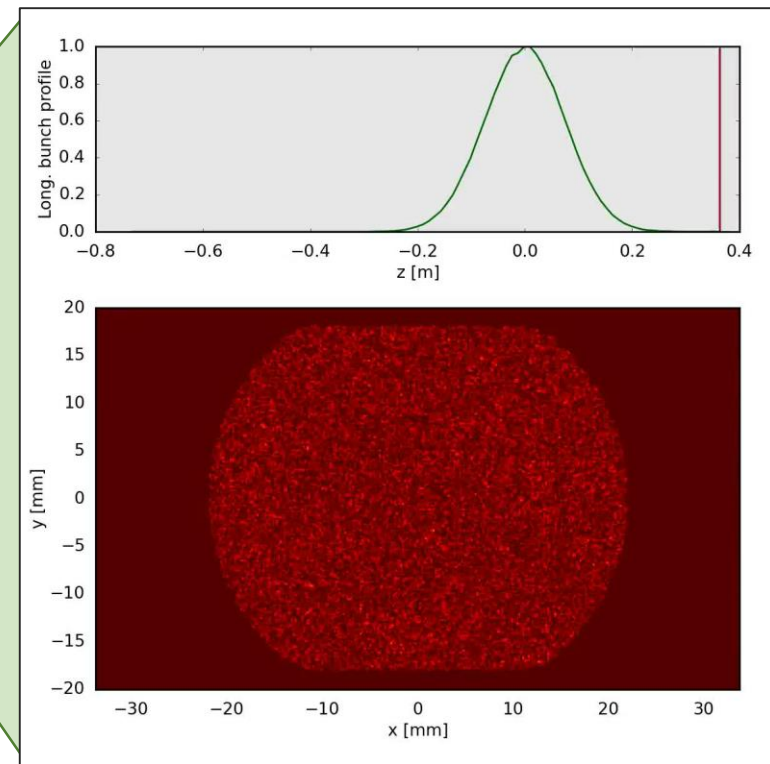
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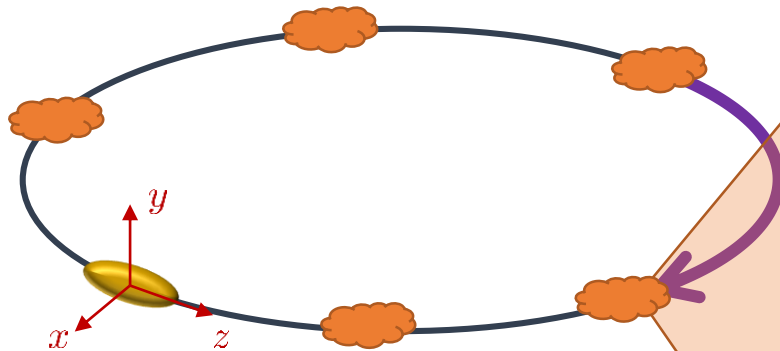
and apply the corresponding kicks to the cloud and the beam

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- Beam passage leads to a **pinch of the cloud** which in turn acts back on the beam – differently each turn

Electron clouds in a quadrupole magnet



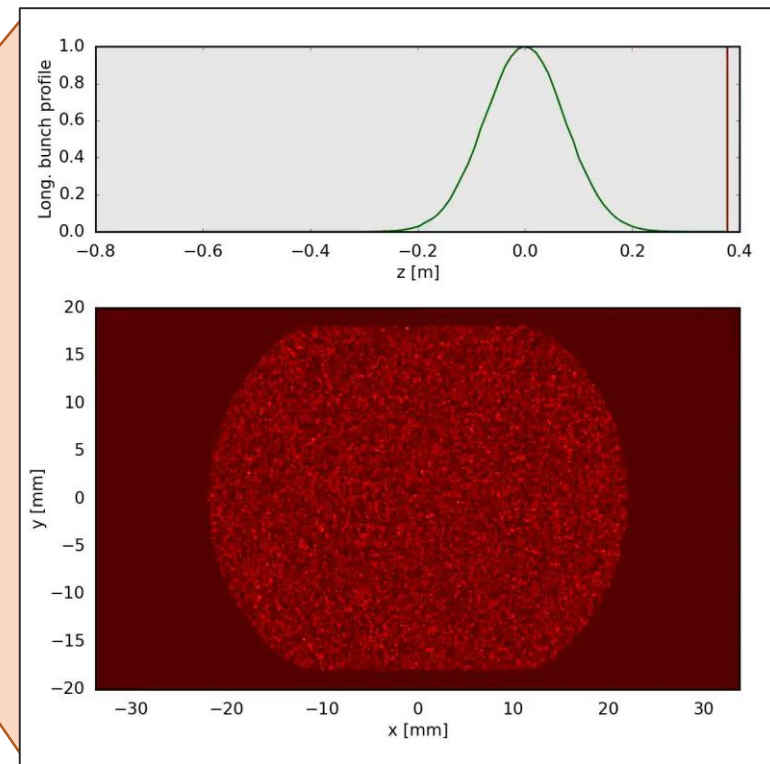
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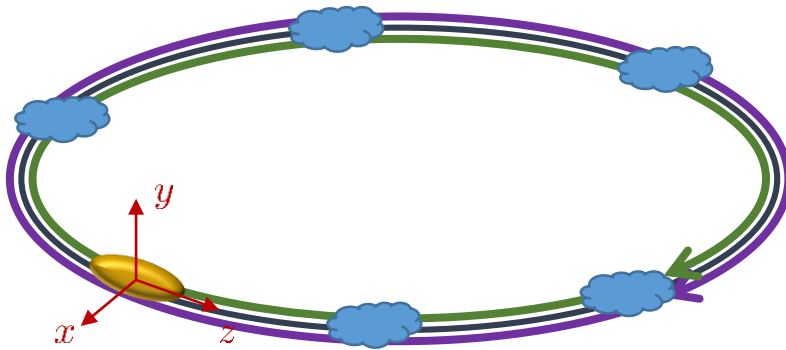
Accelerator-beam system – e-cloud

$$\begin{array}{|l} \left(\begin{array}{c} x_i \\ x'_i \end{array} \right) \Big|_{k+1} = \mathcal{M}_i \left(\begin{array}{c} x_i \\ x'_i \end{array} \right) \Big|_k \\ \left(\begin{array}{c} z_i \\ \delta_i \end{array} \right) \Big|_{k+1} = \mathcal{I} \left[\left(\begin{array}{c} z_i \\ \delta_i \end{array} \right) \Big|_k \right] \end{array}$$

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

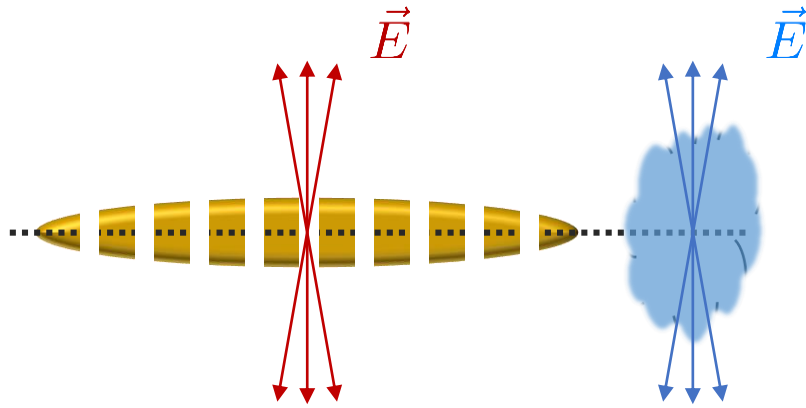
$$\Delta \dot{\vec{x}} = -\frac{e}{m} \left(\vec{E}_{p^+}[i] + \frac{\dot{\vec{x}} \times \vec{B}}{c} \right) \Delta t$$

Particles in/fields from slice i



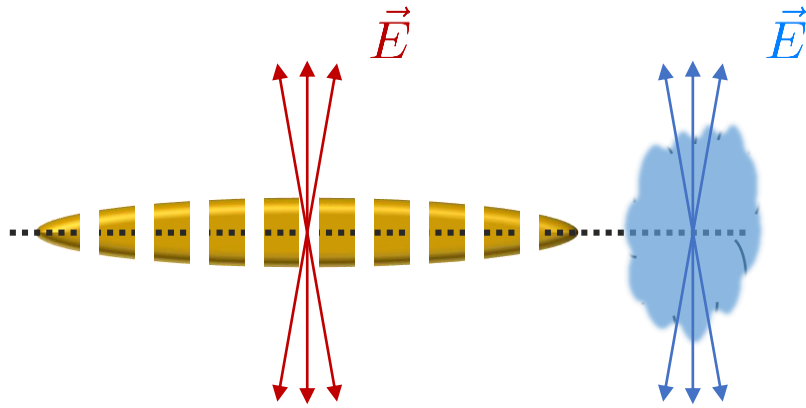
- Basic loop of tracking with wake fields:
 - Transport beam along segment to interaction point
 - Perform **e-cloud interaction** – requires electric fields from macroparticle distributions
 - Electric field computation in this case conveniently handled with **Particle-In-Cell** algorithm

E-cloud beam system



- PIC stands for **Particle-In-Cell**
- We use this method to compute **fields generated by particles** to solve e.g. the Poisson equation
- Electron motion occurs at the time scale of a slice of a bunch length \rightarrow track single slices through the e-cloud and **apply integrated kicks**

E-cloud beam system



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- **Compute electric fields** from one slice and from e-cloud

- **Apply kicks** to protons

- **Advance electrons** by one slice length – this is a **multi-scale dynamics** problem (fast cyclotron motion superposed to slower guiding center drift) → **Boris algorithm** for tracking (per macroparticle)

- Track **next slice** through e-cloud

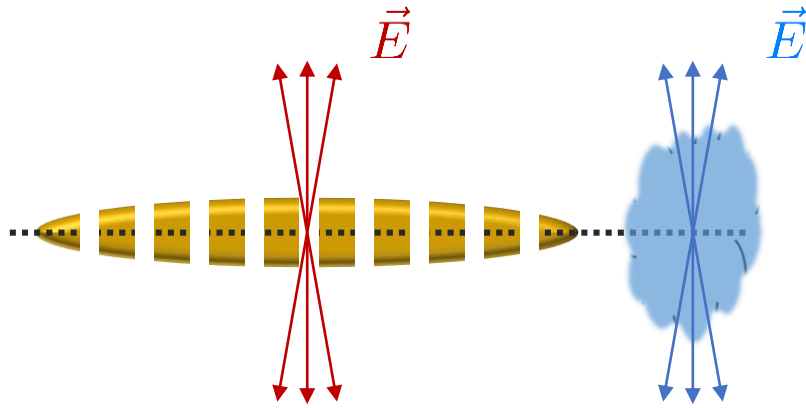
Solve

$$\Delta \phi(x, y)_{p^+} = -\frac{\rho_{p^+}(x, y)}{\epsilon_0}$$

$$\Delta \phi(x, y)_{e^-} = -\frac{\rho_{e^-}(x, y)}{\epsilon_0}$$

using PIC method.

E-cloud beam system

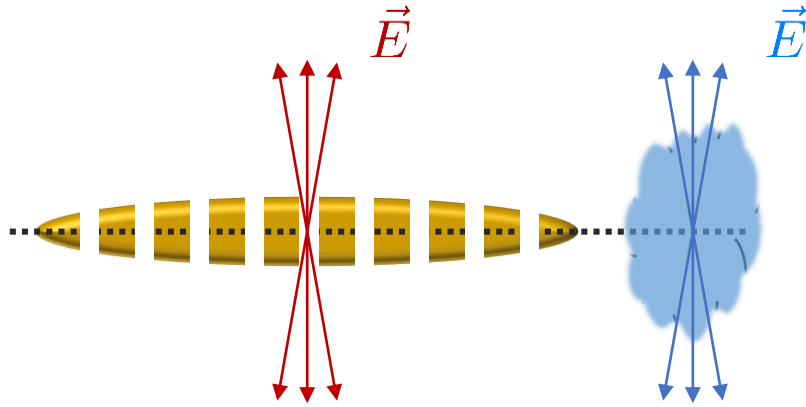


Update momenta in slice i with

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

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E-cloud beam system



$$\dot{\mathbf{x}} = \vec{v}$$

$$\dot{\vec{v}} = \frac{e}{m} \left(\vec{E} + \frac{\vec{v} \times \vec{B}}{c} \right)$$

$$\frac{\mathbf{x}_{k+1} - \mathbf{x}_k}{\Delta t} = \mathbf{v}_{k+1}$$

$$\frac{\mathbf{v}_{k+1} - \mathbf{v}_k}{\Delta t} = \frac{e}{m} \left(\mathbf{E}_k + \frac{(\mathbf{v}_{k+1} + \mathbf{v}_k) \times \mathbf{B}_k}{2c} \right)$$

$$\mathbf{v}^- = \mathbf{v}_k + \frac{e}{m} \mathbf{E}_k \frac{\Delta t}{2}$$

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{e}{2mc} \left((\mathbf{v}^+ + \mathbf{v}^-) \times \mathbf{B}_k \right)$$

$$\mathbf{v}_{k+1} = \mathbf{v}^+ + \frac{e}{m} \mathbf{E}_k \frac{\Delta t}{2}$$

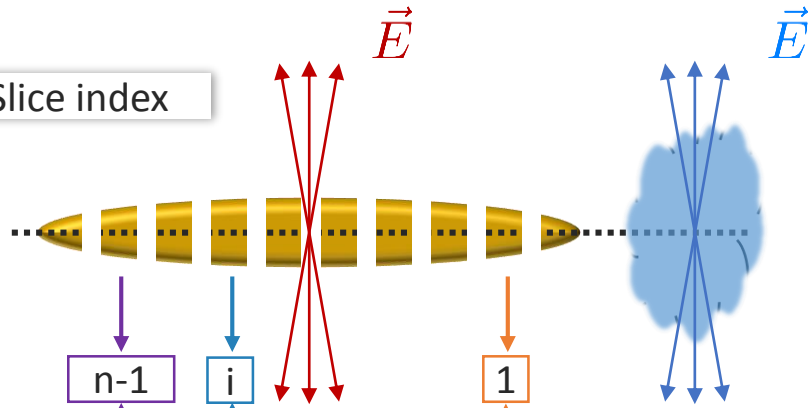
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 - Track **next slice** through e-cloud

C. Birdsall and A. Langdon, *Plasma Physics Via Computer Simulation* (McGraw-Hill, Inc., New York, 1985)

Hong Qin et al. , *Why is Boris algorithm so good?*, Physics of Plasmas 20, 084503 (2013)

E-cloud beam system

Slice index



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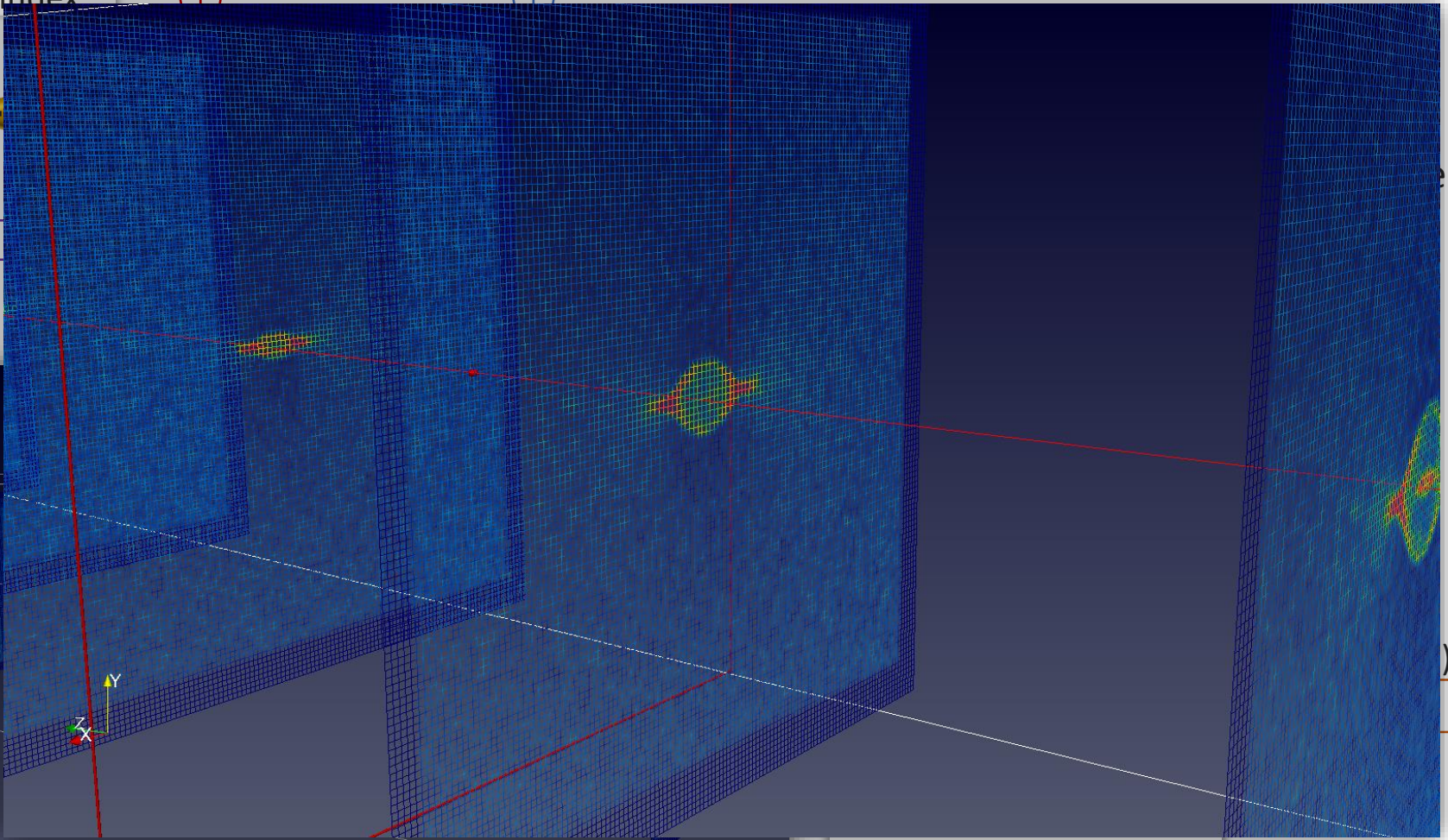
E-cloud at slice index

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E-cloud beam system

- PIC stands for **P**article-**I**n-**C**ell

Slice index



t

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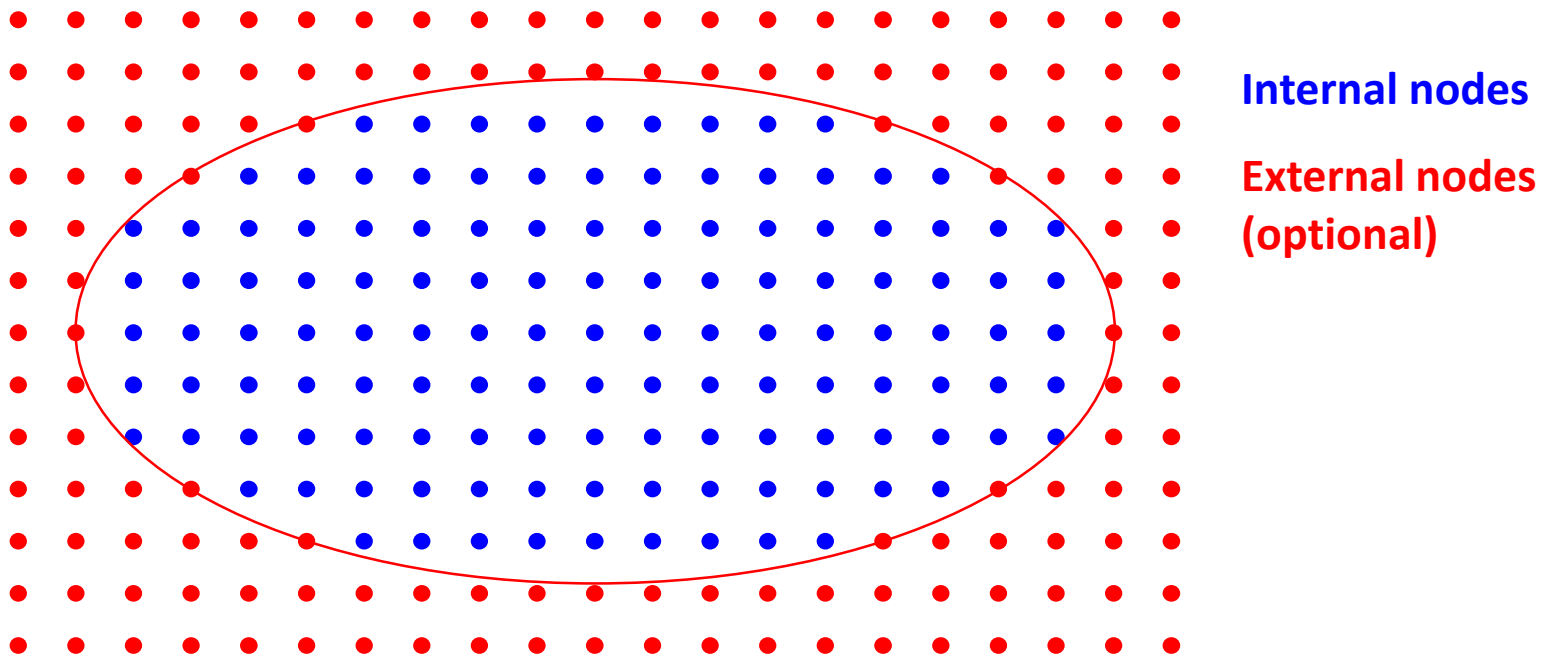
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PIC solvers in brief

- In many of our codes, **Particle in Cell (PIC)** algorithms are used to compute the **electric field** generated by a **set of charged particles** in a **set of discrete points** (can be the locations of the particles themselves, or of another set of particles)
- The solution typically consists of **4 stages**:
 1. **Charge scatter** from macroparticles (MPs) to grid (reduction of macroparticles)
 2. Calculation of the **electrostatic potential at the nodes**
 3. Calculation of the **electric field at the nodes** (gradient evaluation)
 4. **Field gather** from grid to MPs

PIC solvers in brief

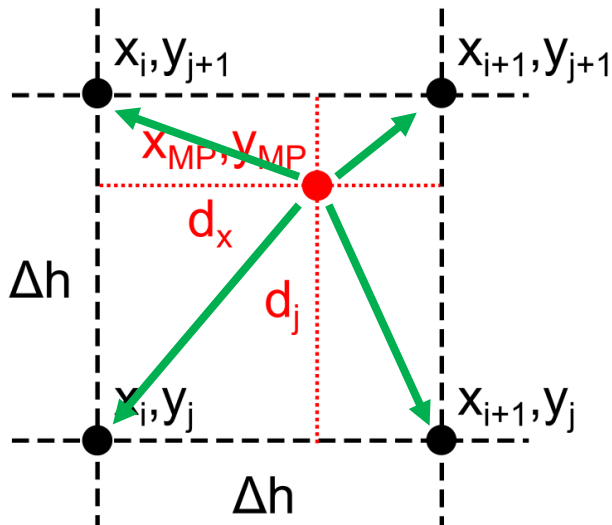
- The solution typically consists of **4 stages**:
 1. **Charge scatter** from macroparticles (MPs) to grid (reduction of macroparticles)
 2. Calculation of the **electrostatic potential at the nodes**
 3. Calculation of the **electric field at the nodes** (gradient evaluation)
 4. **Field gather** from grid to MPs



Uniform square grid

PIC solvers – basic steps

- The solution typically consists of **4 stages**:
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$$\rho_{i,j} = \rho_{i,j} + \frac{q n_{\text{MP}}}{\Delta h} \left(1 - \frac{d_x}{\Delta h}\right) \left(1 - \frac{d_y}{\Delta h}\right)$$
$$\rho_{i+1,j} = \rho_{i+1,j} + \frac{q n_{\text{MP}}}{\Delta h} \left(\frac{d_x}{\Delta h}\right) \left(1 - \frac{d_y}{\Delta h}\right)$$
$$\rho_{i,j+1} = \rho_{i,j+1} + \frac{q n_{\text{MP}}}{\Delta h} \left(1 - \frac{d_x}{\Delta h}\right) \left(\frac{d_y}{\Delta h}\right)$$
$$\rho_{i+1,j+1} = \rho_{i+1,j+1} + \frac{q n_{\text{MP}}}{\Delta h} \left(\frac{d_x}{\Delta h}\right) \left(\frac{d_y}{\Delta h}\right)$$

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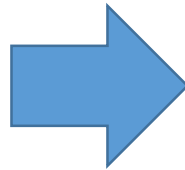
$$\left\{ \begin{array}{l} \nabla^2 \phi(x, y) = -\frac{\rho(x, y)}{\epsilon_0} \\ \text{Boundary conditions (e.g., perfectly} \\ \text{conducting, open, periodic)} \end{array} \right.$$

- Different numerical approaches exist to **solve these types of equations** each with its own advantages and drawbacks:
 - Open space **FFT solver** (explicit, very fast but open boundaries)
 - Rectangular boundary **FFT solver** (explicit, very fast but only rectangular boundaries)
 - **Finite Difference implicit** Poisson solver (arbitrary chamber shape, sparse matrix, possibility to use Shortley Weller boundary refinement, KLU fast routines, computationally more demanding)
 - Dual or multi-grid in combination with direct or iterative solvers

PIC solvers – basic steps

- The solution typically consists of **4 stages**:
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$$\mathbf{E} = -\nabla\phi$$

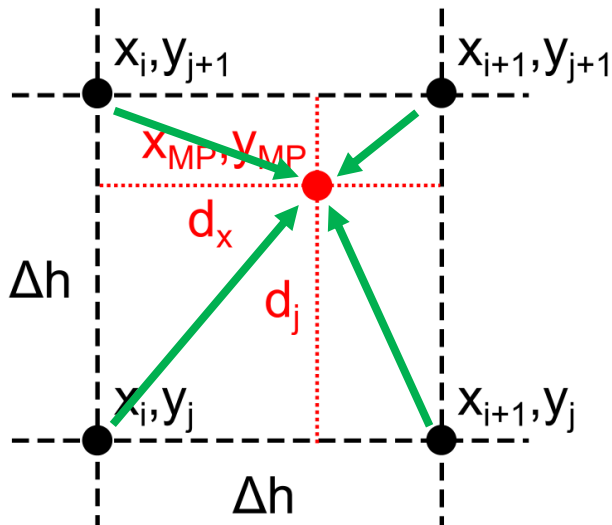


$$(E_x)_{i,j} = -\frac{\phi_{i+1,j} - \phi_{i-1,j}}{2\Delta h}$$

$$(E_y)_{i,j} = -\frac{\phi_{i,j+1} - \phi_{i,j-1}}{2\Delta h}$$

PIC solvers – basic steps

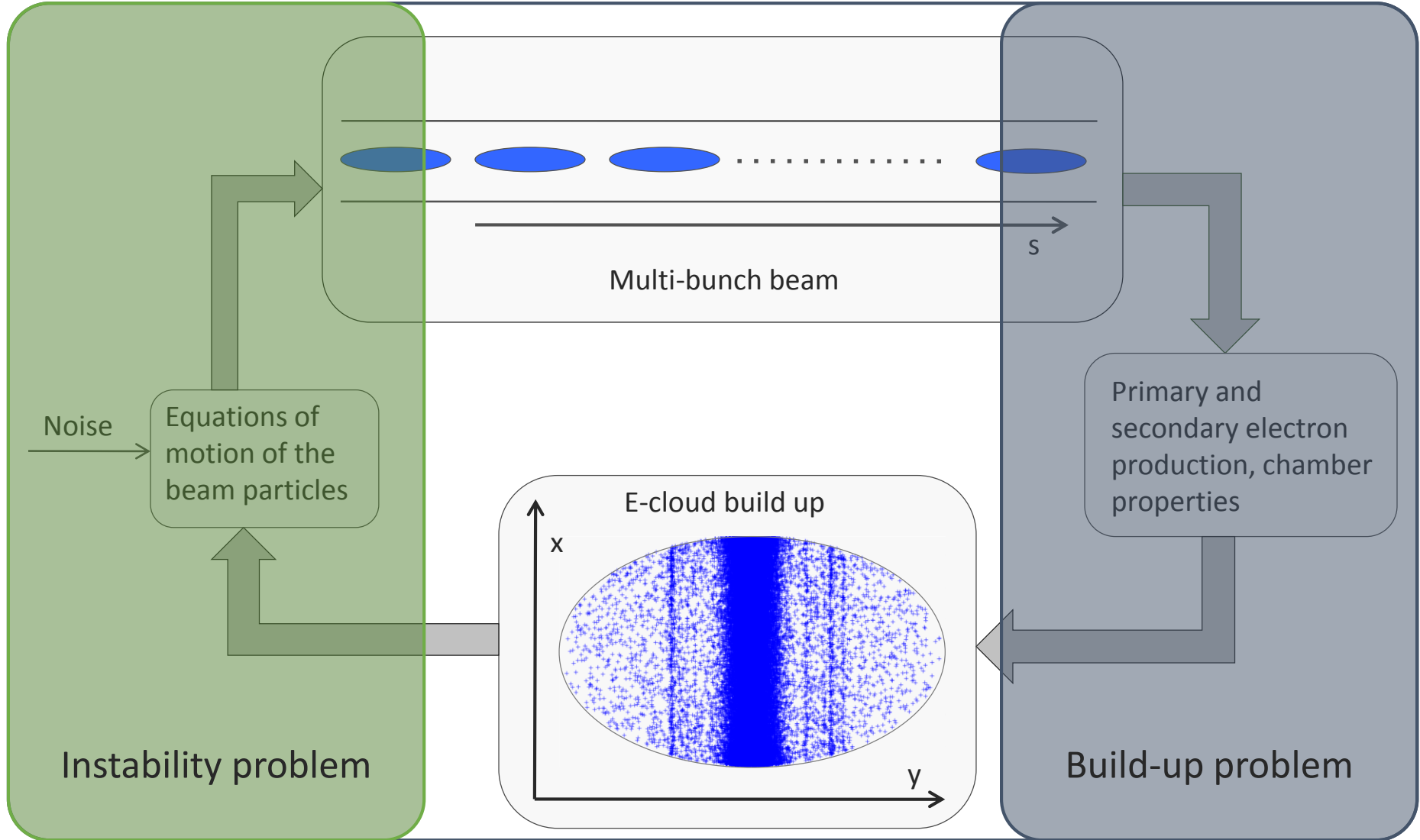
- The solution typically consists of **4 stages**:
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$$\mathbf{E}(x_{MP}, y_{MP}) =$$

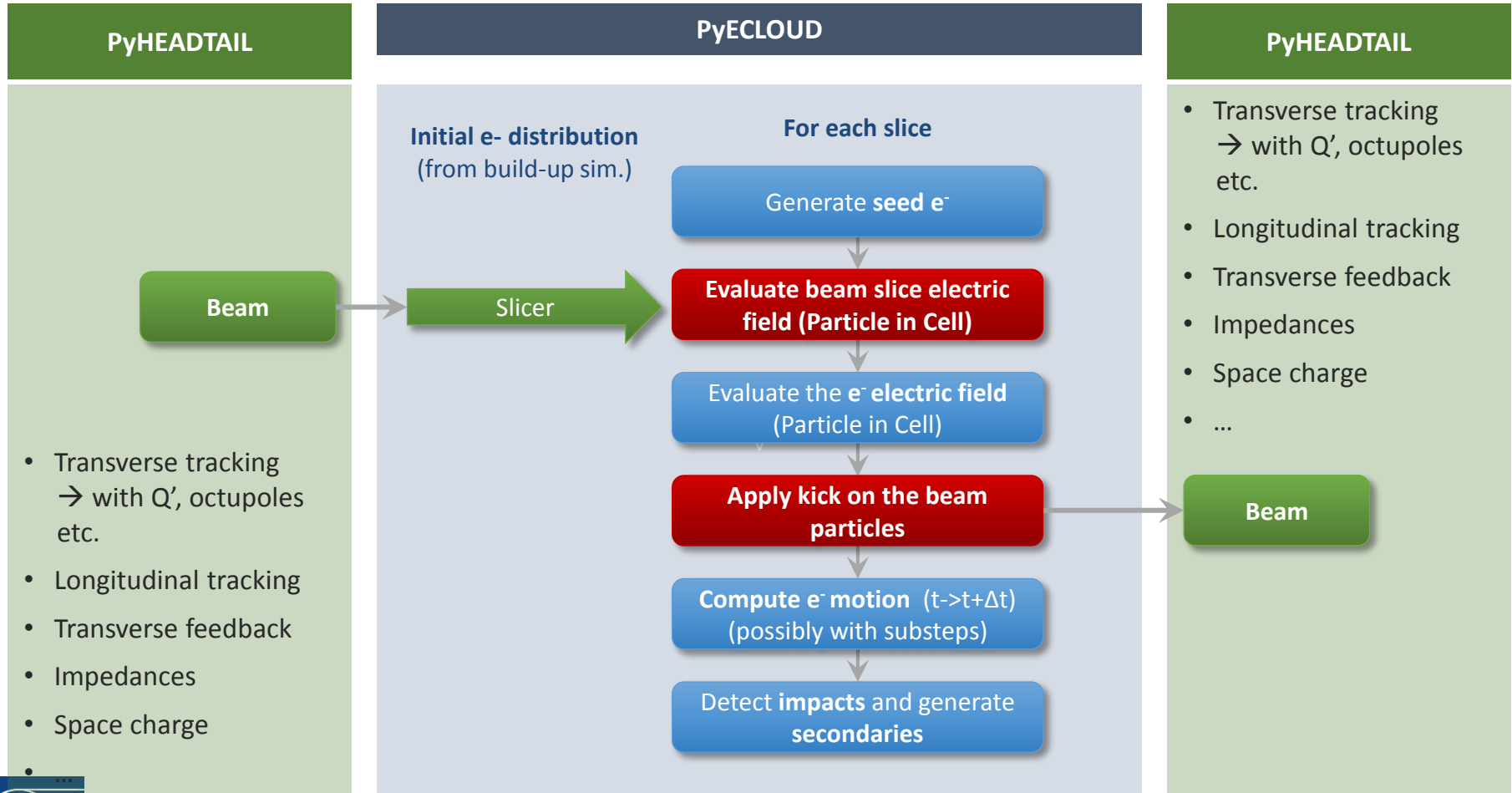
$$\mathbf{E}_{i,j} \left(1 - \frac{d_x}{\Delta h}\right) \left(1 - \frac{d_y}{\Delta h}\right) + \mathbf{E}_{i+1,j} \left(\frac{d_x}{\Delta h}\right) \left(1 - \frac{d_y}{\Delta h}\right) \\ + \mathbf{E}_{i,j+1} \left(1 - \frac{d_x}{\Delta h}\right) \left(\frac{d_y}{\Delta h}\right) + \mathbf{E}_{i+1,j+1} \left(\frac{d_x}{\Delta h}\right) \left(\frac{d_y}{\Delta h}\right)$$

Numerical model of electron cloud effects



Numerical model of electron cloud effects

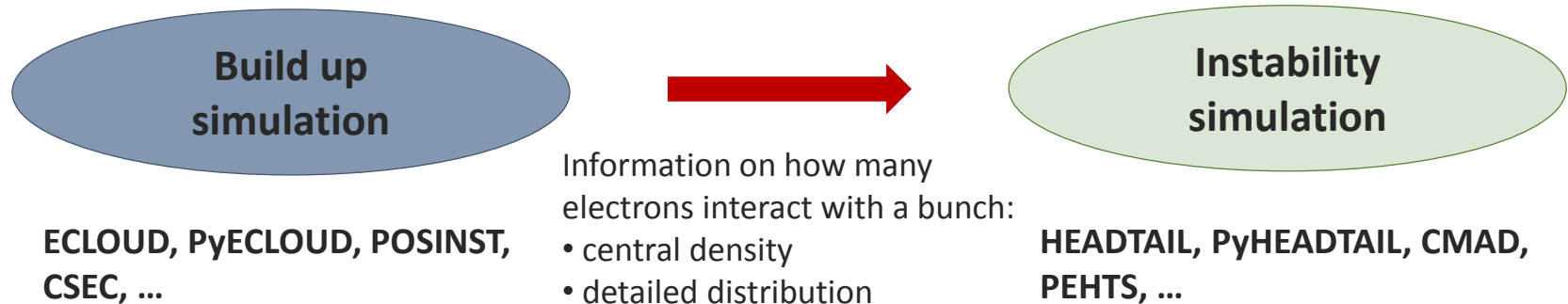
- A self-consistent treatment requires the combination of an instability and a build-up code
- Becomes easily possible with modular structure and good design of codes (e.g. object orientation)



Legend: From instability code – From build-up code – Interaction between the two codes

Numerical model of electron cloud effects

- Coupled bunch electron cloud instability naturally needs a self-consistent solution of the electron cloud problem
 - A broad time scale to cover, currently working on the problem
- For the moment we simulate the two branches separately (similar to what is done for impedances):
 - **Electron cloud build up**
 - ✓ Multi-bunch
 - ✓ Usually single passage, single turn or just few turns
 - **Electron cloud instability**
 - ✓ Single bunch
 - ✓ Multi-turn, or even multi-kick multi-turn



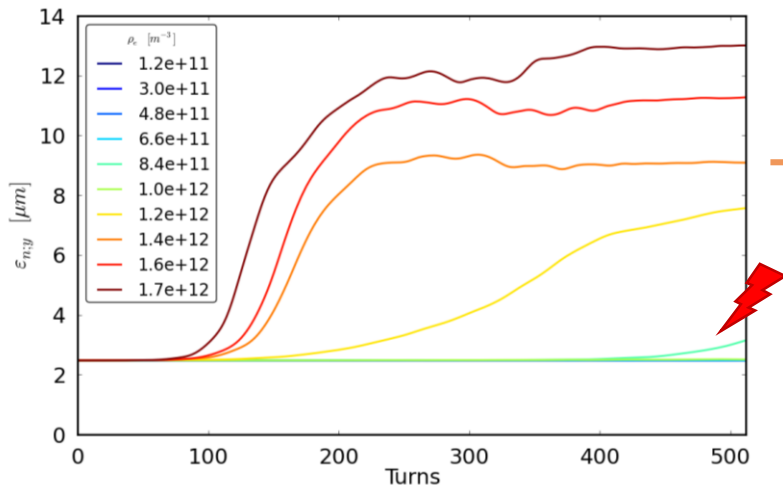
- In principle both **coherent instability** and **incoherent emittance growth** could be predicted by these simulations
- Evolution of a beam interacting with an electron cloud depends on a **significant number of parameters** in a non-trivial way
 - Bunch length (longitudinal emittance)
 - Beam transverse sizes (emittances and beta functions at the electron cloud location)
 - Beam energy
 - Beam current (number of particles per bunch)
 - Chromaticity
 - Magnetic field (field-free, dipole, quadrupole)
 - Electron cloud density and distribution (in reality determined by many of the above parameters, but can be set independently in simulations)

Introduction to macroparticle models – implementations, applications and examples

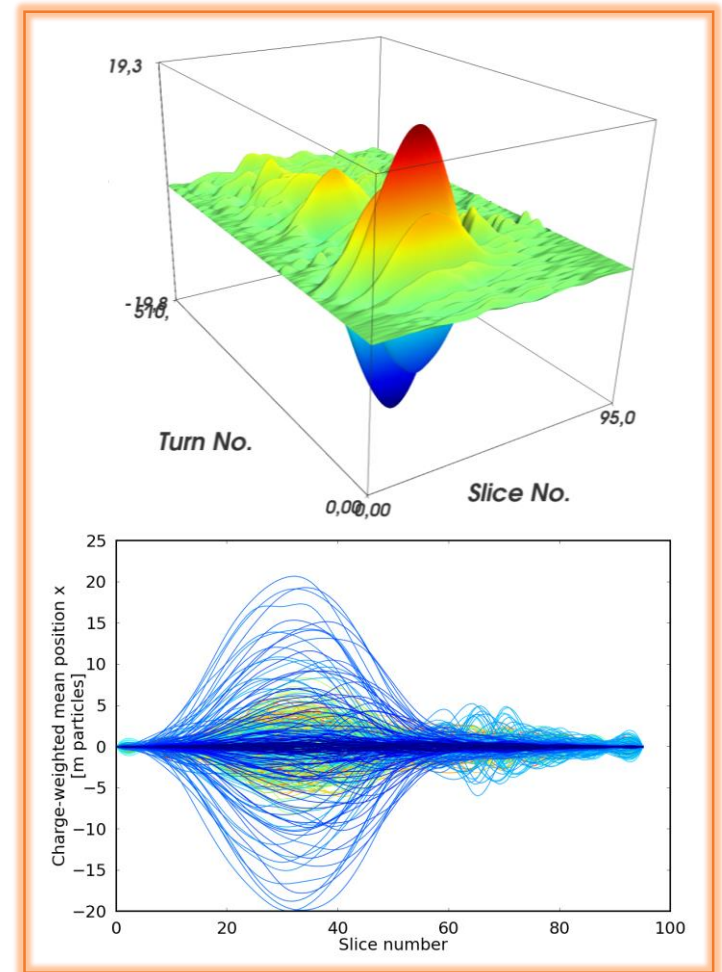
- Part 1 – numerical modelling
 - Initialisation
 - Simple tracking
 - Chromaticity and detuning
 - Wakefields with examples
 - Constant wakes
 - Dipole wakes
 - TMCI & headtail modes
- Part 2 – electron cloud
 - Modelling of e-cloud interactions
 - PIC solvers
 - **Application for e-cloud instabilities**

Electron cloud induced instabilities

- Typical e-cloud simulation try to identify the e-cloud **central density threshold** for an **instability**
- **Scans** in the central density are performed until an **exponential growth** can be observed in the emittance

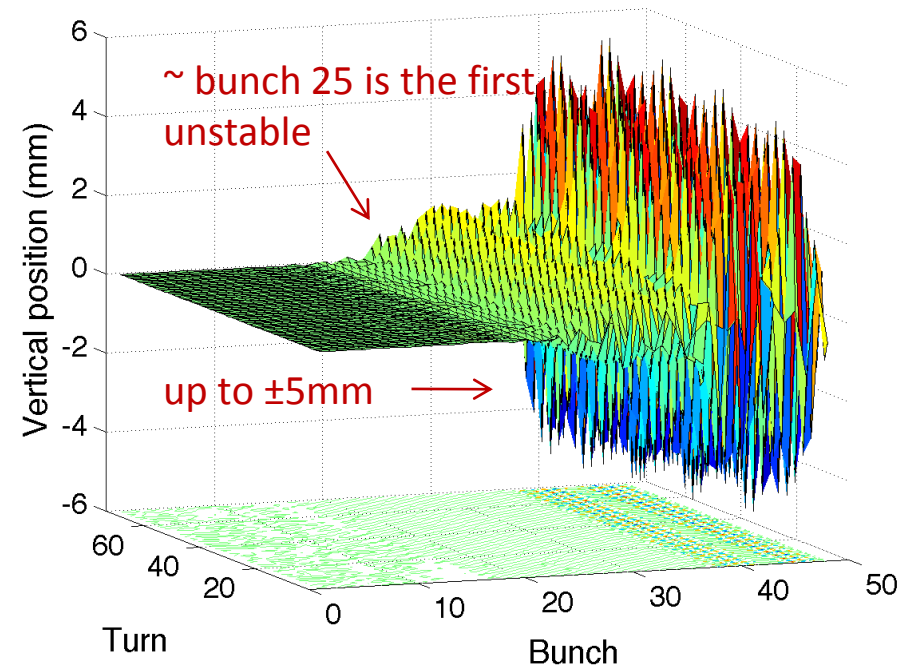
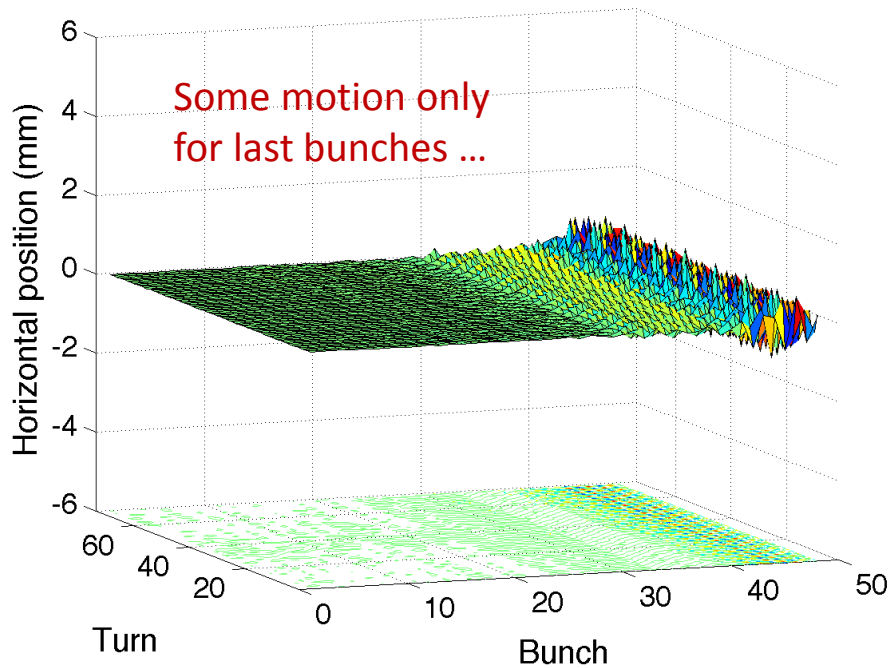


- Coherent instabilities occur when a certain **central cloud density threshold** is breached
- This leads to **coherent intra bunch motion** which grows **exponentially**
- A consequence is **emittance blow-up** and **losses**



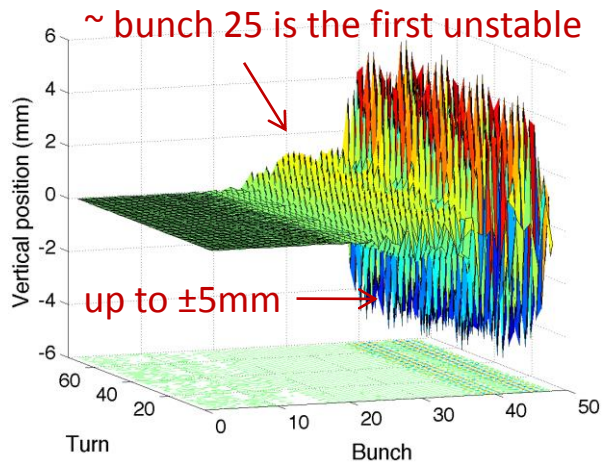
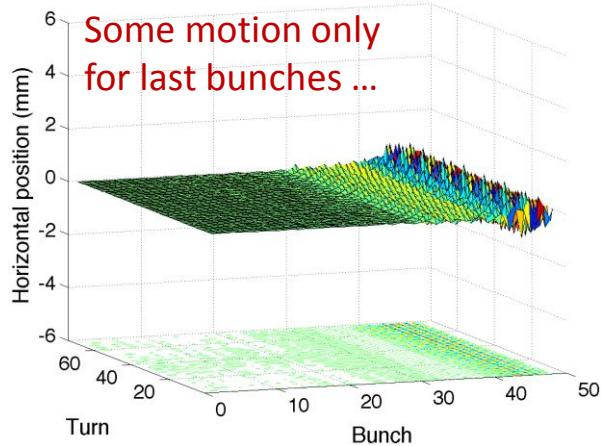
Ex. of coherent e-cloud effects in the LHC

- First injection of 48 bunches of 25 ns beam into the LHC in 2011
- Beam was dumped twice due to a **violent instability** in the vertical plane, causing losses above the interlock threshold



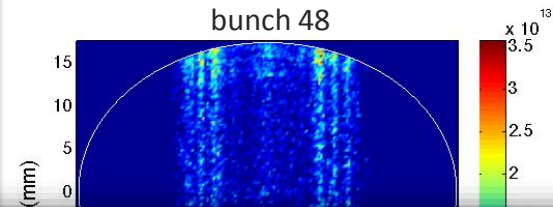
Ex. of coherent e-cloud effects in the LHC

48b injection test (26/08/11)

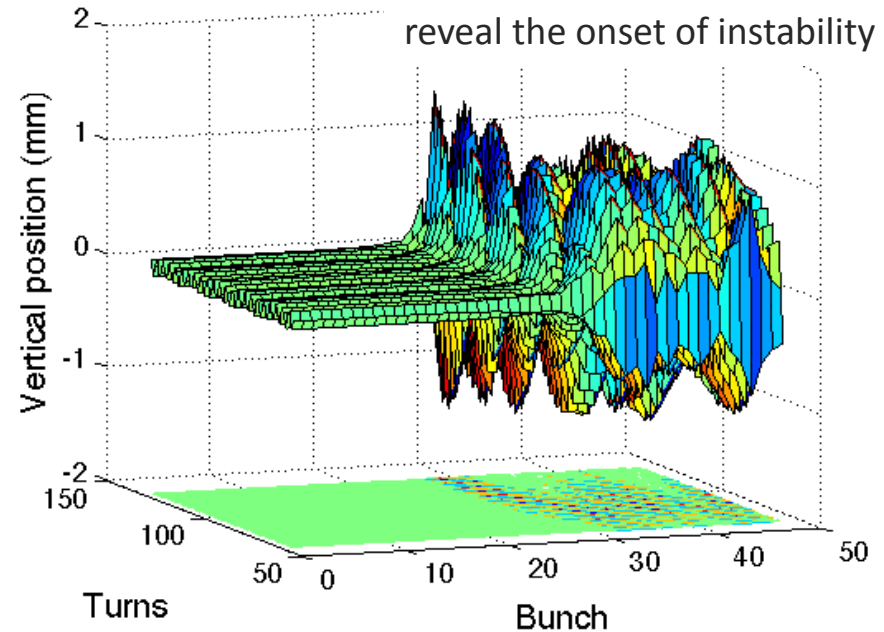


48x

PyECLOUD e^- distribution ($\delta_{\max}=2.1$)

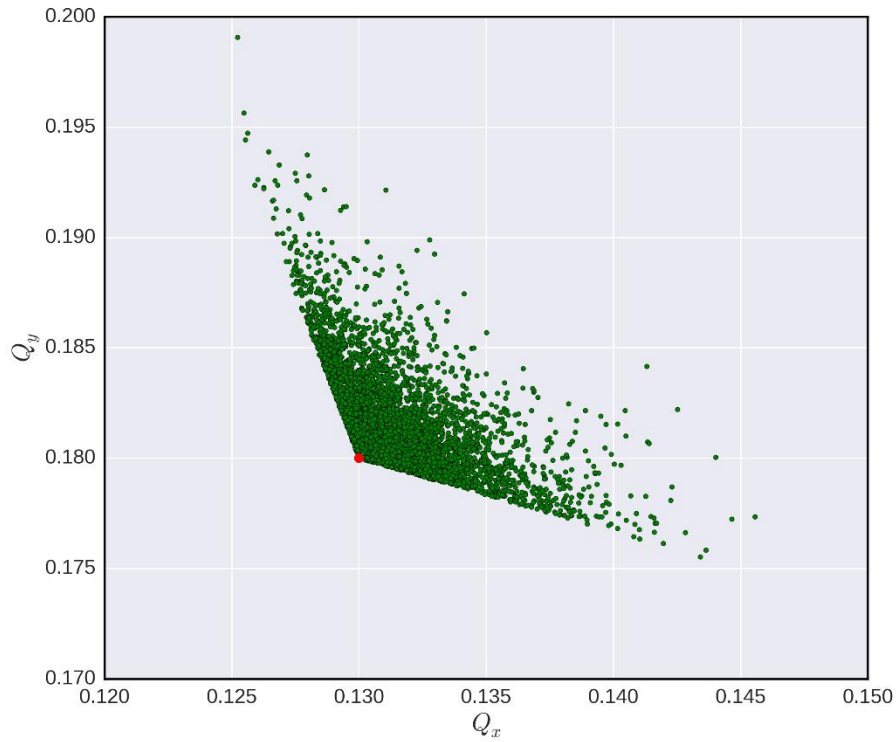


48x HEADTAIL simulations reveal the onset of instability

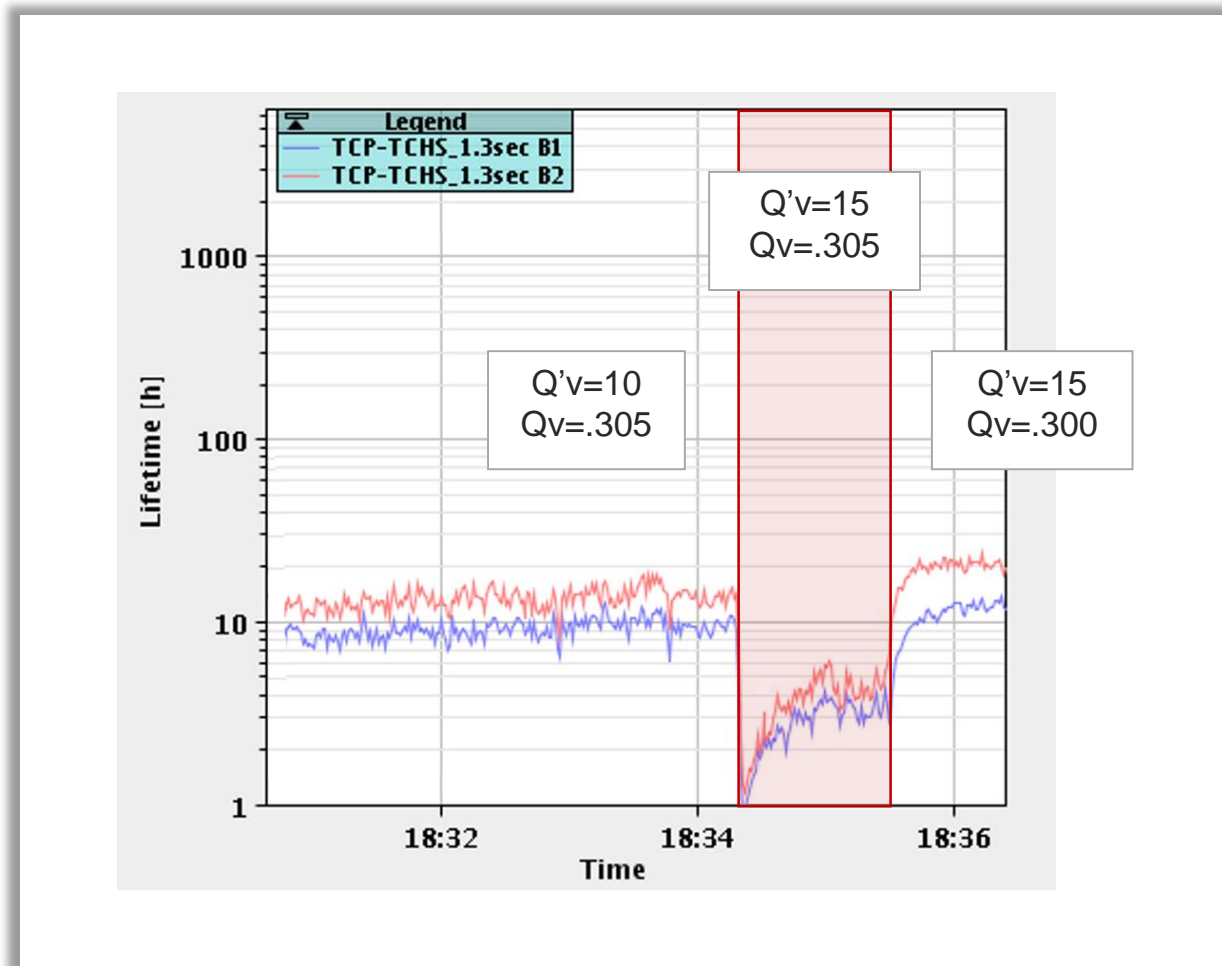


Ex. of incoherent e-cloud effects in the LHC

- Remember tune footprint from octupoles in Part I

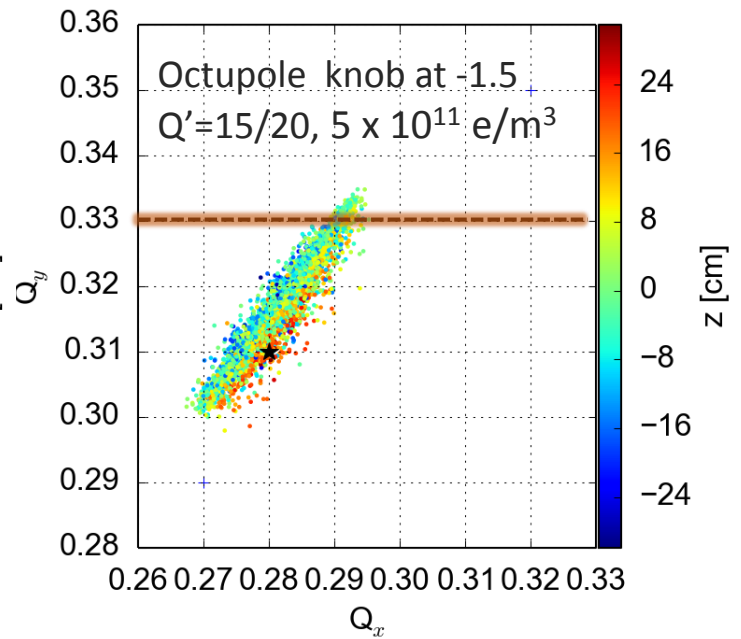
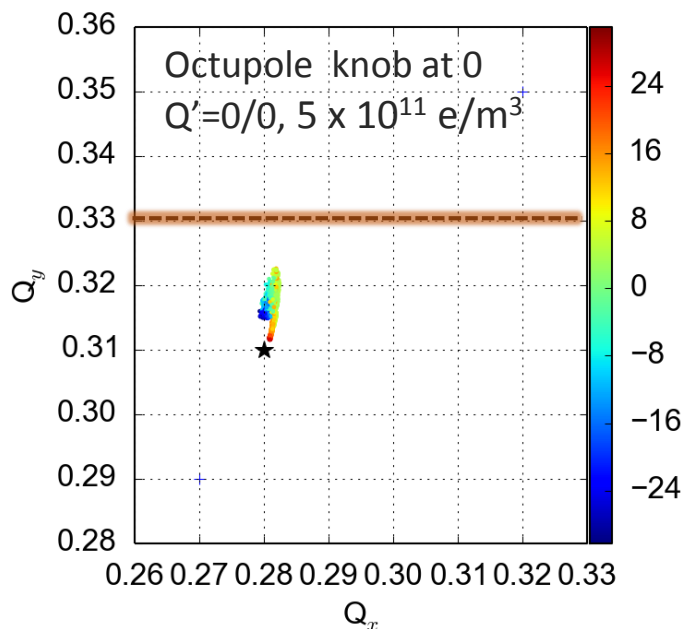
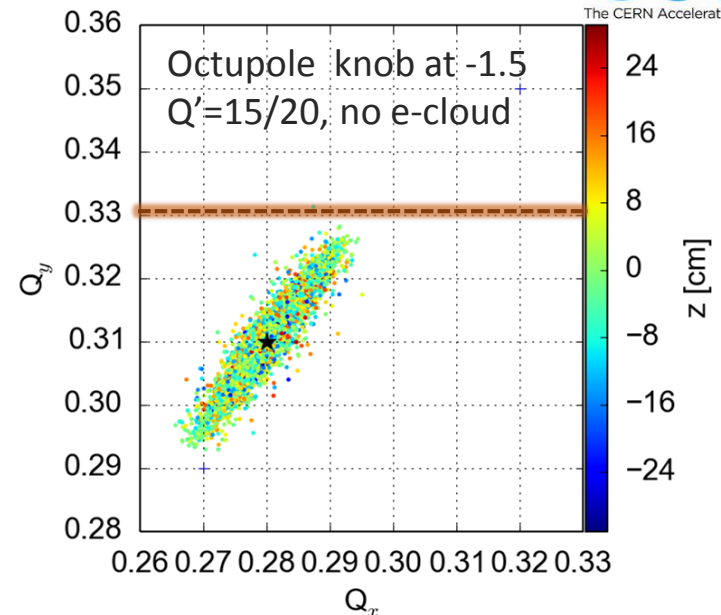
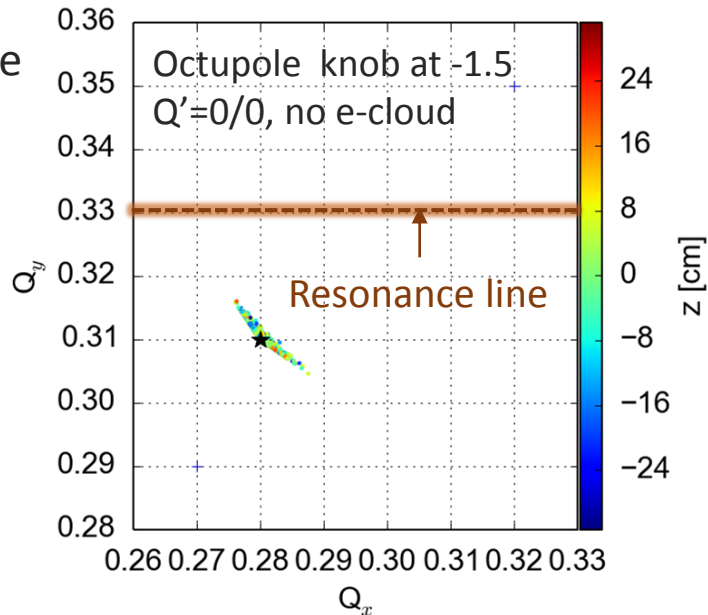


Ex. of incoherent e-cloud effects in the LHC



Ex. of incoherent e-cloud effects in the LHC

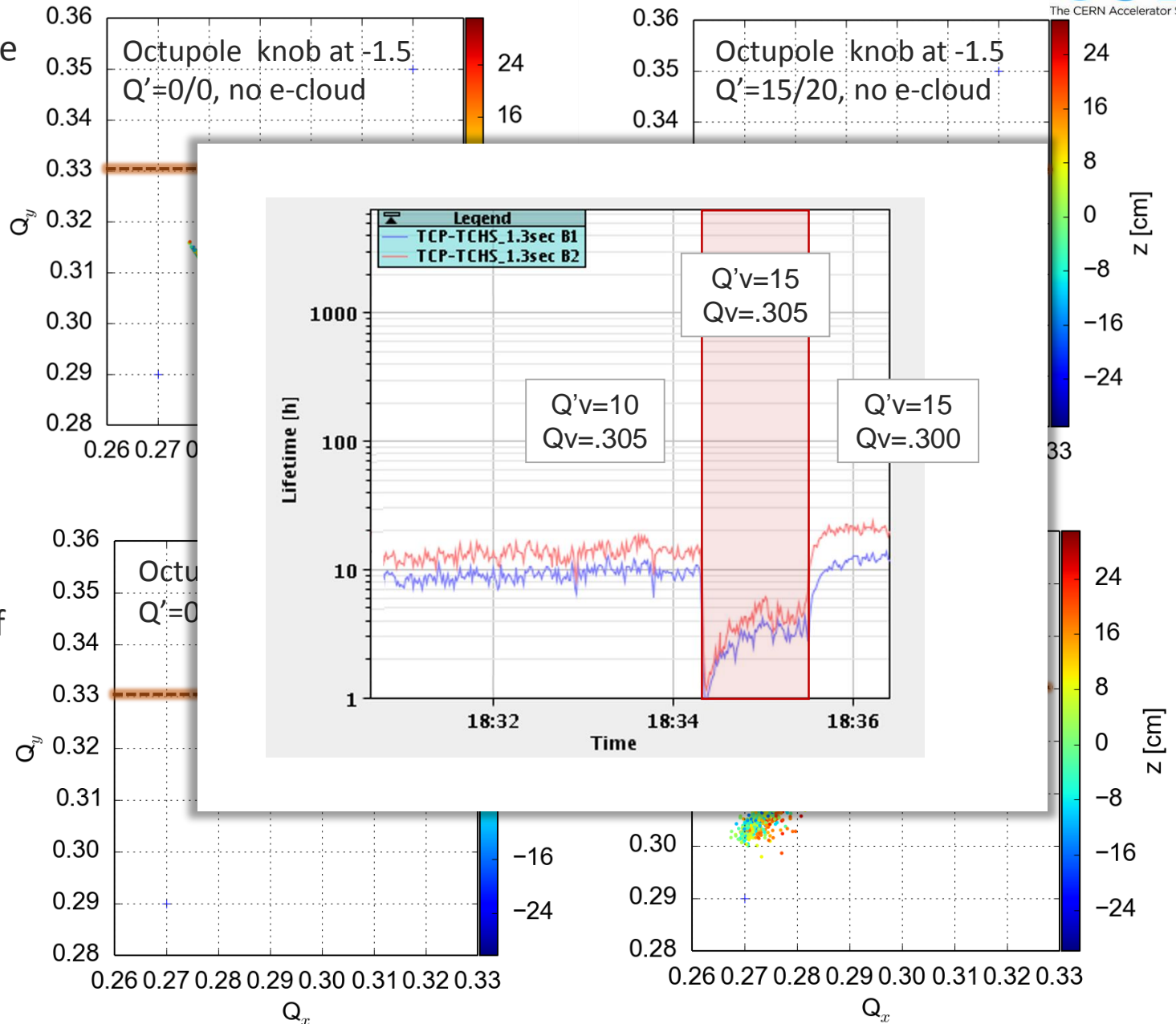
- Macroparticle simulations allow to obtain tune footprint from all effects separated
- ... as well as from all effects combined



A. Romano et al

Ex. of incoherent e-cloud effects in the LHC

- Macroparticle simulations allow to obtain tune footprint from all **effects separated**
- ... as well as from all **effects combined**
- ... to identify the source of **incoherent losses in the LHC**



A. Romano et al



Vlasov solvers

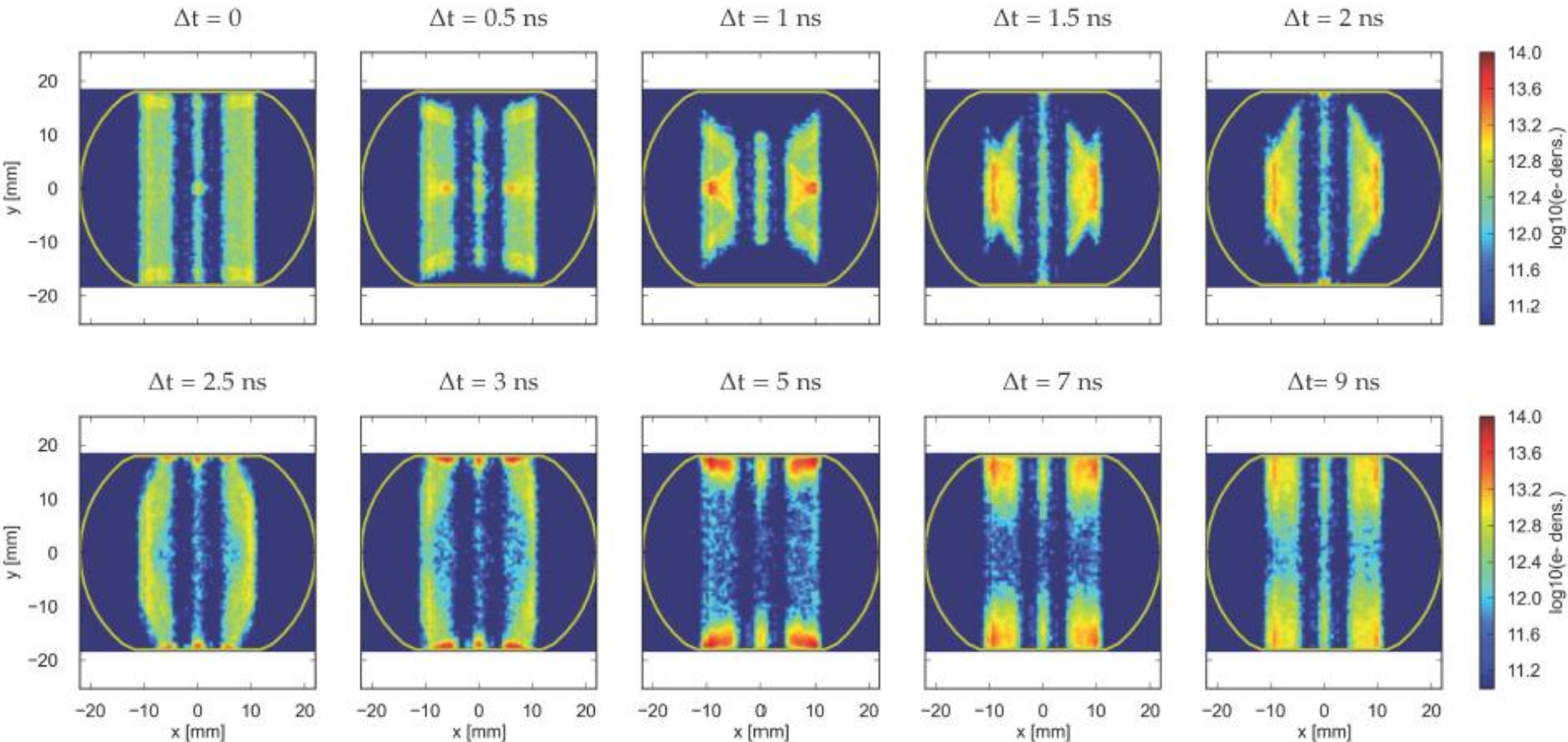
- No time this time...

End part II

Backup

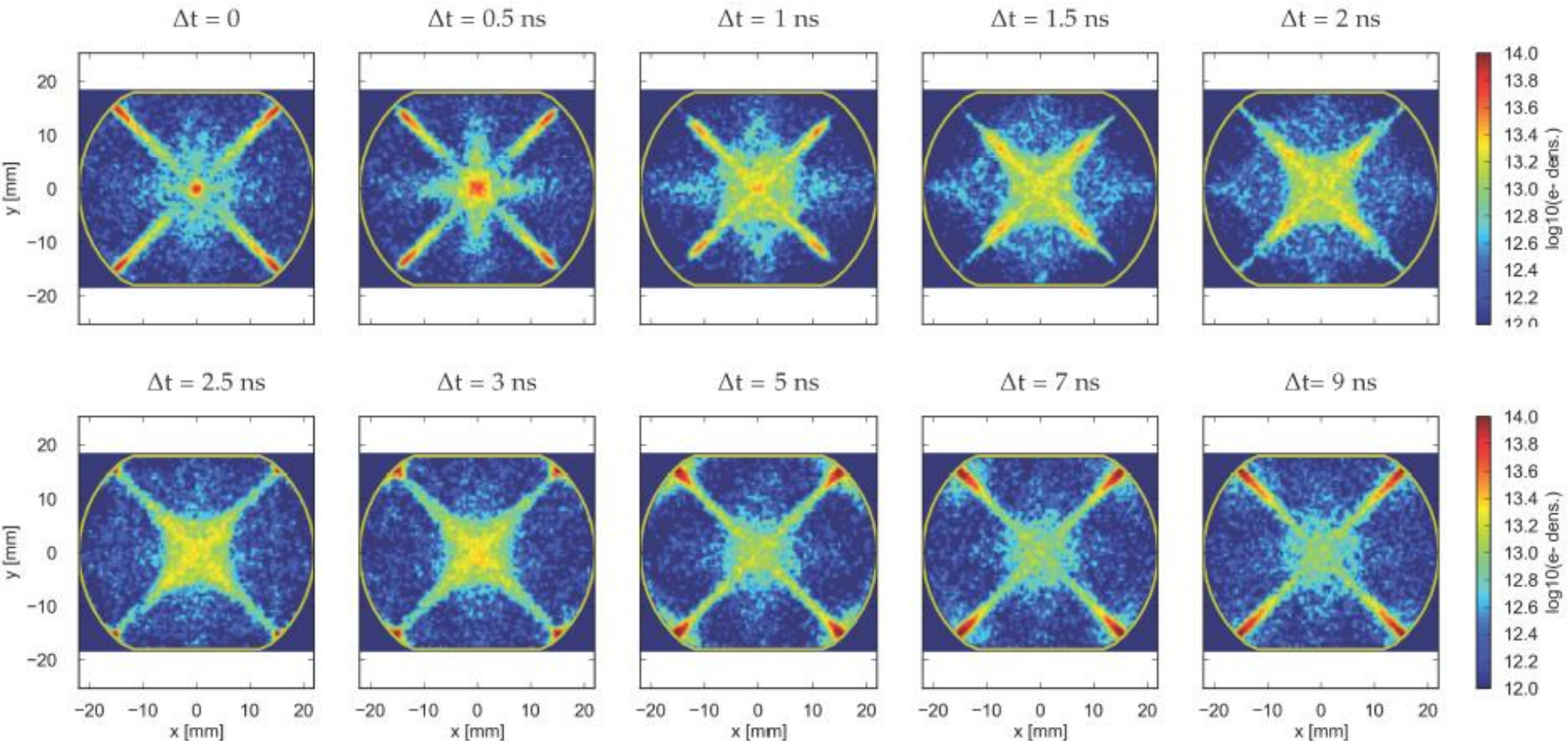
Electron clouds in a bending magnet

- The electrons exhibit different transverse (x, y) distributions, according to the type of region in which the electron cloud is formed
 - In dipole regions, the electron motion is confined along the lines of the magnetic field.
Example: snapshots of multipacting in the dipole of an LHC arc cell during bunch passage and including secondary production.



Electron clouds in a quadrupole magnet

- The electrons exhibit different transverse (x,y) distributions, according to the type of region in which the electron cloud is formed
 - In quadrupole regions, the electrons tend to multipact along the pole-to-pole lines of the cross section (example: snapshots of multipacting in an LHC arc quadrupole). Multipacting thresholds are usually lower in quadrupoles because electrons survive long thanks to trapping due to the magnetic gradient.

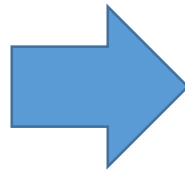


Basic stages of a PIC algorithm

Standard Particle In Cell (PIC) → 4 stages:

1. **Charge scatter** from macroparticles (MPs) to grid
2. Calculation of the **electrostatic potential at the nodes**
3. Calculation of **the electric field at the nodes** (gradient evaluation)
4. **Field gather** from grid to MPs

$$\begin{cases} \nabla^2 \phi(x, y) = -\frac{\rho(x, y)}{\epsilon_0} \\ \phi(x, y) = 0 \quad \text{on the boundary} \end{cases}$$

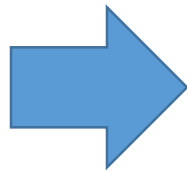


Internal nodes:

$$\frac{\phi_{i-1,j} + \phi_{i,j-1} - 4\phi_{i,j} + \phi_{i+1,j} + \phi_{i,j+1}}{\Delta h^2} = -\frac{\rho_{i,j}}{\epsilon_0}$$

External nodes:

$$\phi_{i,j} = 0$$

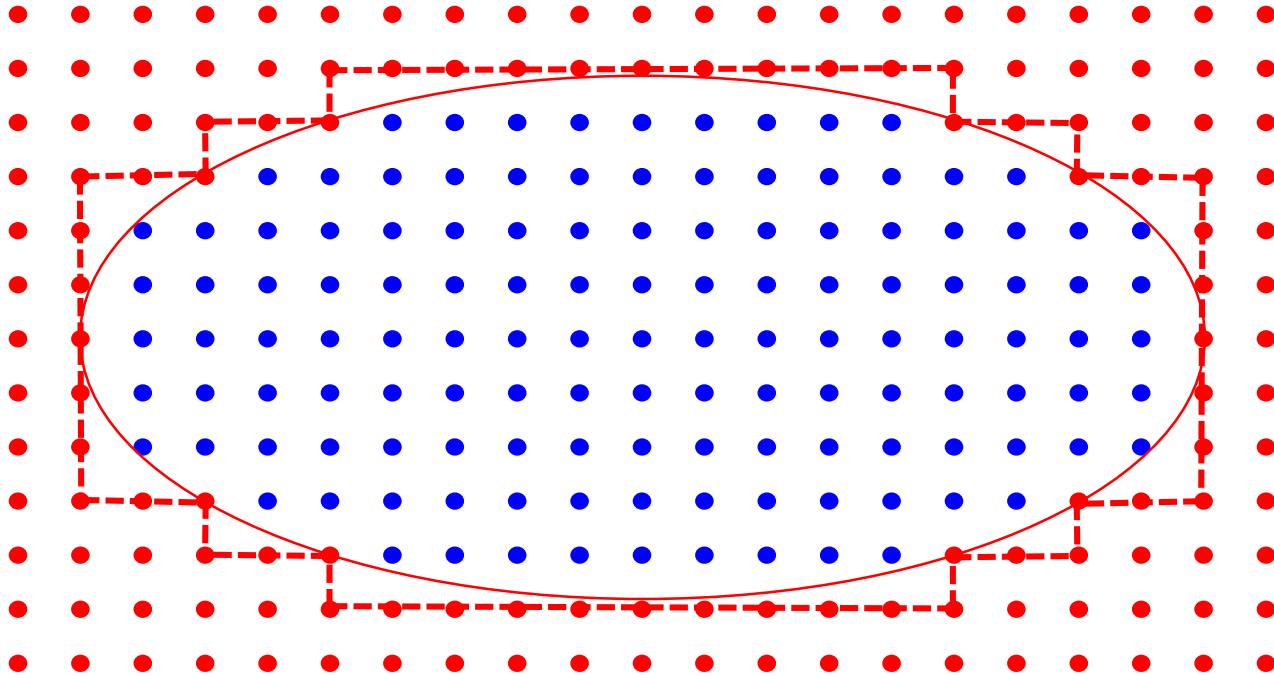


Can be written in matrix form:

$$\underline{\underline{A}}\underline{\underline{\phi}} = \frac{1}{\epsilon_0}\underline{\underline{\rho}}$$

A is sparse and depends only on chamber geometry and grid size

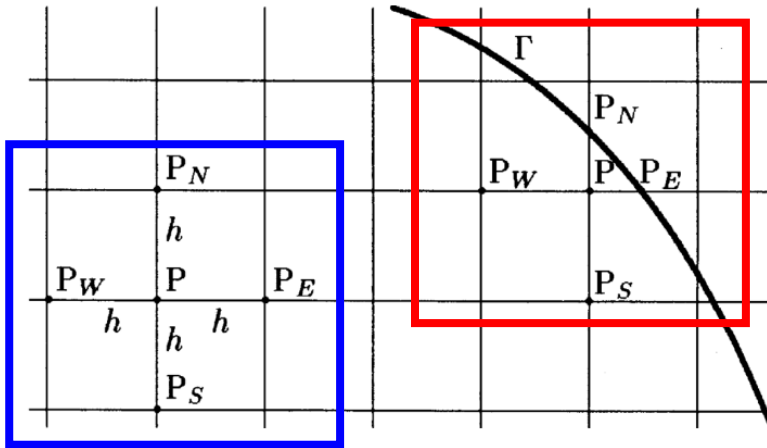
→ It can be computed and LU factorized in the initialization stage to speed up calculation



With this approach a curved boundary is **approximated with a staircase**

Can we do better?

The Shortley - Weller method



Refined approximation of Laplace operator at boundary nodes:

$$\begin{aligned}
 -\Delta_h^{(SW)} U(P) &= \left(\frac{2}{h_E h_W} + \frac{2}{h_S h_N} \right) U(P) \\
 &\quad - \frac{2}{h_E (h_E + h_W)} U(P_E) - \frac{2}{h_W (h_E + h_W)} U(P_W) \\
 &\quad - \frac{2}{h_S (h_S + h_N)} U(P_S) - \frac{2}{h_N (h_S + h_N)} U(P_N)
 \end{aligned}$$

Usual 5-points formula at internal nodes:

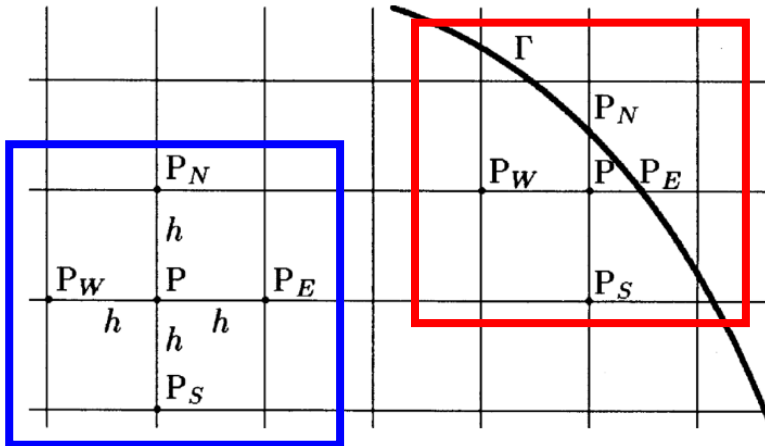
$$\begin{aligned}
 -\Delta_h^{(SW)} U(P) &= \frac{4}{h^2} U(P) - \frac{1}{h^2} U(P_E) - \frac{1}{h^2} U(P_W) \\
 &\quad - \frac{1}{h^2} U(P_S) - \frac{1}{h^2} U(P_N)
 \end{aligned}$$

$O(h^2)$ truncation error is preserved

(see: N. Matsunaga and T. Yamamoto, Journal of Computational and Applied Mathematics 116 – 2000, pp. 263–273)

The Shortley - Weller method

Sorry for the change of notation...



Refined gradient evaluation at boundary nodes:

$$E_x(P) = -\frac{1}{2} \left(\frac{U(P_E) - U(P)}{h_E} + \frac{U(P) - U(P_W)}{h_W} \right)$$

$$E_y(P) = -\frac{1}{2} \left(\frac{U(P_N) - U(P)}{h_N} + \frac{U(P) - U(P_S)}{h_S} \right)$$

Usual central difference for gradient evaluation at internal nodes:

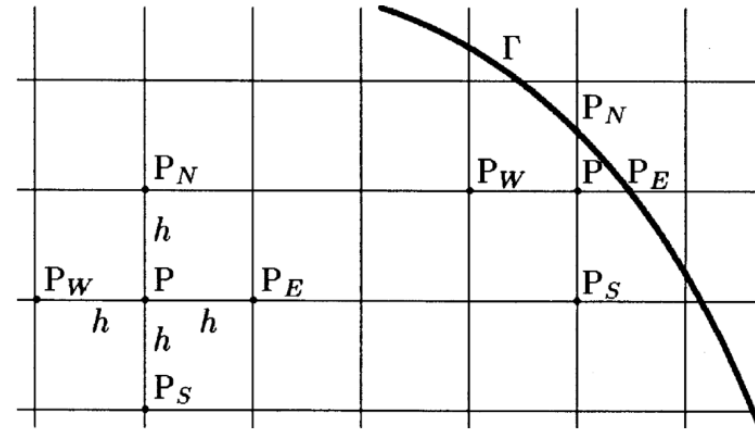
$$E_x(P) = -\frac{1}{2} \left(\frac{U(P_E) - \cancel{U(P)}}{h} + \frac{\cancel{U(P)} - U(P_W)}{h} \right)$$

$$E_y(P) = -\frac{1}{2} \left(\frac{U(P_N) - \cancel{U(P)}}{h} + \frac{\cancel{U(P)} - U(P_S)}{h} \right)$$

The Shortley - Weller method

Tricky implementation:

- **Boundary nodes need to be identified, distances from the curved boundary** need to be evaluated
 - **PyECLLOUD impact routines** have been employed (some refinement was required since they are optimized for robustness while here we need accuracy)
- **Nodes too close to the boundary** can lead to **ill conditioned A matrix** → we identify them and impose $U=0$
 - **Special treatment for gradient evaluation** is needed at these nodes
- Since chamber geometry and grid size stay constant along the simulation **most of the boundary treatment can be handled in the initialization stage**



$$\underline{\underline{A}} \underline{U} = \frac{1}{\epsilon_0} \underline{\rho}$$

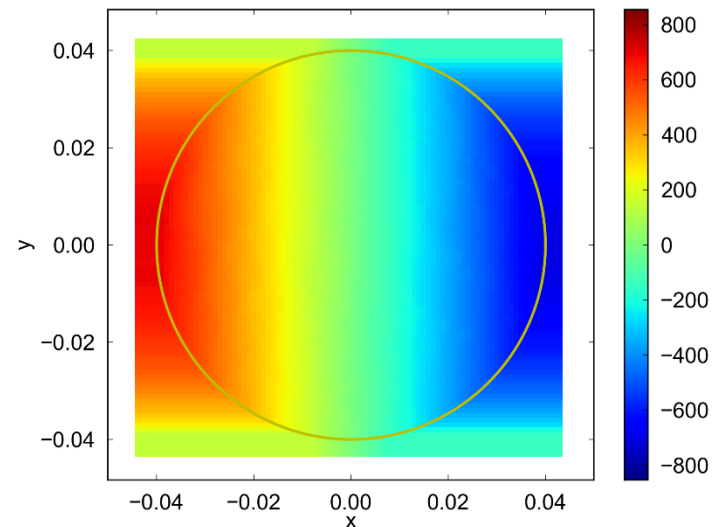
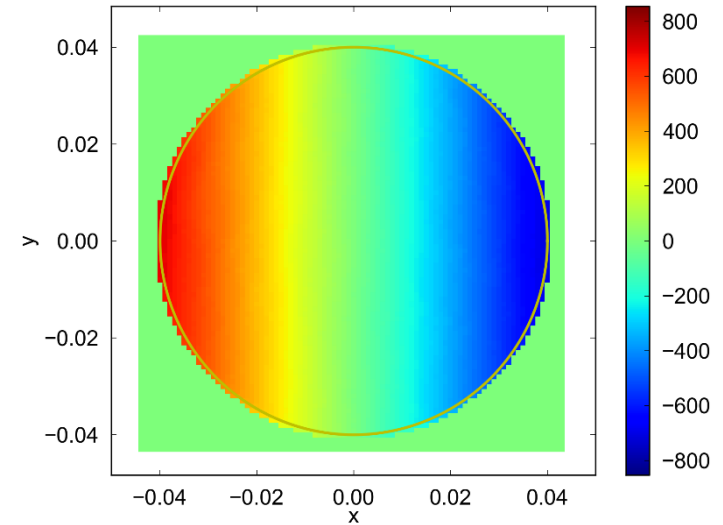
$$\underline{E}_x = \underline{\underline{D}}_x \underline{U}$$

$$\underline{E}_y = \underline{\underline{D}}_y \underline{U}$$

The Shortley - Weller method

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 - **Special treatment for gradient evaluation** is needed at these nodes
- Since chamber geometry and grid size stay constant along the simulation **most of the boundary treatment can be handled in the initialization stage**
- **Field map extrapolated outside the chamber** to simplify field gather for particle close to the chamber's wall



- Alternative approach: use a dual grid solver

