

# Code Development for Collective Effects

K. Li, H. Bartosik, G. Iadarola, L. Mether, A. Oeftiger,  
A. Passarelli, A. Romano, G. Rumolo, M. Schenk

HB2016, 3-8 July, Malmo, Sweden

# CDCE2016!?

K. Li, H. Bartosik, G. Iadarola, L. Mether, A. Oeftiger,  
A. Passarelli, A. Romano, G. Rumolo, M. Schenk

HB2016, 3-8 July, Malmo, Sweden

## Context:

**Collective effects** pose **important limitations** in modern **high brightness circular accelerators**. Studying and understanding these effects can help overcoming these limitations.

**Numerical methods** form one of the **fundamental contemporary tools** used for this purpose. We discuss some modern approaches for numerical modeling of collective effects and show some use-cases employing the example of the **PyHEADTAIL framework**.

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

## Summary:

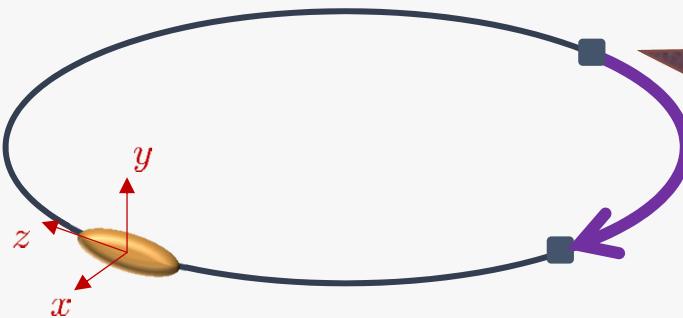
Brief outline of the **nature of collective effects** and why we study them with computer simulation programs.

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

# Modeling collective effects

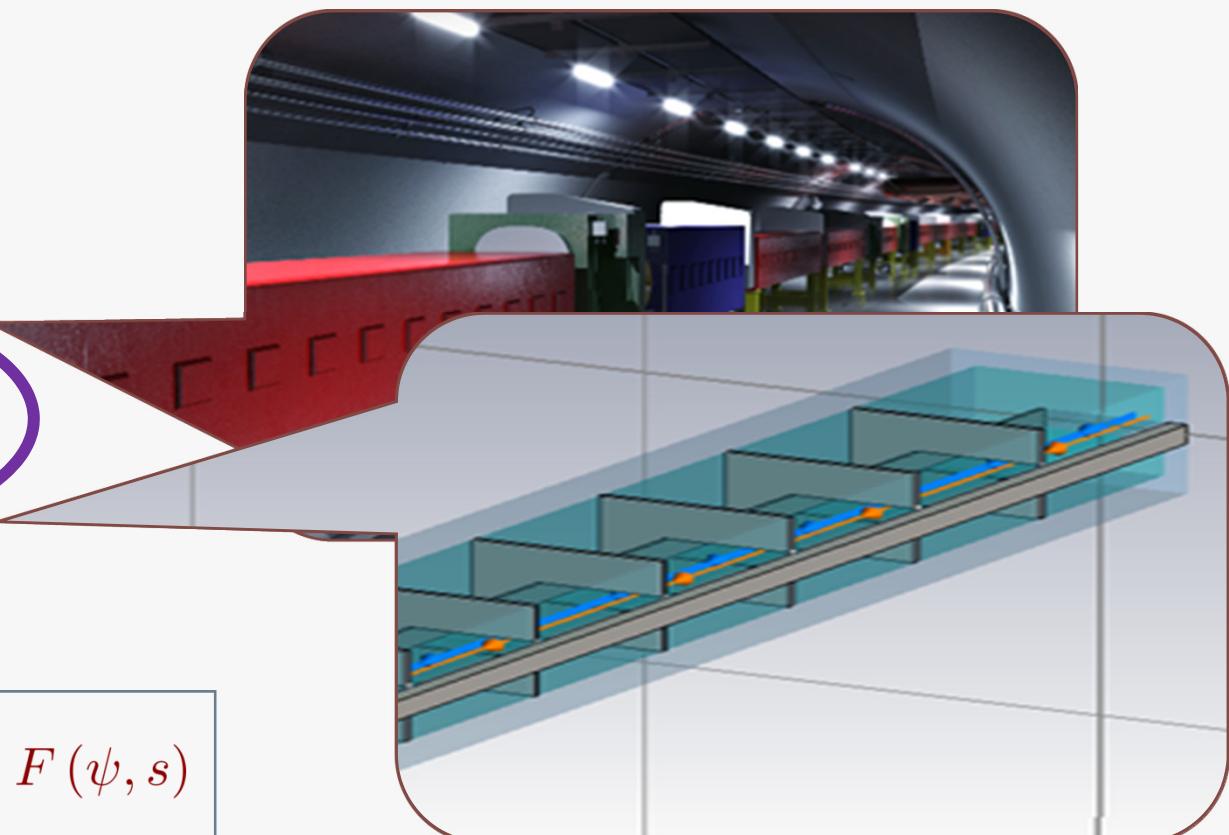
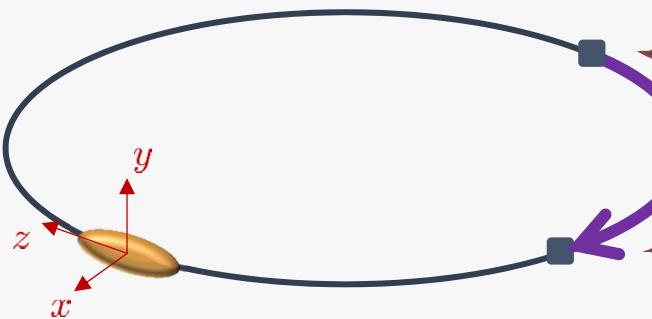
- Beam dynamics deals with studying the **evolution of the phase space variables** i.e., the **generalized coordinates** and **canonically conjugate momenta** of a beam in an accelerator
- Generally this evolution is determined by **external force fields** (magnets, electrostatic fields, RF fields)



$$\frac{d}{dt} \psi(x, x', y, y', z, \delta) = F_{\text{extern}}(x, y, z, s)$$

# Modeling collective effects

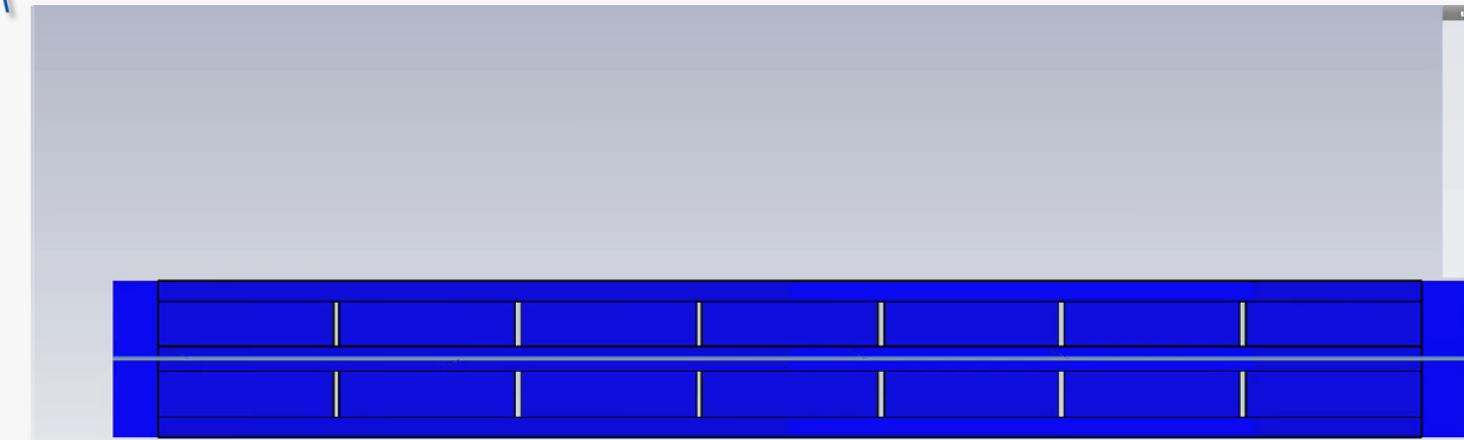
- Beam dynamics deals with studying the **evolution of the phase space variables** i.e., the **generalized coordinates** and **canonically conjugate momenta** of a beam in an accelerator
- Generally this evolution is determined by **external force fields** (magnets, electrostatic fields, RF fields)
- Collective effects add to these fields that depend on the **phase space distribution function** itself (space charge, wake fields)



$$\frac{d}{dt} \psi(x, x', y, y', z, \delta) = F_{\text{extern}}(x, y, z, s) + F(\psi, s)$$

# Modeling collective effects

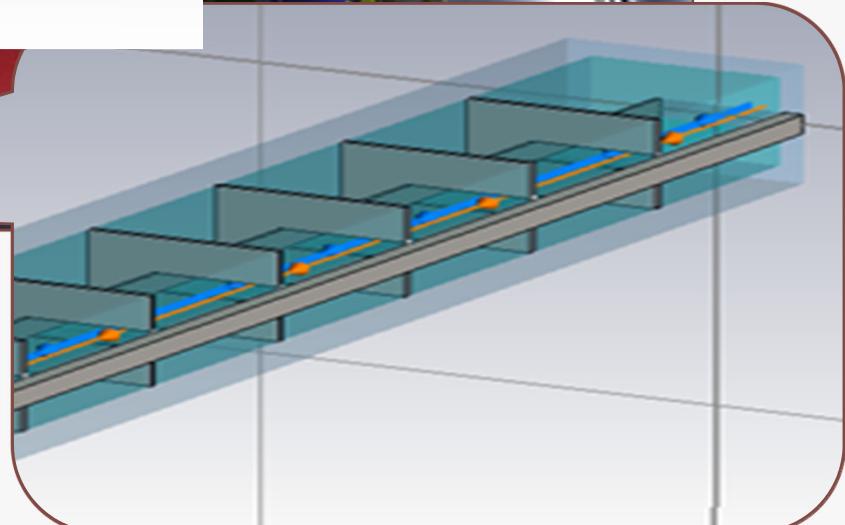
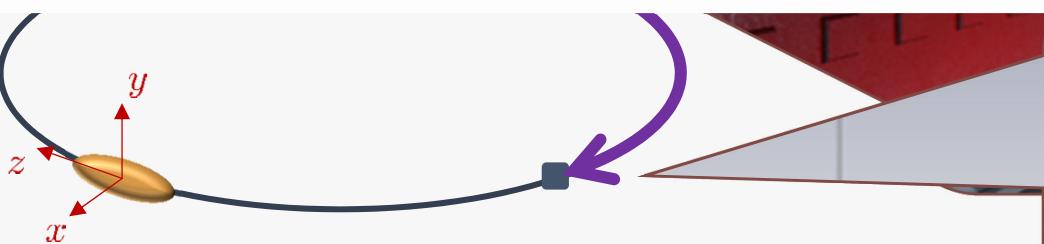
- ...
  - ...
  - ...
- i.e., the **generalized coordinates** and  
rostatic fields, RF fields)  
on function itself (space charge, wake



on function itself (space charge, wake



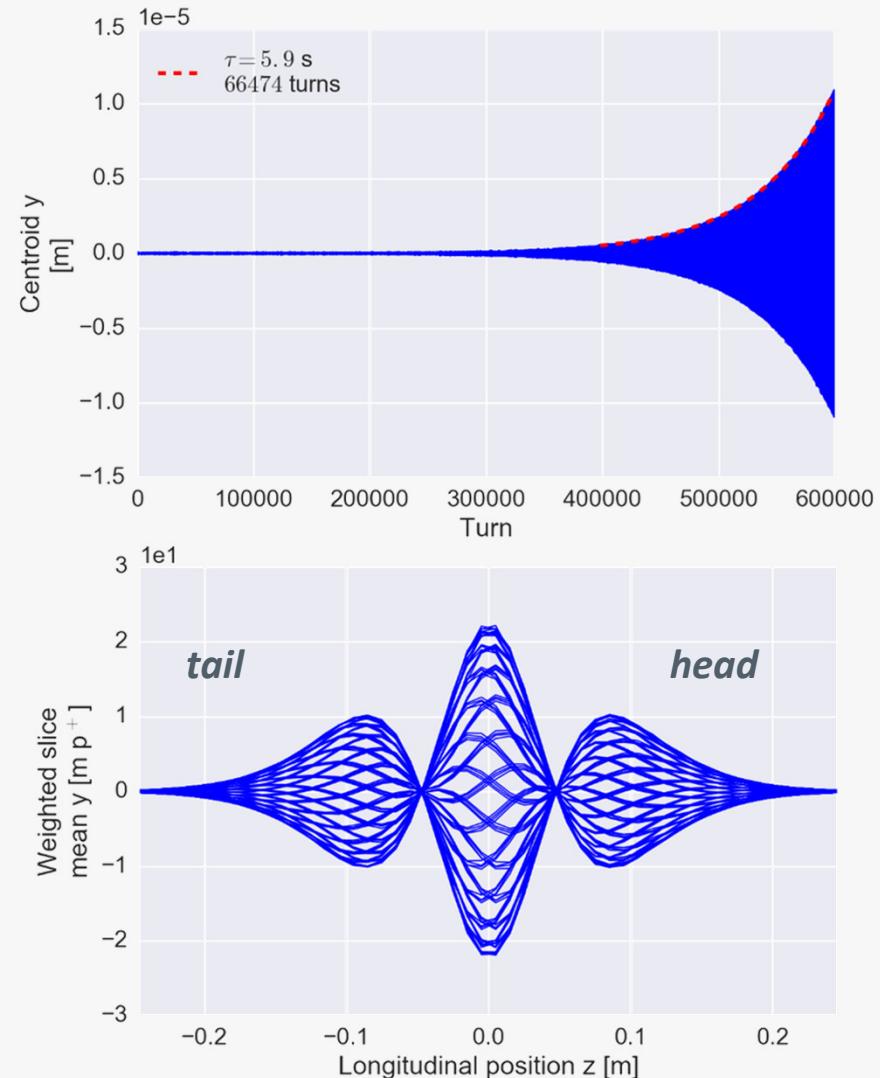
```
#-field (t=0..end(0..)x=0.5)_pb (peak)
Cellsize mm cl: 1, 0, 0
Cellsize position: 0.5
Components: 2
ZL MaxField (V/m): -233.9 dB MAX
Samples (39): 2
Time [ns]: 0.3
```



$$\frac{d}{dt} \psi(x, x', y, y', z, \delta) = F_{\text{extern}}(x, y, z, s) + F(\psi, s)$$

# Modeling collective effects

- Beam parameters
- Generalized coordinates
- Collective fields

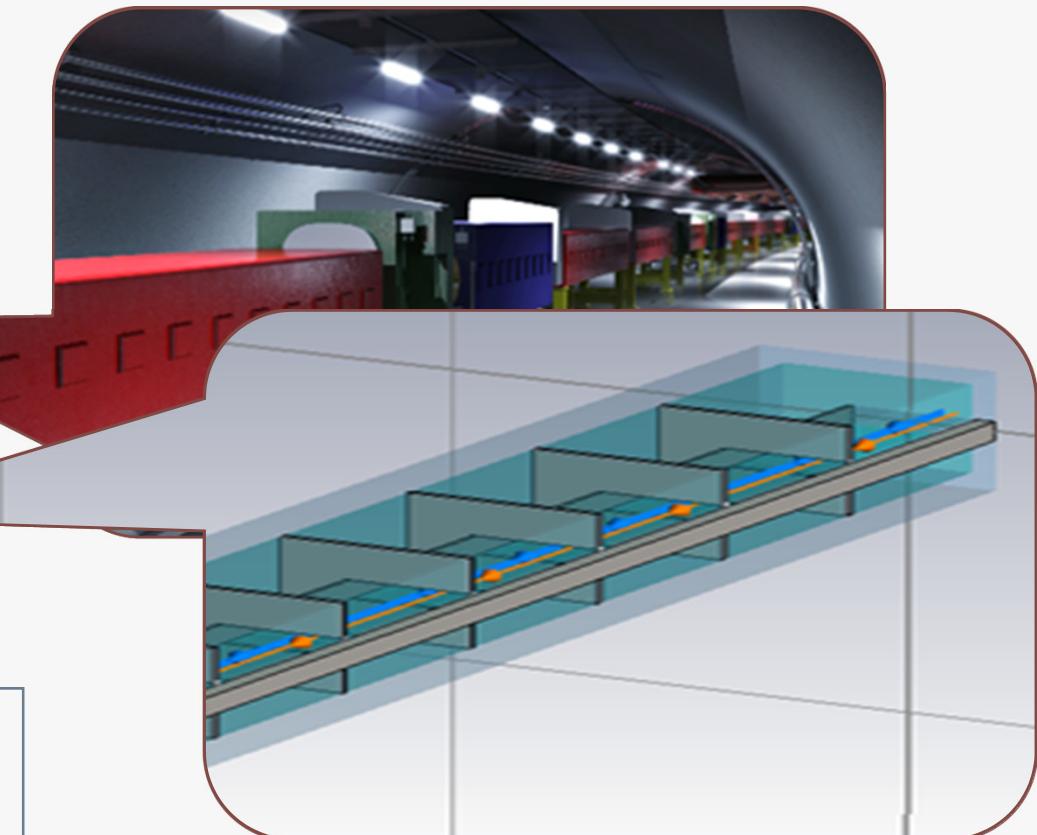


$$\frac{d}{dt} \psi$$

phase space variables i.e., the generalized coordinates and operator

fields (magnets, electrostatic fields, RF fields)

phase space distribution function itself (space charge, wake



- Beam dynamics deals with studying the **evolution of the phase space variables** i.e., the **generalized coordinates** and **canonically conjugate momenta** of a beam in an accelerator
- Generally this evolution is determined by **external force fields** (magnets, electrostatic fields, RF fields)
- Collective fields)

charge, wake

- For a **multi-particle system** this self-consistency equation becomes arbitrarily complex and practically **impossible to solve**
- Obtaining the **multi-particle dynamics** requires **computer simulation codes**

$$\frac{d}{dt} \psi(x, x', y, y', z, \delta) = F_{\text{extern}}(x, y, z, s) + F(\psi, s)$$

## Summary:

Brief explanation of the **numerical modelling** of the accelerator-beam system employed for computer simulation programs to study **collective effects in circular accelerators**.

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

# The PyHEADTAIL Model

## Coordinate system



- Bunch acquires and transports information from elements actions (messenger!)
- Elements imprint their action on bunch.

$$\left[ \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \begin{pmatrix} y_i \\ y'_i \end{pmatrix} \begin{pmatrix} z_i \\ \delta_i \end{pmatrix} \right]_{i=1,\dots,N} \in \mathbb{R}^{2N}$$

# The PyHEADTAIL Model

## Betatron motion



- Bunch acquires and transports information from elements actions (messenger!)
- Elements imprint their action on bunch.

Chromaticity: coupling to longitudinal  
Detuning with amplitude:  
continuous detuning

$$\Delta\mu_i \sim \Delta\mu_0 + (\xi \delta_i) + [\alpha_{xx} J_{x,i} + \alpha_{xy} J_{y,i}] \frac{\Delta\mu_0}{2\pi Q}$$

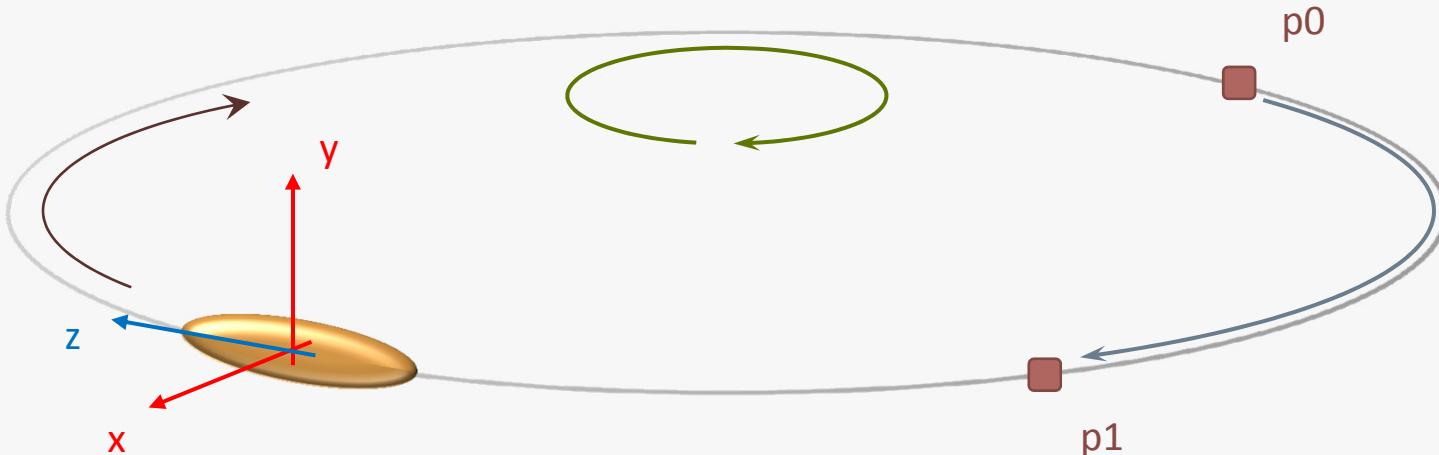
$$\mathcal{M}_i = \begin{pmatrix} \sqrt{\beta_1} & 0 \\ -\frac{\alpha_1}{\sqrt{\beta_1}} & \frac{1}{\sqrt{\beta_1}} \end{pmatrix} \begin{pmatrix} \cos(\Delta\mu_i) & \sin(\Delta\mu_i) \\ -\sin(\Delta\mu_i) & \cos(\Delta\mu_i) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{\beta_0}} & 0 \\ \frac{\alpha_0}{\sqrt{\beta_0}}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

$$\left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_1 = \mathcal{M}_i \left. \begin{pmatrix} x_i \\ x'_i \end{pmatrix} \right|_0$$

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

# The PyHEADTAIL Model

## Synchrotron motion



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

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

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

$i = 1, \dots, N$

$k$ : iteration/turn

- Bunch acquires and transports information from elements actions (messenger!)
- Elements imprint their action on bunch.

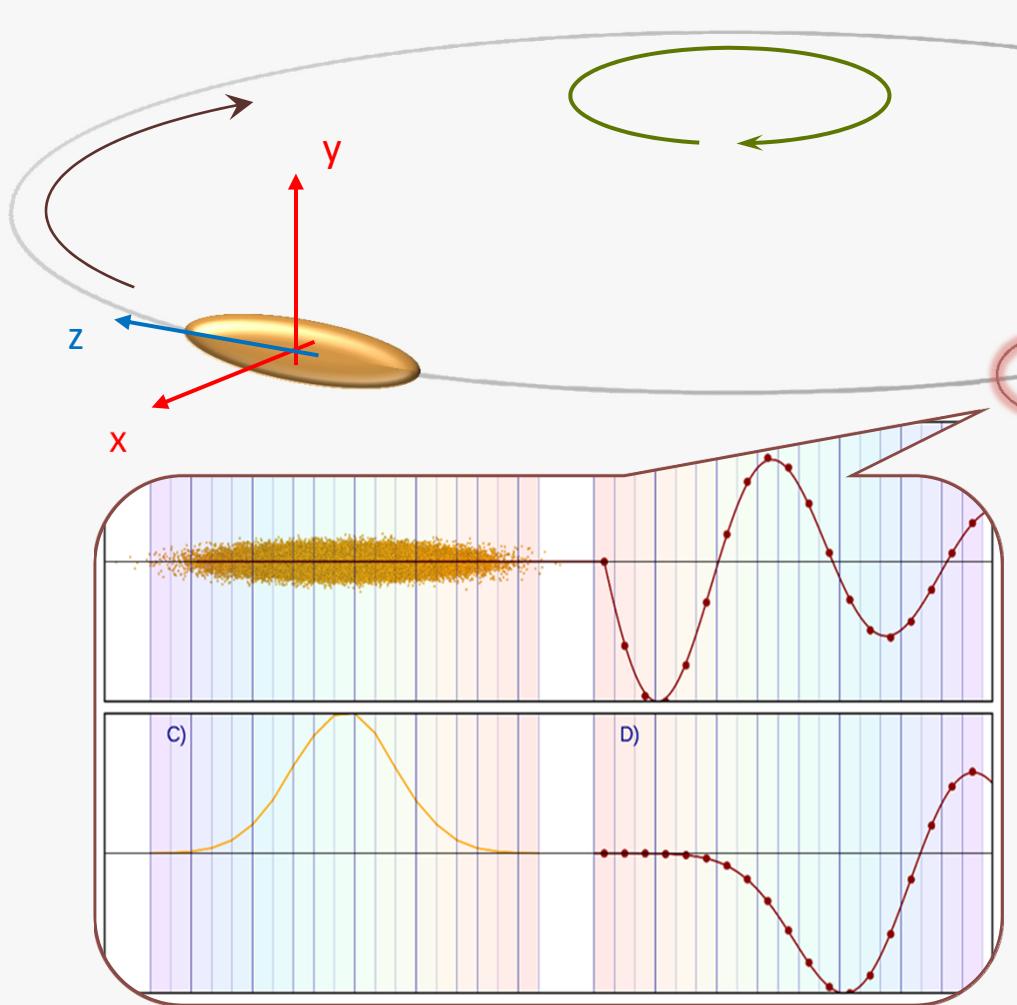
$$z' = -\eta \delta$$

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

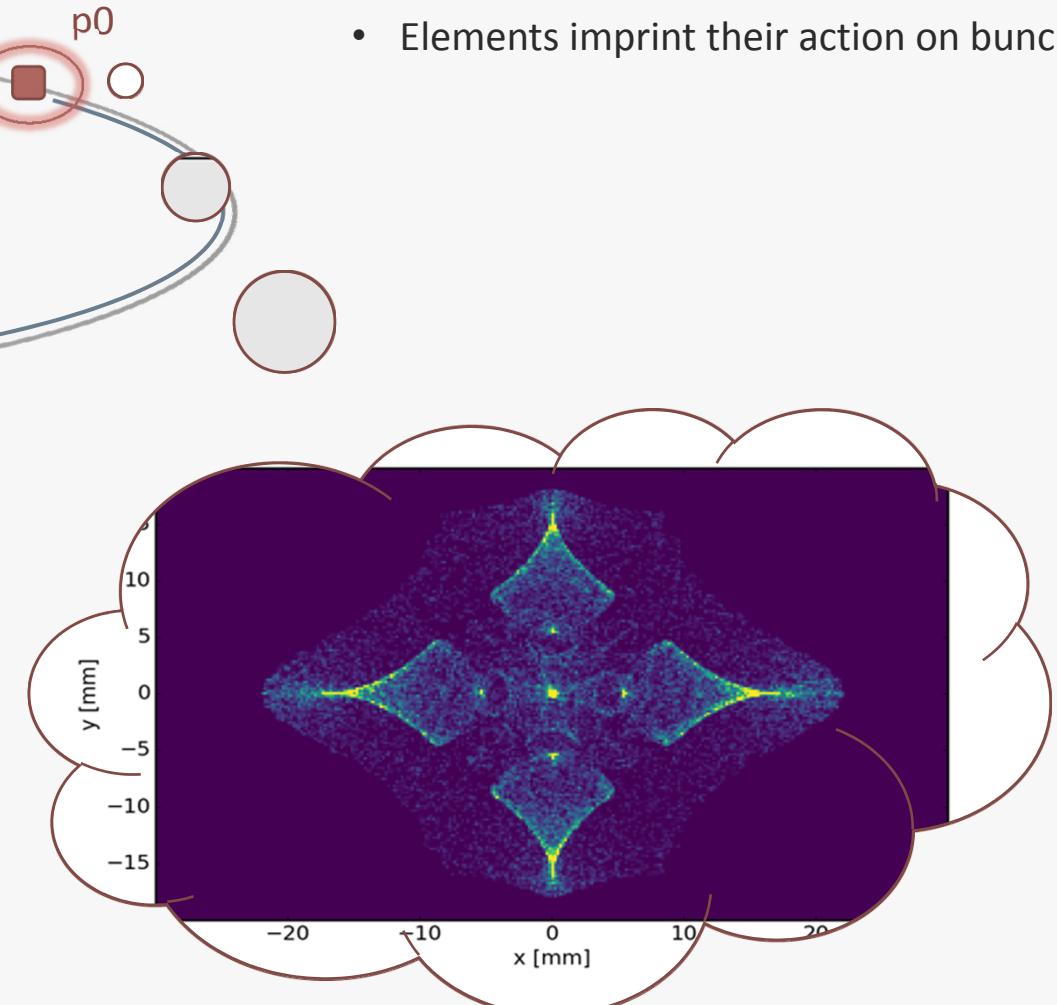
- $V_{\text{RF}}$ : RF voltage
- $h = \frac{\omega_{\text{RF}}}{\omega_0}$ : harmonic number
- $\omega_0$ : Revolution frequency
- $C$ : circumference

# The PyHEADTAIL Model

Wake fields, e-clouds etc.



- Bunch acquires and transports information from elements actions (messenger!)
- Elements imprint their action on bunch.



## Summary:

Some guidelines on programming strategies with their advantages and limitations.

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

# Modeling collective effects

- What are the demands of modern computer codes?



## Simple

- Easy to fix
- Easy to read
- Easy to maintain

## Modular

- Easy to extend
- Easy to combine
- Easy to maintain

## Dynamic

- Fast
- Flexible
- Interactive

... and each individual module becomes a carefully engineered piece of software.

## Be minimalist

- keep number of lines to the minimum necessary

## Be pragmatic

- use available libraries and don't re-invent the wheel

## Be paranoid

- write clear and well-formatted code

*“Always code as if the guy who ends up maintaining your code will be a violent psychopath who knows where you live”*

*John Woods*

## Repository (PyHEADTAIL)

...

feedback

gpu

impedances

machines

monitors

multipoles

particles

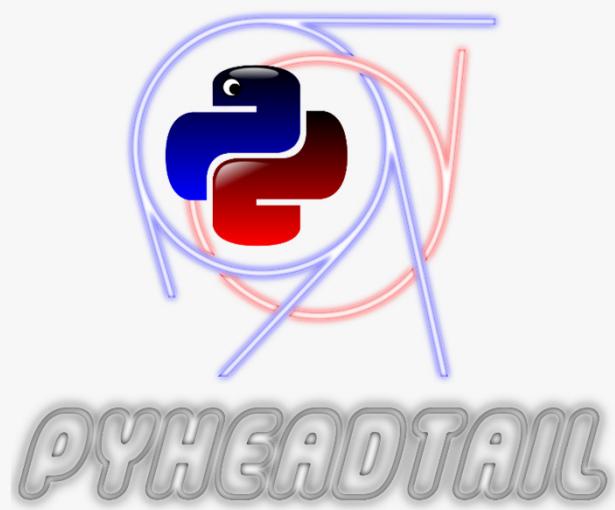
radiation

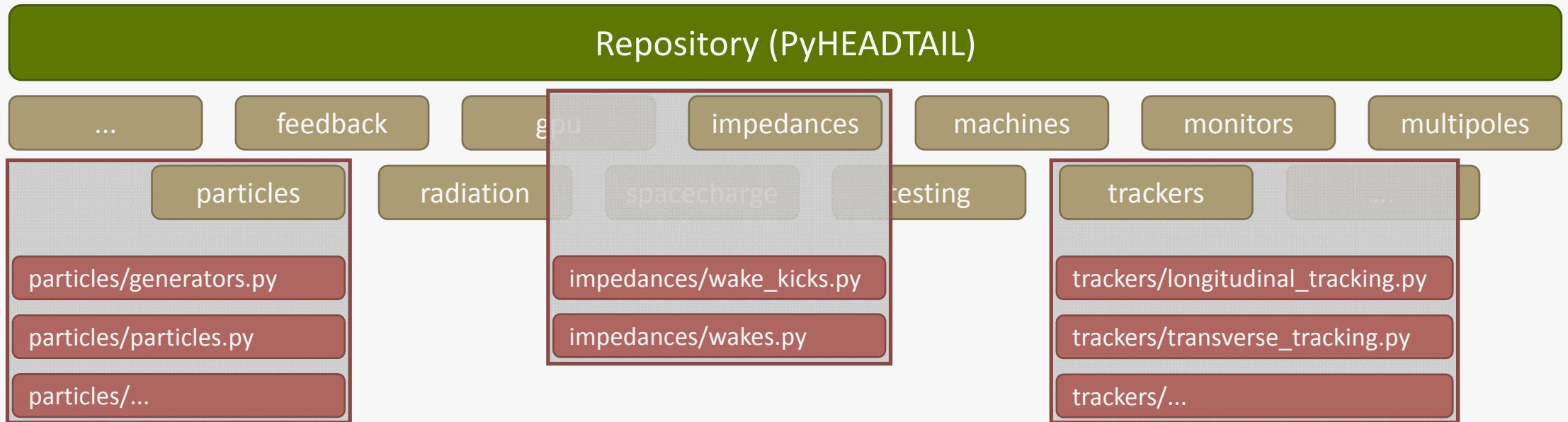
spacecharge

testing

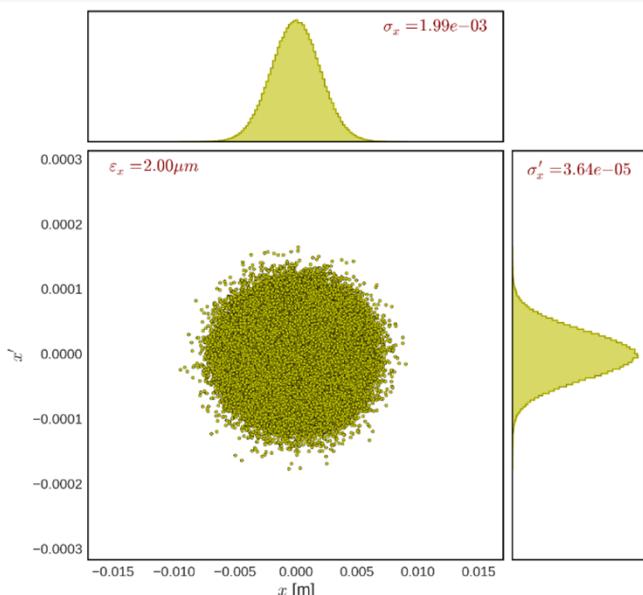
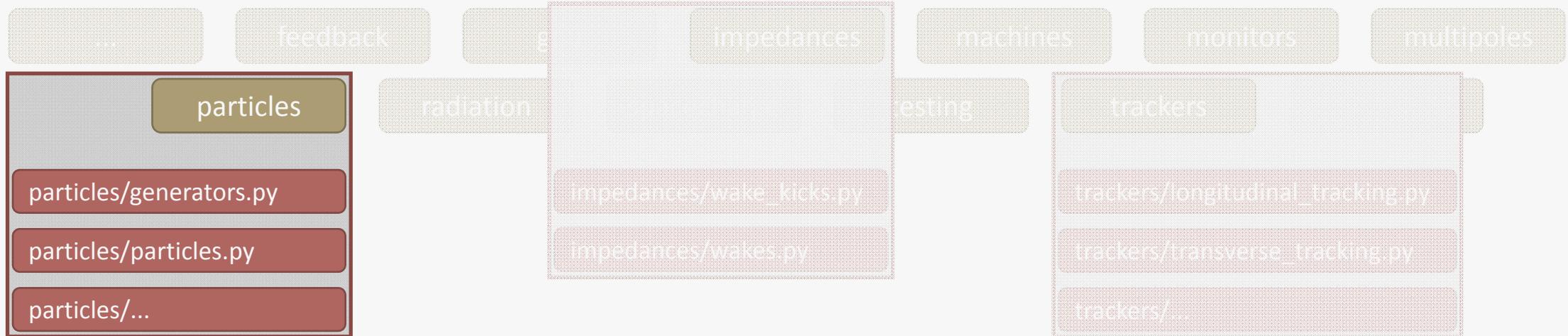
trackers

...



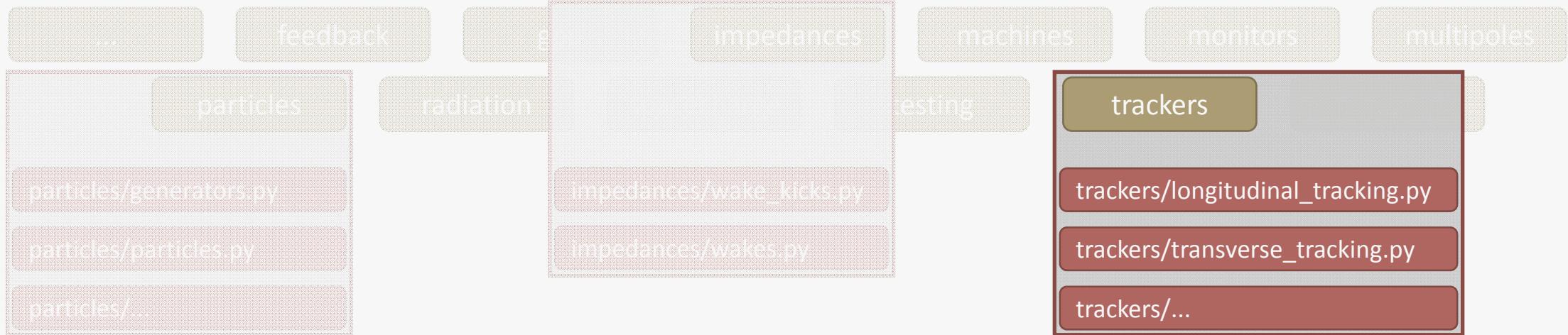


## Repository (PyHEADTAIL)

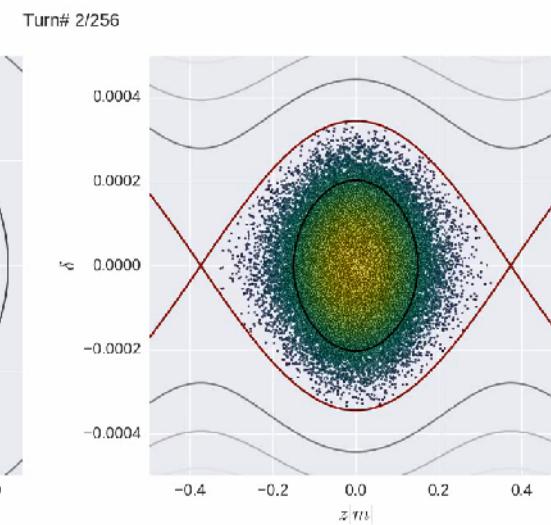
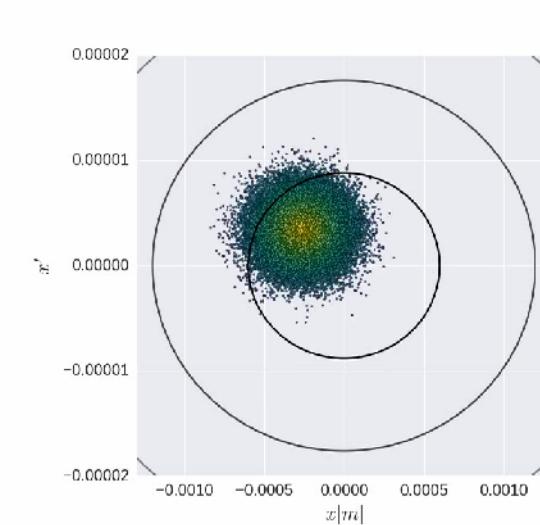


$$\begin{aligned}\varepsilon_{\perp} &= \beta\gamma\sqrt{\langle x^2 \rangle \langle x'^2 \rangle - \langle xx' \rangle^2} \\ &= \beta\gamma\sigma_x\sigma_{x'} \\ \varepsilon_{\parallel} &= 4\pi\sigma_z\sigma_{\delta} \frac{p_0}{e}\end{aligned}$$

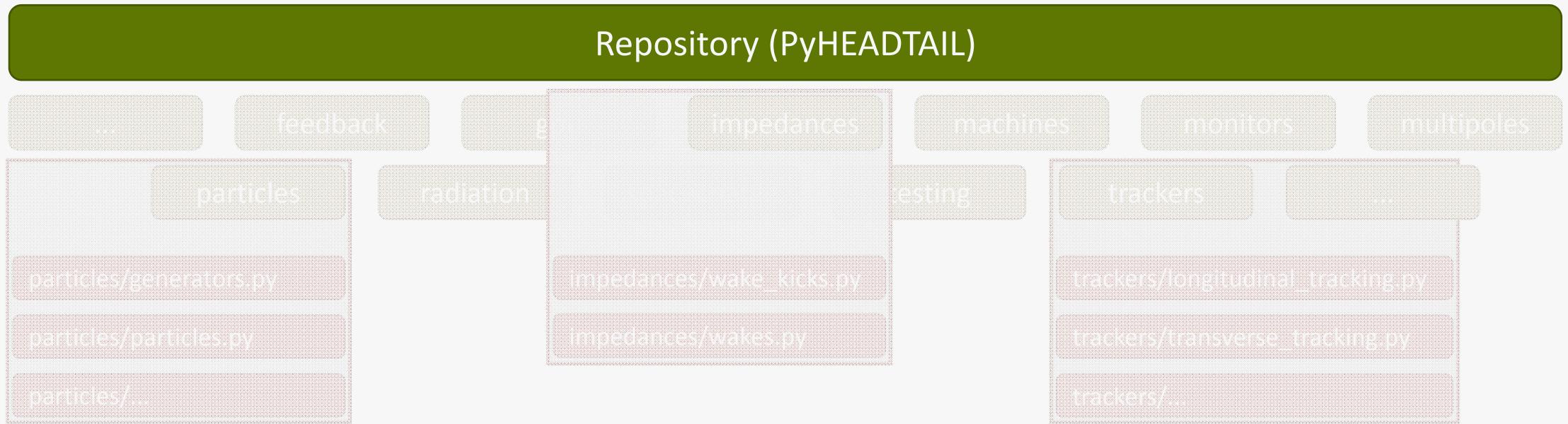
## Repository (PyHEADTAIL)



Transverse



Longitudinal



*"Just as Code Style, API Design, and Automation are essential for a healthy development cycle,  
Repository structure is a crucial part of your project's architecture."*

*The Hitchhiker's Guide to Python*

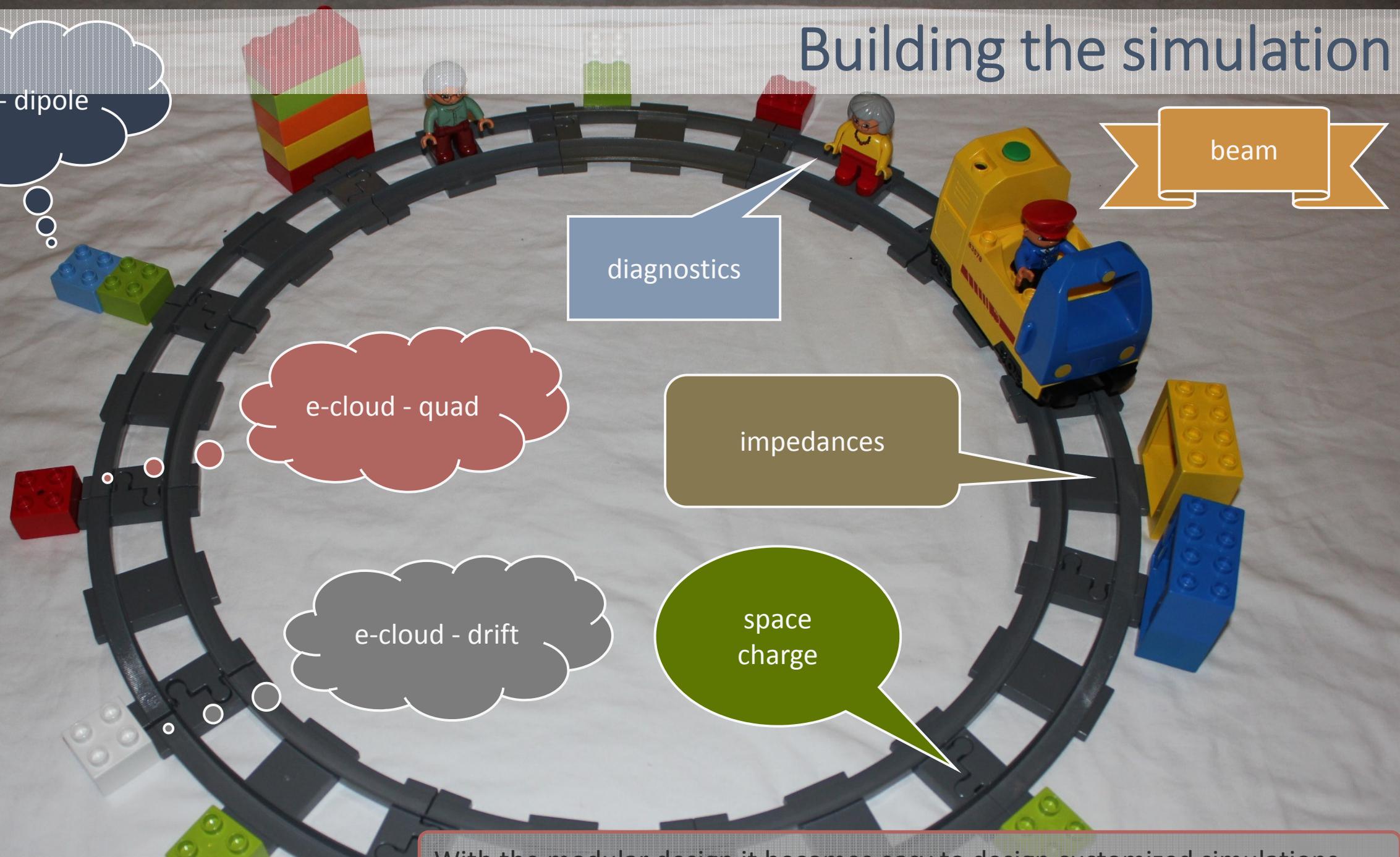
A good repository structure forms the backbone of a project. Object-oriented programming adds to this a defined programming structure.

# Building the simulation



With the modular design it becomes easy to design customized simulations.

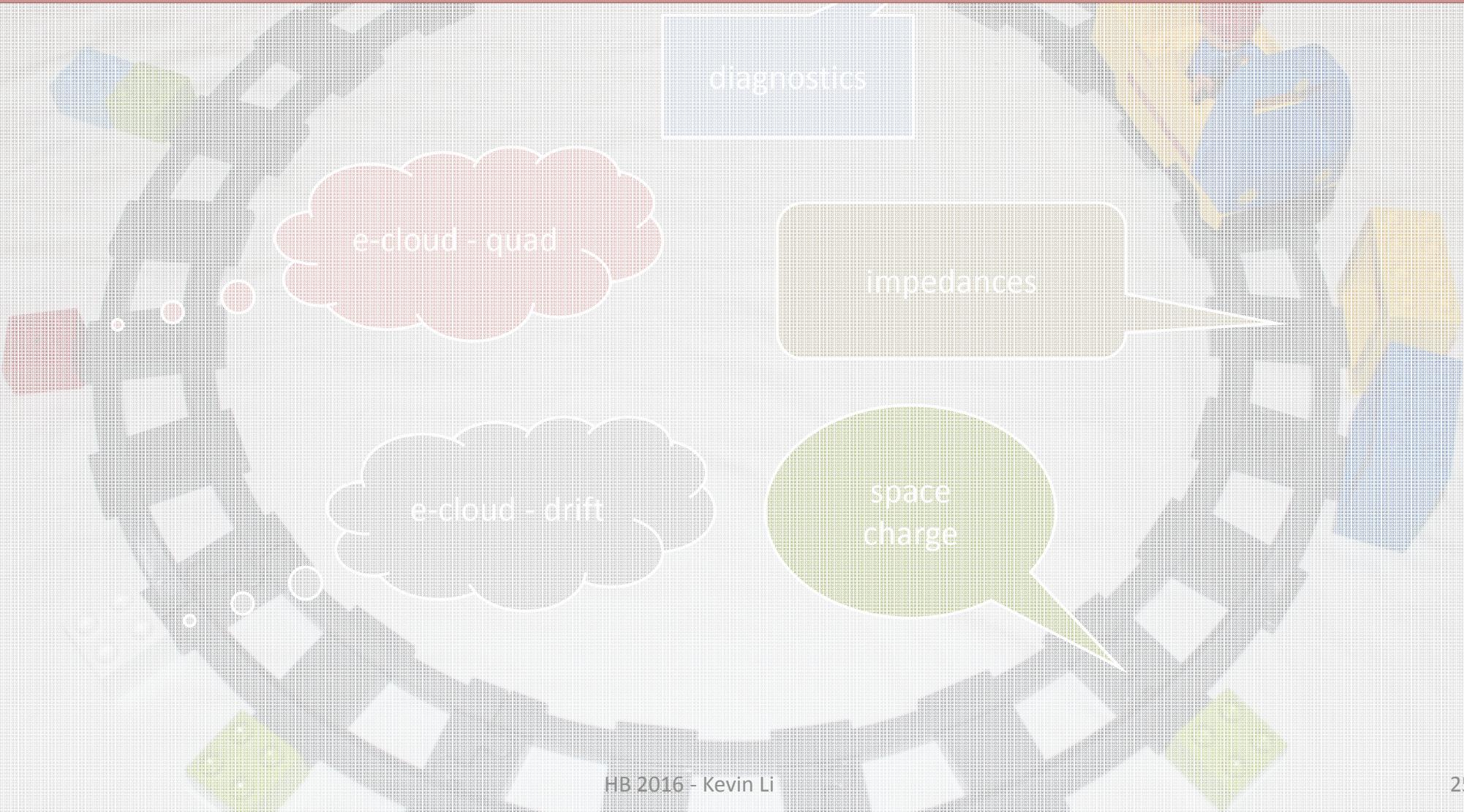
# Building the simulation



With the modular design it becomes easy to design customized simulations.

# Building the simulation

We need to think of a clever inputfile language that reflects this modularity (example of MAD-X, MAFIA etc.).



# Building the simulation

~~We need to think of a clever inputfile language that reflects this modularity (example of MAD-X, MAFIA etc.).~~

Why invent yet another language/syntax when there are established and popular languages most programmers already know:

*“It was nice to learn Python;  
a nice afternoon.”*

*Donald Knuth*

Input file becomes simply **a Python script** → inject the full power of the Python programming language to the input file

- Control flows
- Third party libraries
- Data analysis and visualization
- ...

Setting up a simulation becomes writing a small program/script – simple, highly customizable, interactive

# Building the simulation

Import modules

Choice of parameters

Instantiate objects

Assemble ring

Tracking loop –  
scriptable with  
Python control flows

See backup slides

```
File Edit Options Buffers Tools Python Virtual Envs Elpy YASnippet Help
166
167 s_cnt = 0
168 n_turns = 256
169 monitorswitch = False
170
171 print '\n--> Begin tracking\n'
172
173 for i in range(n_turns):
174     t0 = time.clock()
175     for m in one_turn_map:
176         m.track(bunch)
177
178     bunchmonitor.dump(bunch)
179
180     if not monitorswitch:
181         if (bunch.mean_x() >= 1.1 or bunch.mean_y() > 1e3 or i > n_turns-8192):
182             print "Monitoring"
183             monitorswitch = True
184
185         if s_cnt < 8192:
186             slicemonitor.dump(bunch)
187             s_cnt += 1
188
189     if (i+1) % 1 is not 0:
190         continue
191
192 Jx = np.sqrt((bunch.x-bunch.mean_x())**2 +
193               transverse_map.beta_x[0] * (bunch.xp-bunch.mean_xp()))**2)
194 contour(XX, YY, JJ, 6, lw=1)
195 ax1.scatter(bunch.x, bunch.xp, c=Jx, cmap=plt.cm.viridis_r, s=6)
196 contour(ZZ, PP, HH, 6, lw=1)
197 contour(ZZ, PP, HH, levels=[0], colors='darkred', lw=3)
198 ax2.scatter(bunch.z, bunch.dp, c=rfbucket.hamiltonian(bunch.z, bunch.dp),
199             cmap=plt.cm.viridis, s=6)
200 ax1.set_xlim(-1.3e-3, 1.3e-3)
201 ax1.set_ylim(-2e-5, 2e-5)
202 ax2.set_xlim(-.5, .5)
203 ax2.set_ylim(-5e-4, 5e-4)
204 ax1.set_xlabel("$x [m]$", fontsize=24)
205 ax1.set_ylabel("$x'$", fontsize=24)
206 ax2.set_xlabel("$z [m]$", fontsize=24)
207 ax2.set_ylabel("$\delta$]", fontsize=24)
```

## Summary:

Some ideas and examples how to improve performance limitations encountered when working with interpreted languages (Python).

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

An important hitch remains on the **FAST** requirement:

*"Python was not made to be fast... ... but to make developers fast."*

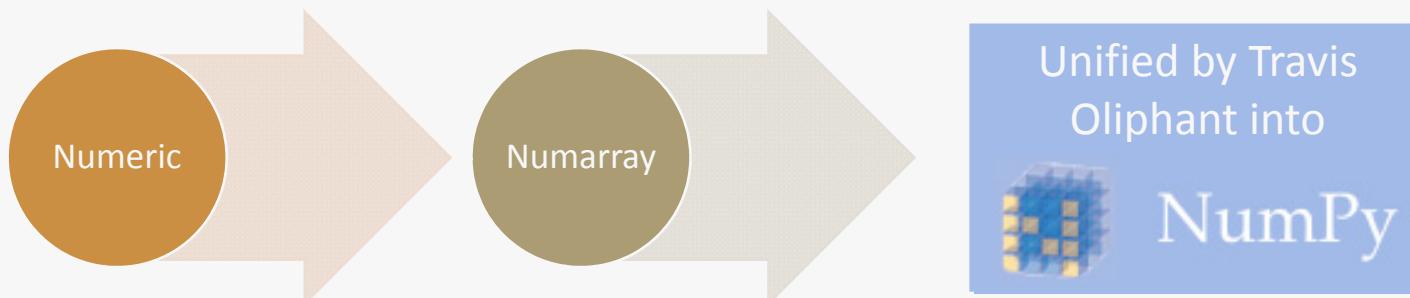
*Writing faster Python,  
Sebastian Witowski*

Being an interpreted language, strongly but dynamically typed, **Python can be slow in execution!** This needs to be handled.

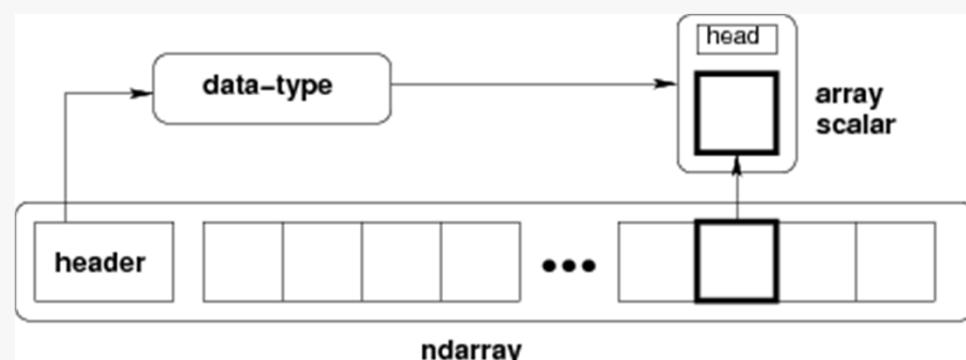
# Performance considerations

Python used as it is usually is slow for number crunching!

In the late 90s the Python scientific community worked on bringing the computationally intensive parts to a lower level:



The core functionality of NumPy is its "ndarray", for  $n$ -dimensional array, data structure.



Today, NumPy is the unrivaled basis for nearly all scientific tools in Python.

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi

The screenshot shows a Pyheadtail notebook interface. At the top, there's a toolbar with File, Edit, View, Insert, Cell, Kernel, and Help. Below the toolbar, the title bar says "012b\_optimisation\_example Last Checkpoint: 4 hours". The main area is divided into sections: "Profile" and "Python sin". In the "Profile" section, there are three code cells:

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)
```

1 loop, best of 3: 171 ms per loop

The screenshot shows a Pyheadtail notebook interface with a red callout box pointing to a line of code in a cell. The cell title is "Python sin". The code is:

```
In [4]: def pysin(x):
    y = [math.sin(i) for i in x]
    return y
```

A red callout box contains the text "for loop in Python – never do this!" with an arrow pointing to the line of code.

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi

The screenshot shows a Jupyter Notebook interface. The title bar says "PYHEADTAIL notebook" and "012b\_optimisation\_example Last Checkpoint: 4 hours". The menu bar includes File, Edit, View, Insert, Cell, Kernel, and Help. A sidebar on the left is titled "Profile" and contains the following code:

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)
```

Below the sidebar, the output of the %timeit commands is shown:

```
1 loop, best of 3: 171 ms per loop
10 loops, best of 3: 26.4 ms per loop
```

The screenshot shows a Jupyter Notebook interface. The title bar says "PYHEADTAIL notebook" and "012b\_optimisation\_example Last Checkpoint: 4 minutes ago (autosaved)". The menu bar includes File, Edit, View, Insert, Cell, Kernel, and Help. The main content area has two sections:

### Python sin

```
In [4]: def pysin(x):
    y = [math.sin(i) for i in x]
    return y
```

### Numpy sin

```
In [5]: import numpy as np
def npsin(x):
    return np.sin(x)
```

A red callout bubble points from the text "Vectorization: the array is interpreted by NumPy and the loop is executed at C level" to the NumPy import statement in cell [5].

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi



**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 4 hours ago

File Edit View Insert Cell Kernel Help

### Profile

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)

1 loop, best of 3: 171 ms per loop
10 loops, best of 3: 26.4 ms per loop
10 loops, best of 3: 26.8 ms per loop
```



**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 11 minutes ago (unsaved changes)

File Edit View Insert Cell Kernel Help

Generated by Cython 0.23.4

Yellow lines hint at Python interaction.  
Click on a line that starts with a "+" to see the C code that Cython generated.

```
01:
+02: import numpy as np
03: cimport numpy as np
04: cimport cython
05: from cython.parallel import prange
06: from libc.math cimport sin
07:
08: @cython.boundscheck(False)
09: @cython.wraparound(False)
10: @cython.cdivision(False)
+11: def cmsin(double[:,:] x, double[:,:] s):
12:
13:     cdef int n = x.shape[0]
14:     cdef int i
15:     for i in prange(n, nogil=True, num_threads=4):
16:         s[i] = sin(x[i])
```



Small low-level extensions for Python accessing native Python data structures – core coding in Python

Typed Memoryviews: efficient data access and handling

Explicit loop at C level; yellow lines indicate Python overhead

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 4 hours ago

File Edit View Insert Cell Kernel Help

## Profile

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)

1 loop, best of 3: 171 ms per loop
10 loops, best of 3: 26.4 ms per loop
10 loops, best of 3: 26.8 ms per loop

%timeit vdt_sin(x, a)
%timeit vdt_sinv(x, a)
%timeit vdt_sincos(x, a, b)

100 loops, best of 3: 11 ms per loop
100 loops, best of 3: 8.23 ms per loop
100 loops, best of 3: 17.2 ms per loop
```

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 8 minutes ago (autosaved)

Generated by Cython 0.23.4

Yellow lines hint at Python interaction.  
Click on a line that starts with a "+" to see the C code that Cython generates.

```
+01: #export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/jc73/vdt/lib
02: #cython boundscheck=False
03:
04: cimport cython
+05: import numpy as np
06: cimport numpy as np
07: from cython.parallel import prange
08:
09: cdef extern from "sin.h" namespace "vdt":
10:     cdef double fast_sin(double x) nogil
11:     cdef void fast_sinv(int n, double *x, double *s) nogil
12:
13: cdef extern from "sincos.h" namespace "vdt":
14:     cdef void fast_sincos(double x, double &s, double &c) nogil
15:
16: @cython.boundscheck(False)
+17: def vdt_sin(double[:,:] x, double[:,:] s):
18:
19:     cdef int n = x.shape[0]
20:     cdef int i
21:     for i in prange(n, nogil=True, num_threads=1):
22:         s[i] = fast_sin(x[i])
23:
24: @cython.boundscheck(False)
+25: def vdt_sincos(double[:,:] x, double[:,:] s, double[:,:] c):
26:
27:     cdef int n = x.shape[0]
28:     cdef int i
29:     for i in prange(n, nogil=True, num_threads=1):
30:         fast_sincos(x[i], s[i], c[i])
31:
32: @cython.boundscheck(False)
+33: def vdt_sinv(double[:,:] x, double[:,:] s):
34:
35:     cdef int n = x.shape[0]
36:     fast_sinv(n, &x[0], &s[0])
```

**Cython**  
Small low-level extensions for Python, accessing native Python data structures – core coding in Python

(here, vdtmath:  
D. Piparo et al. 2014 J. Phys.: Conf. Ser. 513 052027  
"Speeding up HEP experiment software with a library of fast and auto-vectorisable mathematical functions")

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 4 hours ago

File Edit View Insert Cell Kernel Help

### Profile

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)

1 loop, best of 3: 171 ms per loop
10 loops, best of 3: 26.4 ms per loop
10 loops, best of 3: 26.8 ms per loop

%timeit vdt_sin(x, a)
%timeit vdt_sinv(x, a)
%timeit vdt_sincos(x, a, b)

100 loops, best of 3: 11 ms per loop
100 loops, best of 3: 8.23 ms per loop
100 loops, best of 3: 17.2 ms per loop
```

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 8 minutes ago (autosaved)

Generated by Cython 0.23.4

Yellow lines hint at Python interaction.  
Click on a line that starts with a "+" to see the C code that Cython generates.

```
+01: #export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/jl23/vdtmath/lib
02: #cython boundscheck=False
03:
04: cimport cython
+05: import numpy as np
06: cimport numpy as np
07: from cython.parallel import prange
08:
09: cdef extern from "sin.h" namespace "vdt":
10:     cdef double fast_sin(double x) nogil
11:     cdef void fast_sinv(int n, double *x, double *s) nogil
12:
13: cdef extern from "sincos.h" namespace "vdt":
14:     cdef void fast_sincos(double x, double &s, double &c) nogil
15:
16: @cython.boundscheck(False)
+17: def vdt_sin(double[:,:] x, double[:,:] s):
18:
19:     cdef int n = x.shape[0]
20:     cdef int i
21:     for i in prange(n, nogil=True, num_threads=1):
22:         s[i] = fast_sin(x[i])
23:
24: @cython.boundscheck(False)
+25: def vdt_sincos(double[:,:] x, double[:,:] s, double[:,:] c):
26:
27:     cdef int n = x.shape[0]
28:     cdef int i
29:     for i in prange(n, nogil=True, num_threads=1):
30:         fast_sincos(x[i], s[i], c[i])
31:
32: @cython.boundscheck(False)
+33: def vdt_sinv(double[:,:] x, double[:,:] s):
34:
35:     cdef int n = x.shape[0]
36:     fast_sinv(n, &x[0], &s[0])
```

**Cython**  
Small low-level extensions for Python, accessing native Python data structures – core coding in Python

(here, vdtmath:  
D. Piparo et al. 2014 J. Phys.: Conf. Ser. 513 052027  
"Speeding up HEP experiment software with a library of fast and auto-vectorisable mathematical functions")

OpenMP multithreading parallelization; move from e.g. 1 to 4 threads

# A very simple example for speed-up

- Profile the evaluation of the sine function over an array
- x is an array with 6M entries ranging uniformly from 0 to 2 pi

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 4 hours ago

File Edit View Insert Cell Kernel Help

### Profile

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)

1 loop, best of 3: 176 ms per loop
10 loops, best of 3: 26.4 ms per loop
100 loops, best of 3: 13 ms per loop

%timeit vdt_sin(x, a)
%timeit vdt_sinv(x, a)
%timeit vdt_sincos(x, a, b)

100 loops, best of 3: 6.12 ms per loop
100 loops, best of 3: 8.19 ms per loop
100 loops, best of 3: 8.26 ms per loop
```

**PYHEADTAIL notebook**

012b\_optimisation\_example Last Checkpoint: 8 minutes ago (autosaved)

Generated by Cython 0.23.4

Yellow lines hint at Python interaction.  
Click on a line that starts with a "+" to see the C code that Cython generates.

```
+01: #export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/kf3/vdt/lib
02: #cython boundscheck=False
03:
04: cimport cython
+05: import numpy as np
06: cimport numpy as np
07: from cython.parallel import prange
08:
09: cdef extern from "sin.h" namespace "vdt":
10:     cdef double fast_sin(double x) nogil
11:     cdef void fast_sinv(int n, double *x, double *s) nogil
12:
13: cdef extern from "sincos.h" namespace "vdt":
14:     cdef void fast_sincos(double x, double &s, double &c) nogil
15:
16: @cython.boundscheck(False)
+17: def vdt_sin(double[:,:] x, double[:,:] s):
18:
19:     cdef int n = x.shape[0]
20:     cdef int i
21:     for i in prange(n, nogil=True, num_threads=1):
22:         s[i] = fast_sin(x[i])
23:
24: @cython.boundscheck(False)
+25: def vdt_sincos(double[:,:] x, double[:,:] s, double[:,:] c):
26:
27:     cdef int n = x.shape[0]
28:     cdef int i
29:     for i in prange(n, nogil=True, num_threads=1):
30:         fast_sincos(x[i], s[i], c[i])
31:
32: @cython.boundscheck(False)
+33: def vdt_sinv(double[:,:] x, double[:,:] s):
34:
35:     cdef int n = x.shape[0]
36:     fast_sinv(n, &x[0], &s[0])
```

**Cython**  
Small low-level extensions for Python, accessing native Python data structures – core coding in Python

(here, vdtmath:  
D. Piparo et al. 2014 J. Phys.: Conf. Ser. 513 052027  
"Speeding up HEP experiment software with a library of fast and auto-vectorisable mathematical functions")

OpenMP multithreading parallelization; move from e.g. 1 to 4 threads

4

# A very simple example for speed-up

- Profile the evaluation of the sine

- There are an abundance of tools out there for embedding and extending Python:

 **C**Python API, *ctypes*, *f2py*, *SWIG*, *Boost::Python*, *Numexpr*, *Cython*, *PyCUDA*, *Numba*, *cffi*...

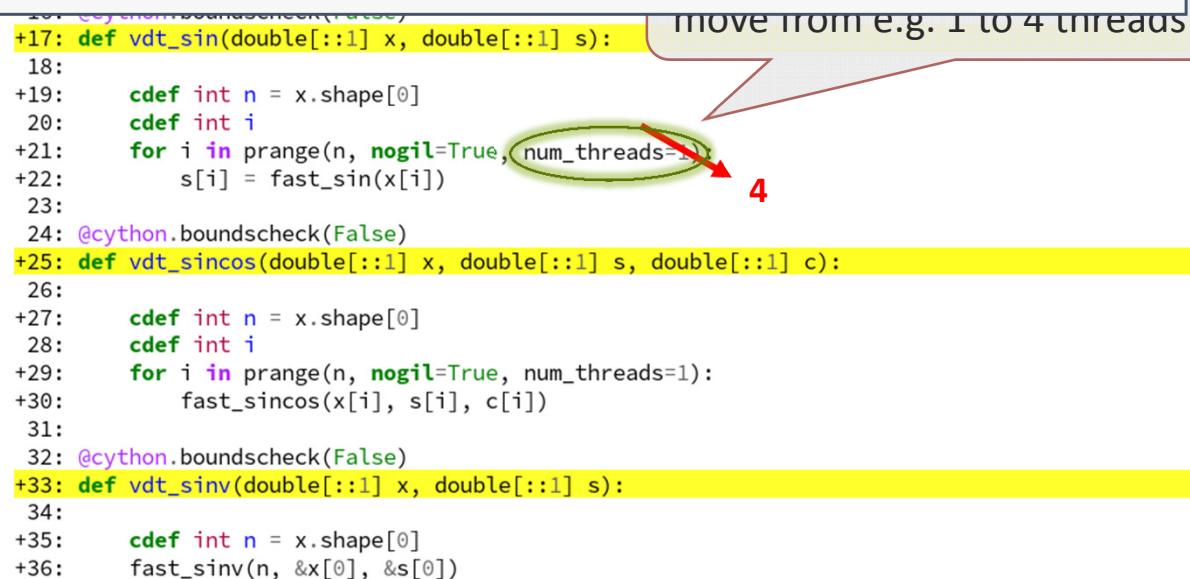
Today, Cython provides a very most modern and flexible approach. However the world is changing fast. Writing simple (and little) code will enable us to remain adaptable.

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x, a)

1 loop, best of 3: 176 ms per loop
10 loops, best of 3: 26.4 ms per loop
100 loops, best of 3: 13 ms per loop
```

```
%timeit vdt_sin(x, a)
%timeit vdt_sinv(x, a)
%timeit vdt_sincos(x, a, b)

100 loops, best of 3: 6.12 ms per loop
100 loops, best of 3: 8.19 ms per loop
100 loops, best of 3: 8.26 ms per loop
```



```
+17: def vdt_sin(double[:,:] x, double[:,:] s):
+18:
+19:     cdef int n = x.shape[0]
+20:
+21:     for i in prange(n, nogil=True, num_threads=1):
+22:         s[i] = fast_sin(x[i])
+23:
+24:     @cython.boundscheck(False)
+25: def vdt_sincos(double[:,:] x, double[:,:] s, double[:,:] c):
+26:
+27:     cdef int n = x.shape[0]
+28:
+29:     for i in prange(n, nogil=True, num_threads=1):
+30:         fast_sincos(x[i], s[i], c[i])
+31:
+32:     @cython.boundscheck(False)
+33: def vdt_sinv(double[:,:] x, double[:,:] s):
+34:
+35:     cdef int n = x.shape[0]
+36:     fast_sinv(n, &x[0], &s[0])
```

# A very simple example for speed-up

- Profile the evaluation of the sine

- There are an abundance of tools out there for embedding and extending Python:

 *CPython API, ctypes, f2py, SWIG, Boost::Python, Numexpr, Cython, PyCUDA, Numba, cffi...*

Today, Cython provides a very most modern and flexible approach. However the world is changing fast. Writing simple (and little) code will enable us to remain adaptable.

```
%timeit pysin(x)
%timeit npsin(x)
%timeit cmsin(x)
```

1 loop, best of  
10 loops, best of  
100 loops, best

```
%timeit vdt_sin()
%timeit vdt_sinv()
%timeit vdt_sinc()
```

100 loops, best  
100 loops, best  
100 loops, best of 3: 8.26 ms per loop



nsions for  
ve Python  
itory and  
coding in

513 052027  
th a library of  
unctions")

lelization;

+17: def vdt\_sin(double[:1] x, double[:1] s): move from e.g. 1 to 4 threads

The next Travis Oliphant:

*"Yep. Theano, Numba, numexpr, Cython and PyPy shall one day all merge to form  
Numtron, defender of sanity, runner of fast numerics."*

Dave Warde-Farley

```
32: @cython.boundscheck(False)
+33: def vdt_sinv(double[:1] x, double[:1] s):
34:
+35:     cdef int n = x.shape[0]
+36:     fast_sinv(n, &x[0], &s[0])
```

## Summary:

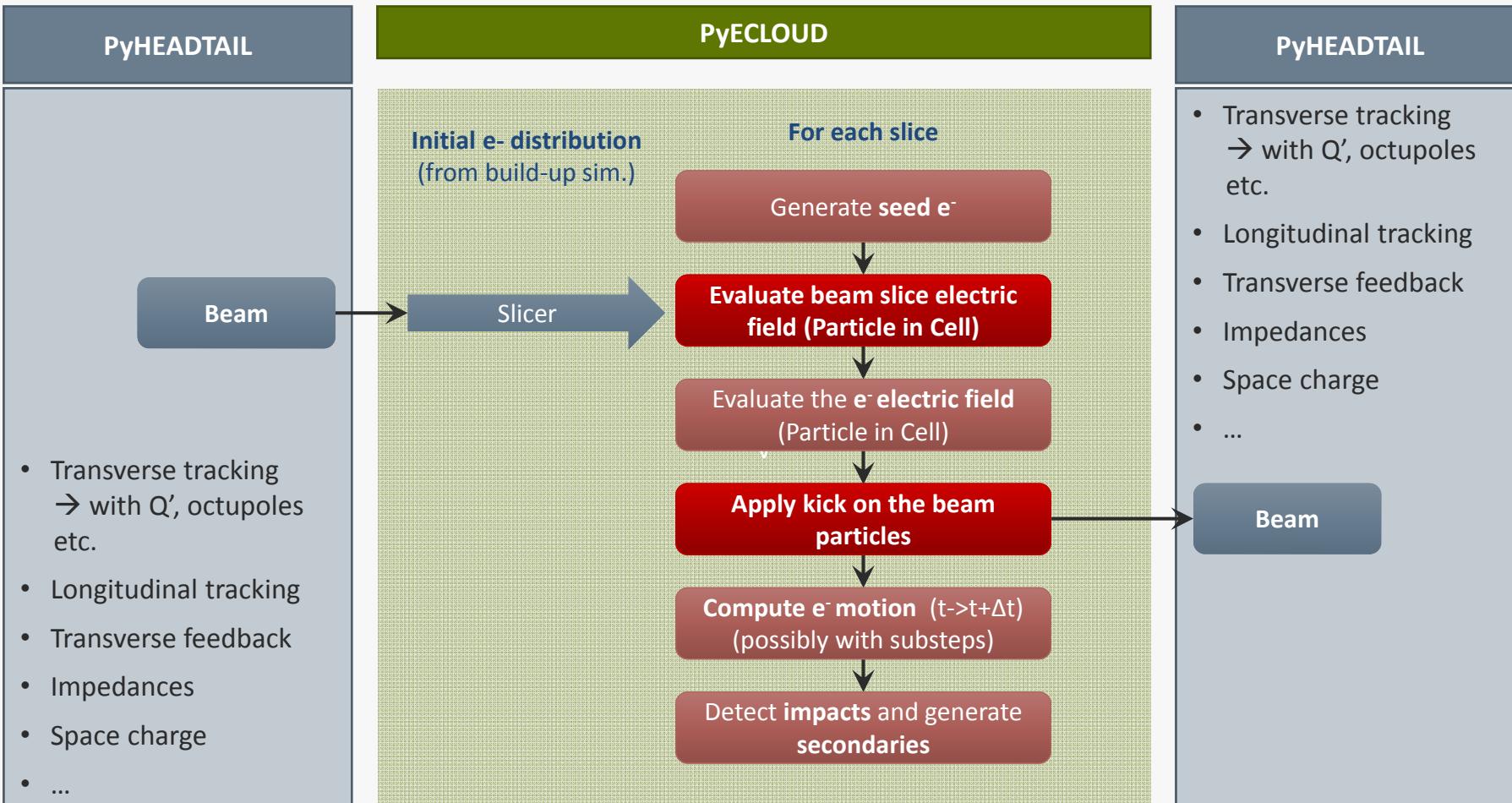
Illustration of a few examples which exploit the architecture and design promoted earlier.

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

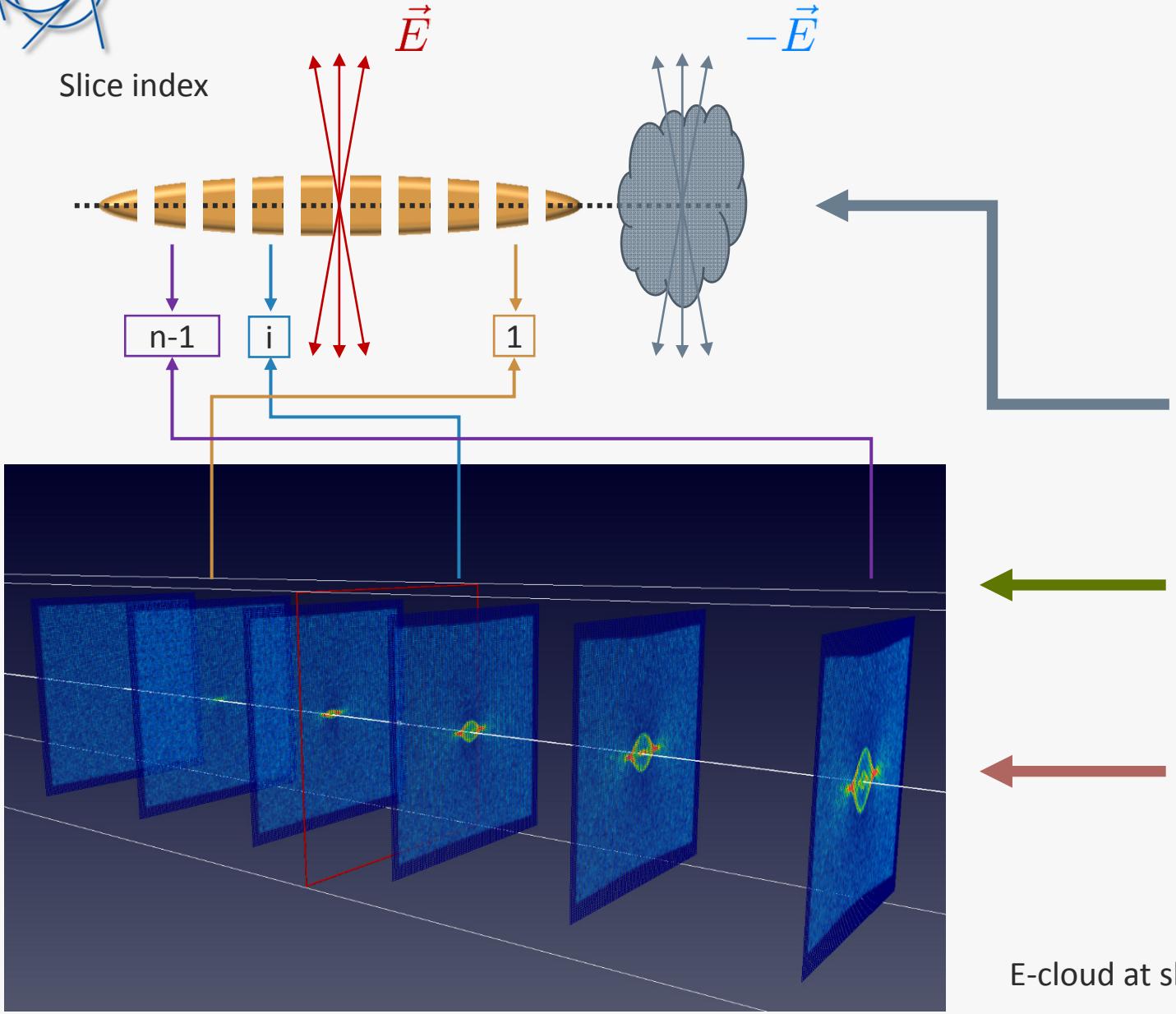
# Interfacing with PyPIC and PyELCOUD

- 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

Courtesy  
Giovanni Iadarola



# E-cloud beam system

## Modules

PyHEADTAIL

beam dynamics

PyECLLOUD

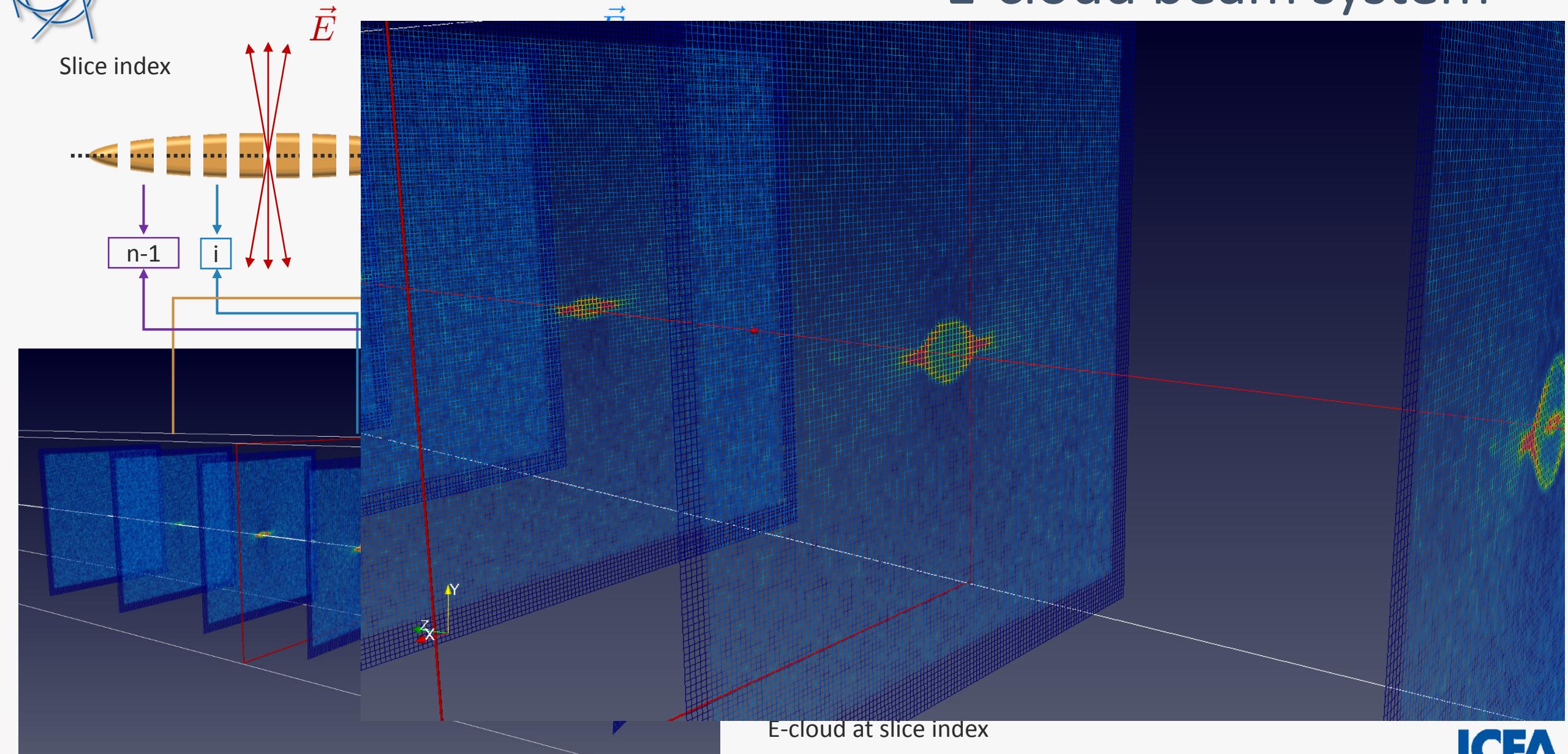
electron build-up  
and dynamics

PyPIC

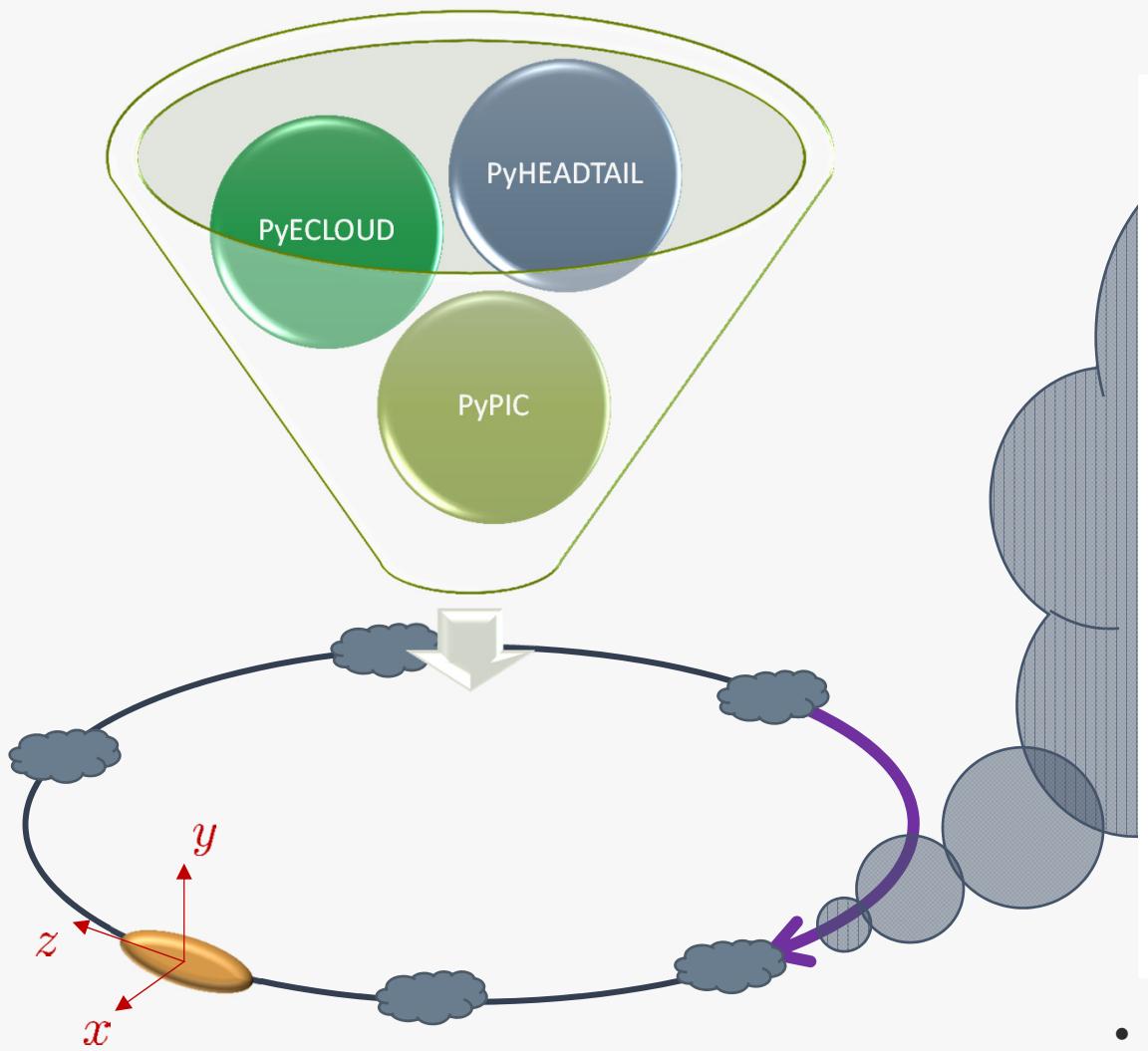
electromagnetic  
field dynamics

## Functions

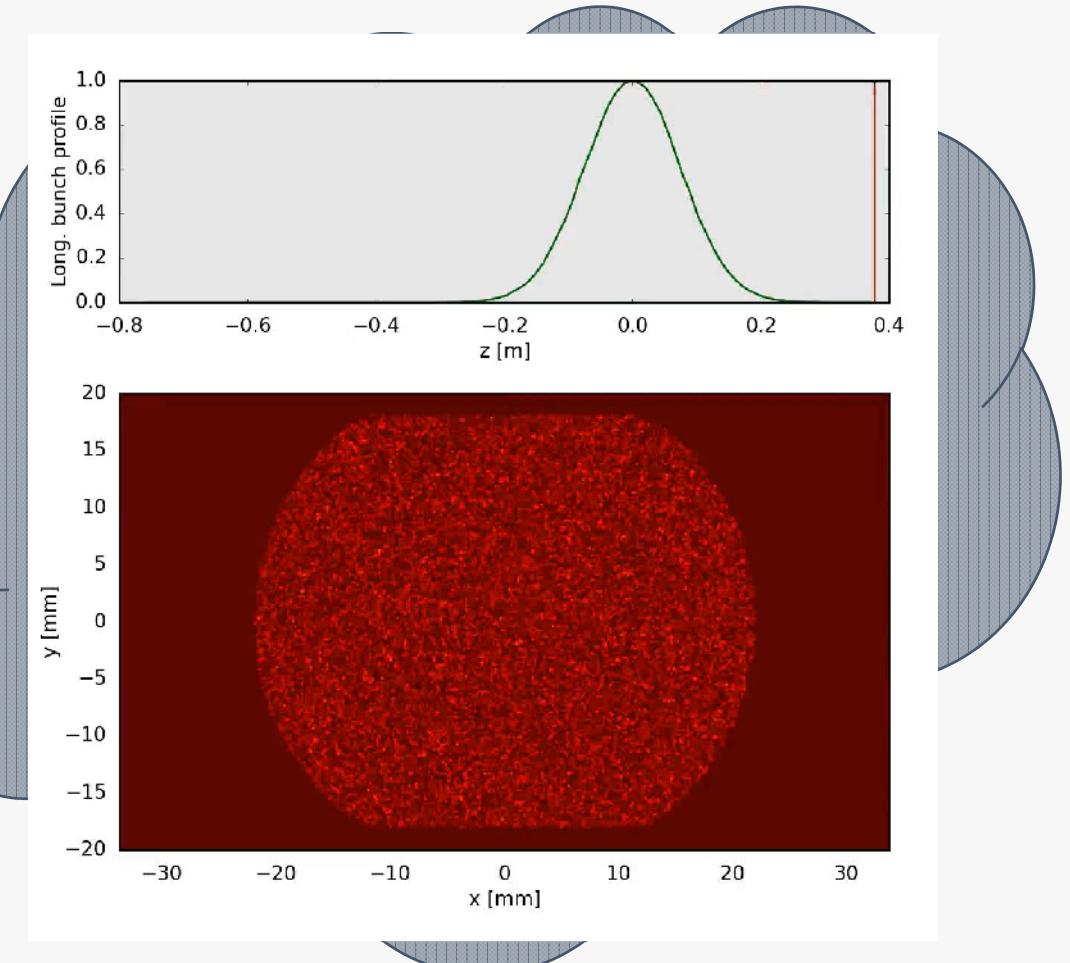
# E-cloud beam system



# Electron clouds in a quadrupole magnet

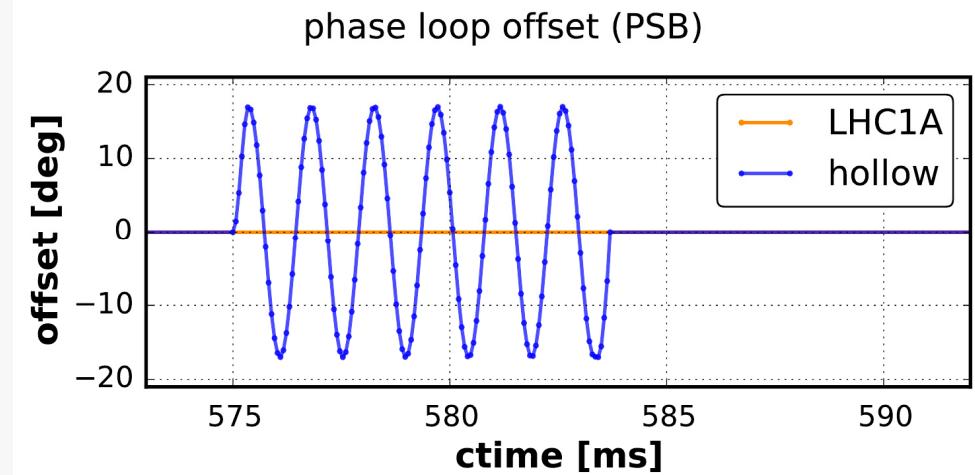
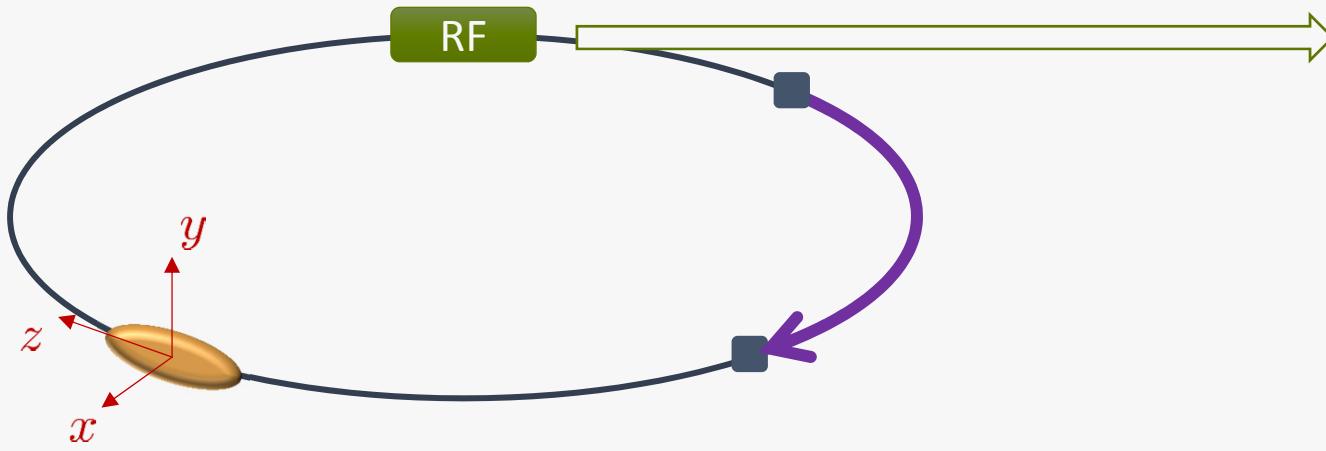


- Two stream collective interaction – much more involved

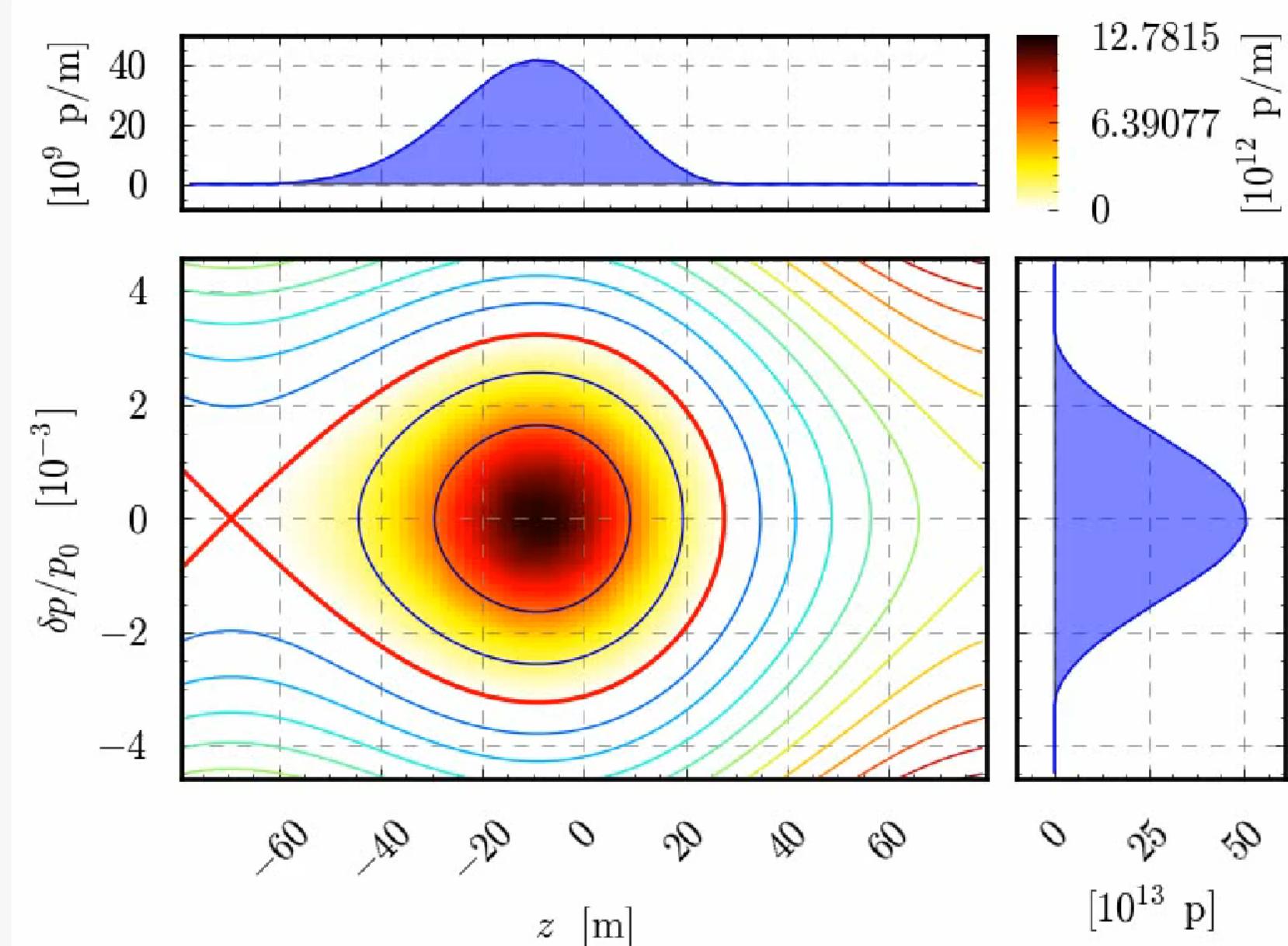


- Beam passage leads to a **pinch of the cloud** which in turn acts back on the beam – differently each turn

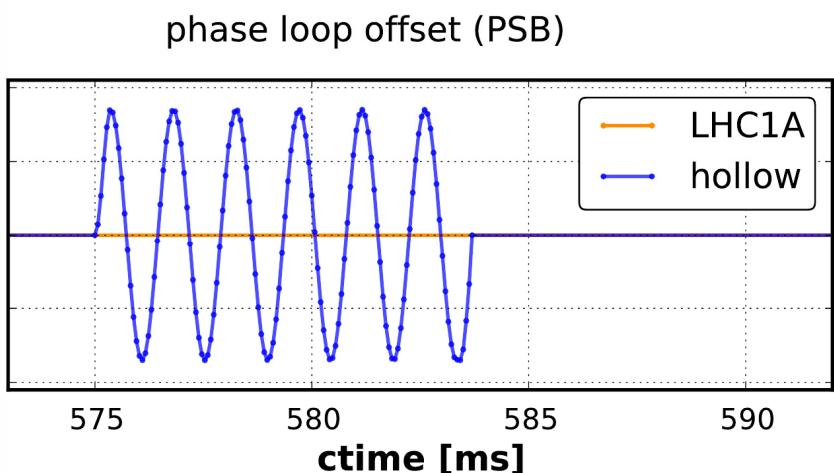
Trim function:  
dynamically change property of RF cavity



# Hollow Bunches

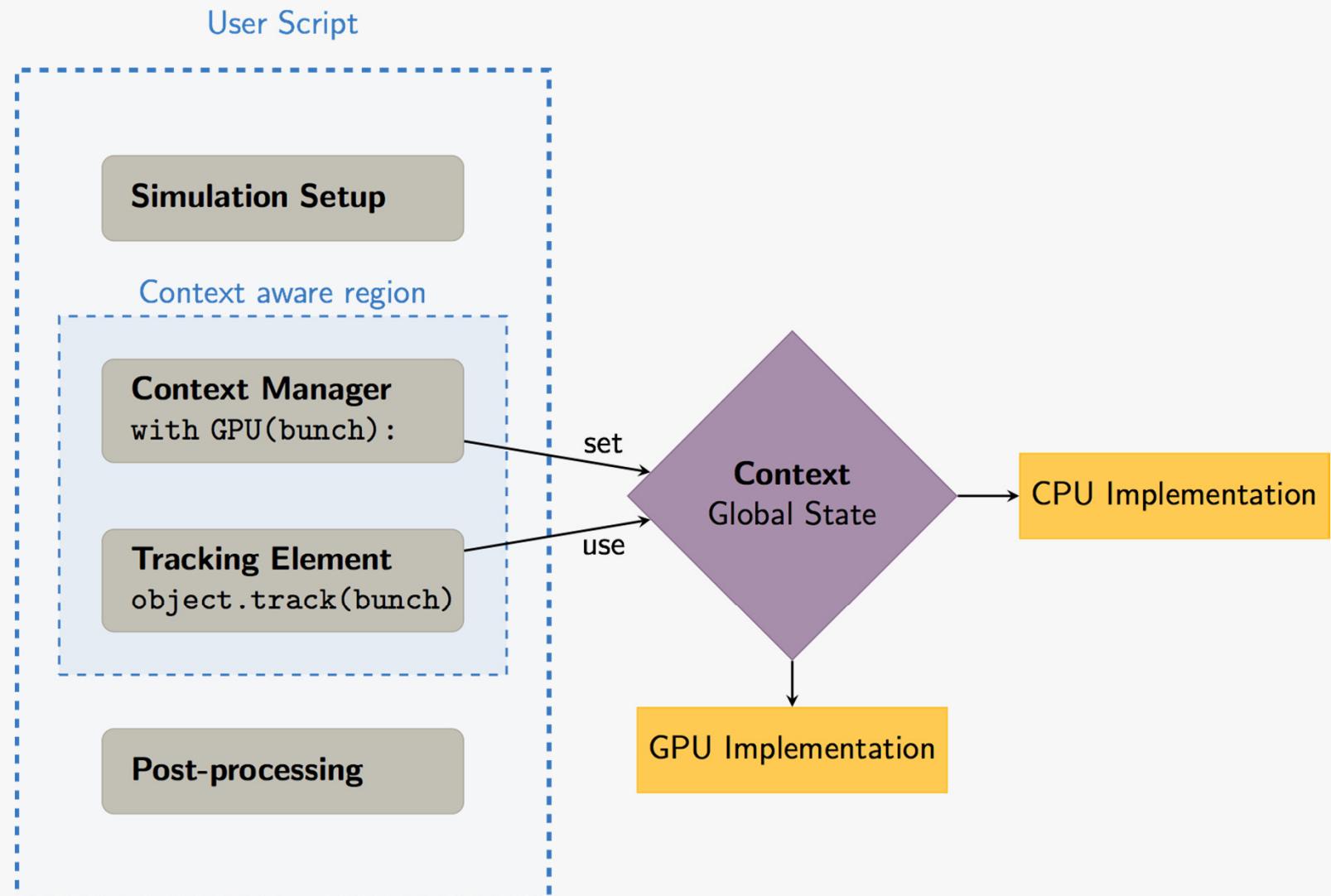


Courtesy Adrian Oeftiger



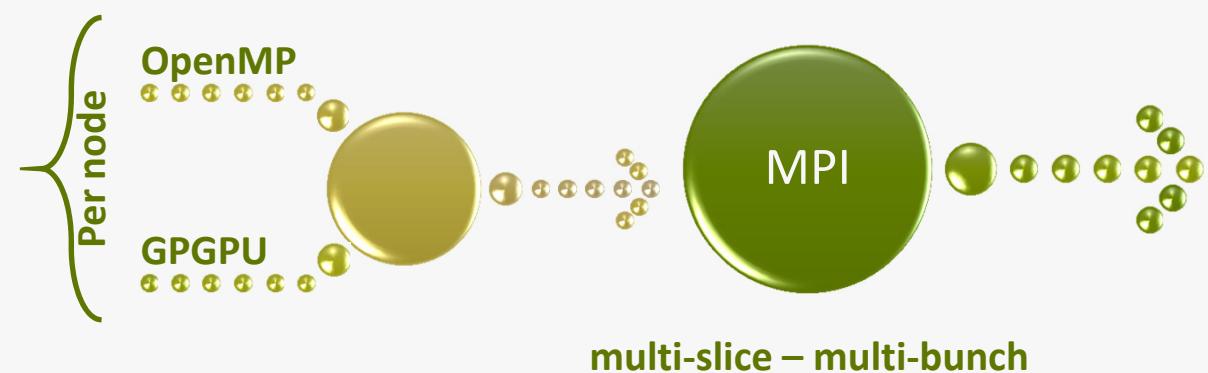
# Context manager for GPU supported functions

1. Setup simulation
2. Set context with context manager
3. Track bunch: correct implementation automatically chosen
4. Move data back to CPU



A user does not need to care about the system internals

- Introduced collective effects and basic model of accelerator-beam systems used for simulations
- Highlighted some requirements for developers of modern computer simulation codes
- Highlighted the importance of performance and possibilities for improvement
- Showed some examples and applications
- Did not go into parallelisation techniques which **for collective effects become challenging**
- Parallelisation strategy would be to exploit all technics using a **hybrid approach**:



# BACKUP

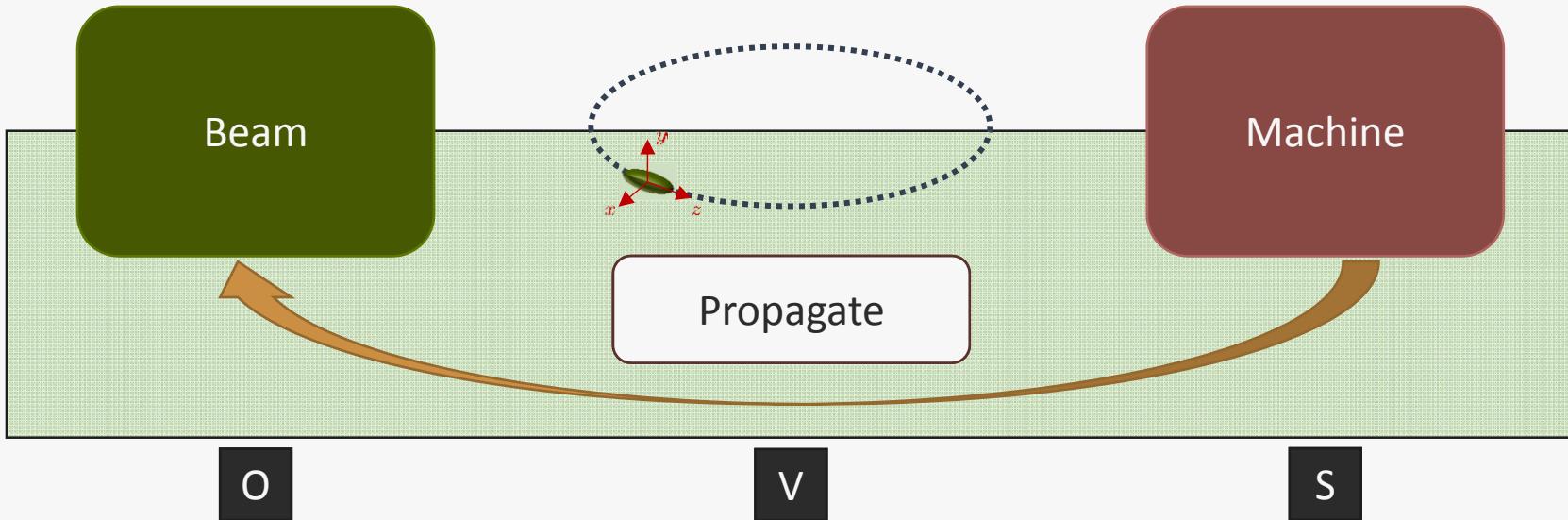
BACKUP

## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

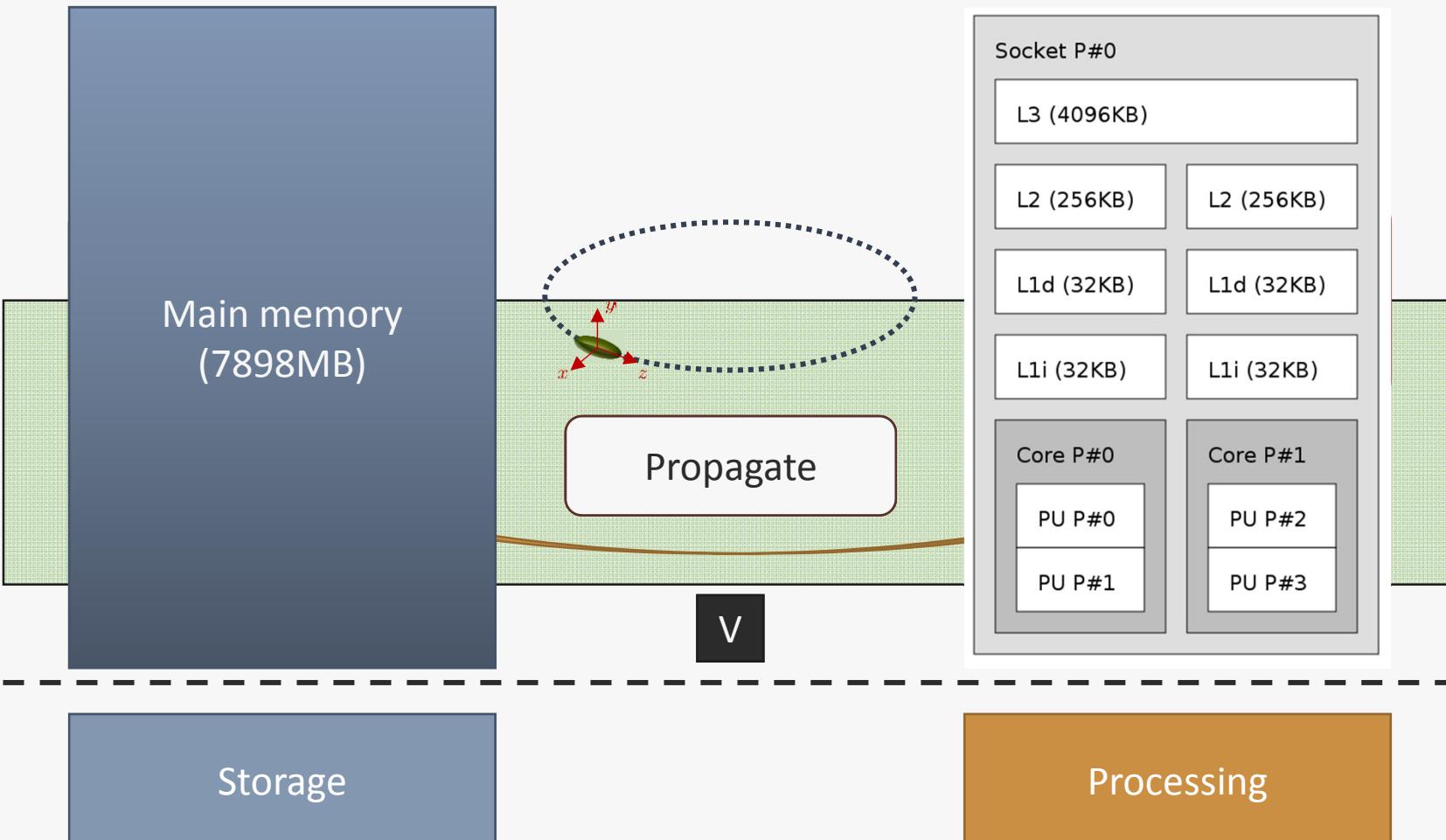
# Mapping accelerator-beam to computer system

- Possible program layout



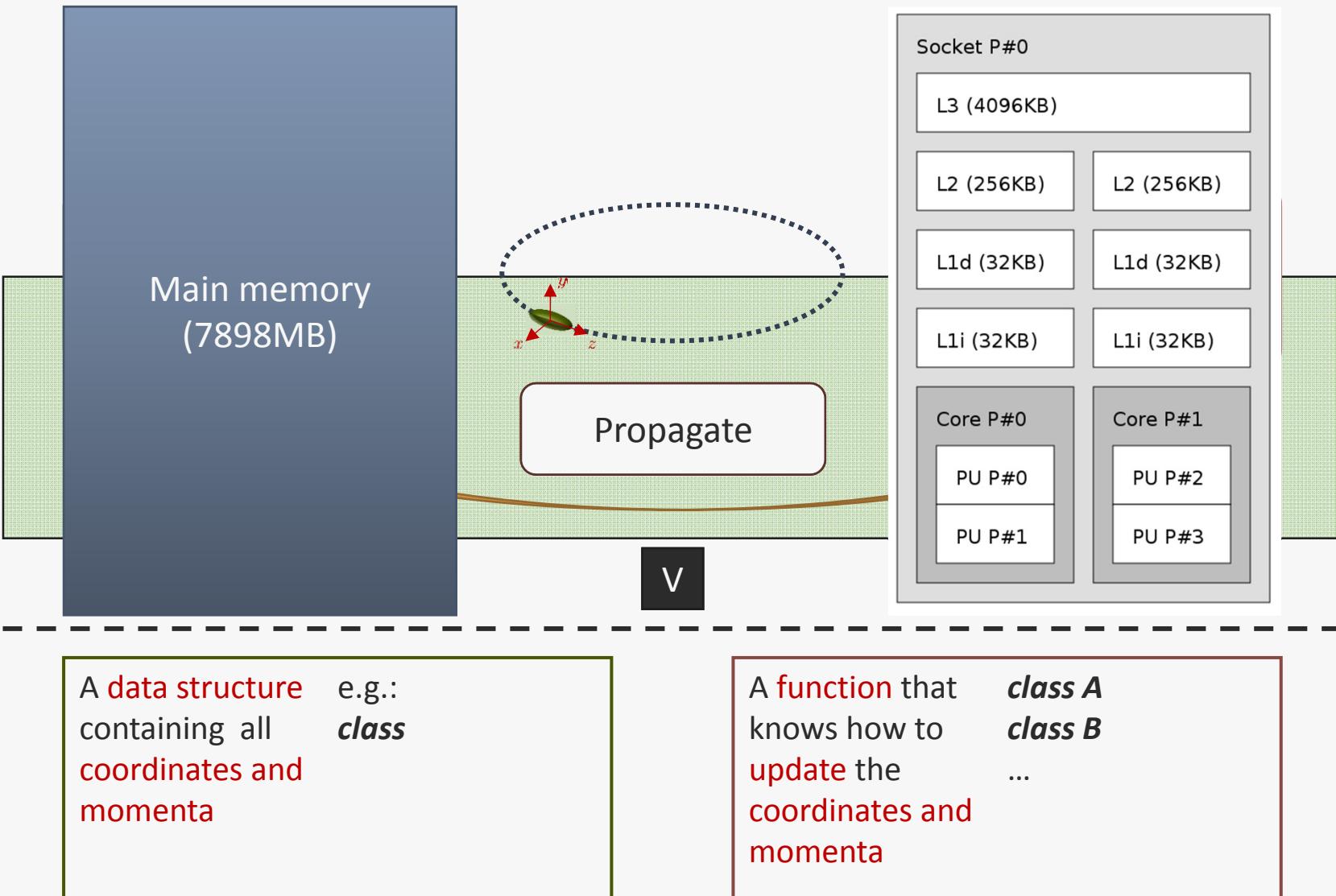
# Mapping accelerator-beam to computer system

- Possible program layout



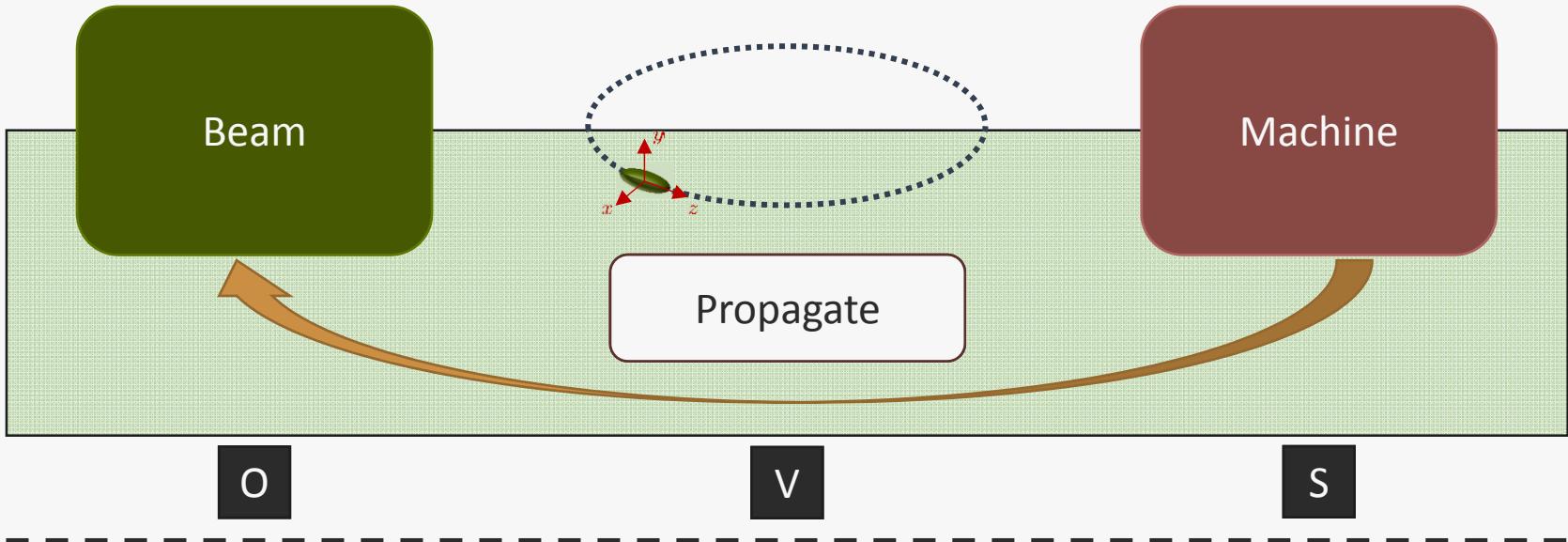
# Mapping accelerator-beam to computer system

- Possible program layout



# Mapping accelerator-beam to computer system

- Possible program layout

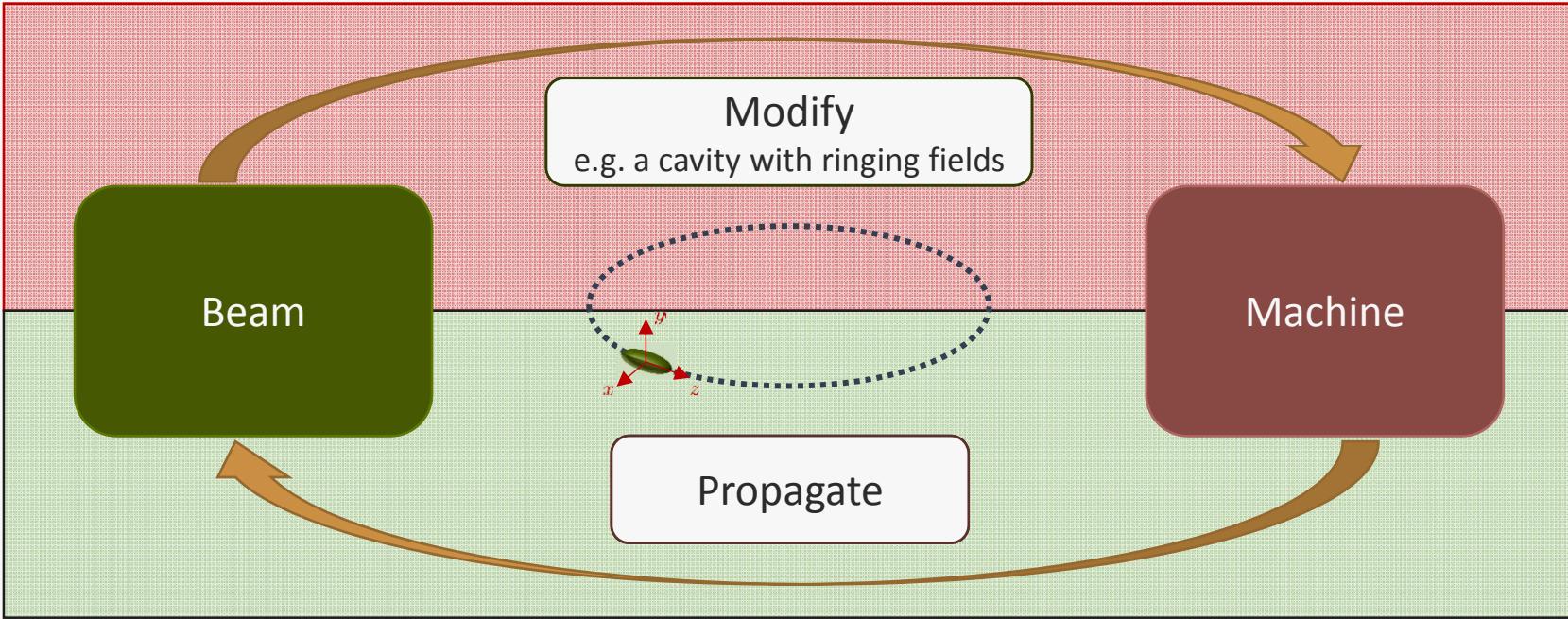


A **data structure** e.g.:  
containing all **class**  
coordinates and  
momenta

A **function** that **class A**  
knows how to **class B**  
**update** the ...  
coordinates and  
momenta

# Mapping accelerator-beam to computer system

- Possible program layout



S

V

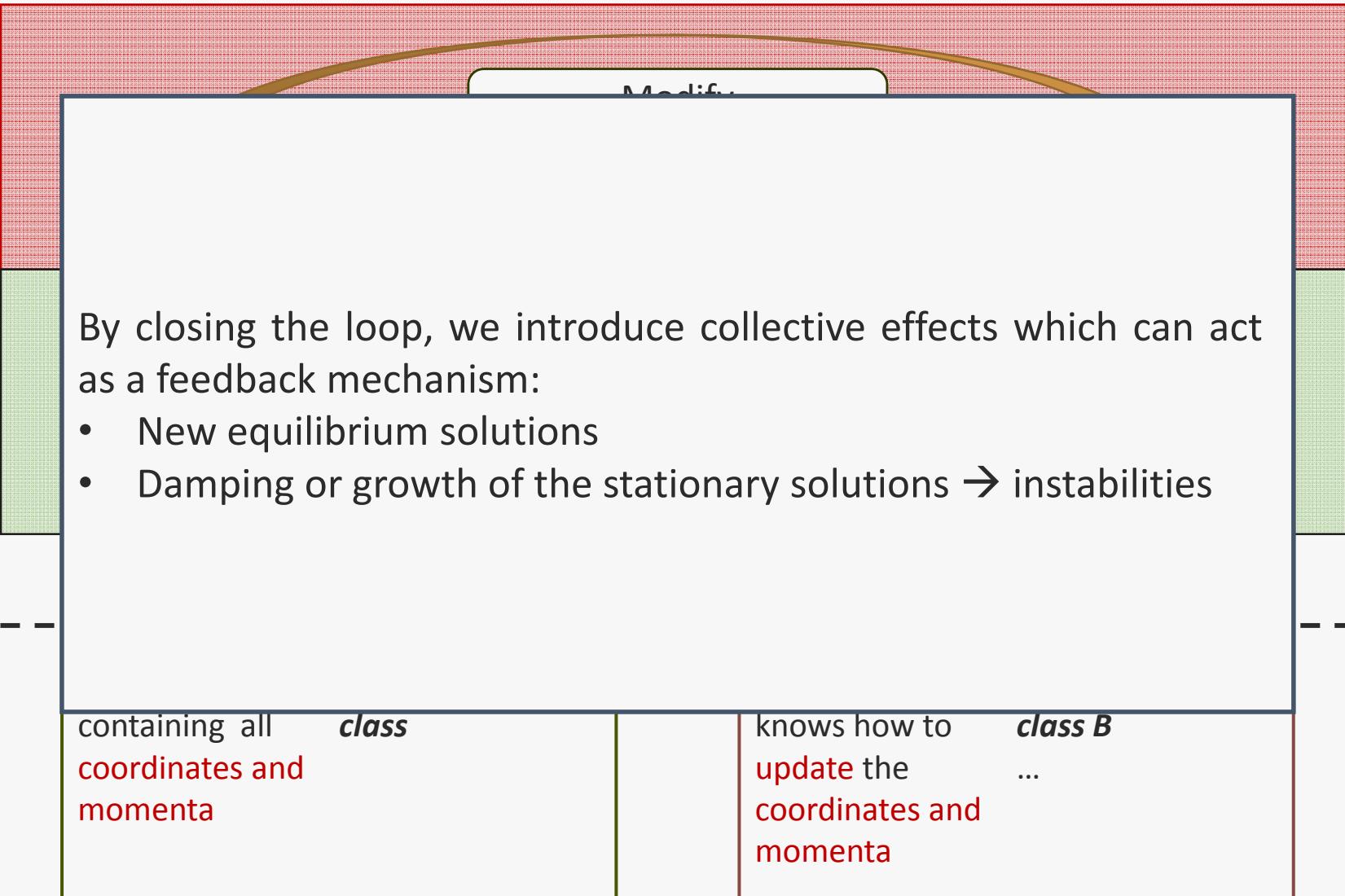
O

A **data structure** e.g.:  
containing all **class**  
coordinates and  
momenta

A **function** that **class A**  
knows how to **class B**  
**update** the ...  
coordinates and  
momenta

# Mapping accelerator-beam to computer system

- Possible program layout



## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

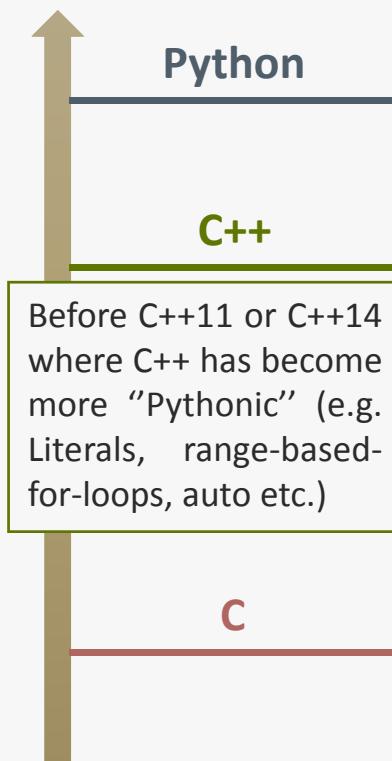
- We work today with **rapidly changing simulation** demands – this requires frequent and rapid code development which should preferably be **close to physics** rather than **close to the hardware**.

### Abstraction (example)



- We work today with **rapidly changing simulation** demands – this requires frequent and rapid code development which should preferably be **close to physics** rather than **close to the hardware**.

### Abstraction (example)



Python is an object oriented **script language** while C++ is an object oriented **compiling language**.

Python code is ... often **5-10 times shorter** than equivalent C++ code! Anecdotal evidence suggests that one Python programmer can finish in two months what two C++ programmers can't complete in a year.

Classical  
rigid

Boilerplate code

Rather static code basis

Edit, compile,  
debug – cycle

Highly  
dynamic

Interactive testing  
and deployment

Incremental  
development

Fast prototyping

- We work today with **rapidly changing simulation** demands – this requires frequent and rapid code development which should preferably be **close to physics** rather than **close to the hardware**.

### Abstraction (example)

An important hitch remains on the **FAST** requirement:

*“Python was not made to be fast... ... but to make developers fast.”*

*Writing faster Python,  
Sebastian Witowski*

Being an interpreted language, strongly but dynamically typed, **Python can be slow in execution!** This needs to be handled.

- We work today with **rapidly changing simulation** demands – this requires frequent and rapid code development which should preferably be **close to physics** rather than **close to the hardware**.

**Abstraction**

An implementation of the crawler example in Java and Python.

**Coding. Crawler**

**Java**

```
public class CrawlerExample {
    public static void main(String[] args) throws IOException {
        PrintWriter textfile = null;
        try {
            textfile = new PrintWriter("result.txt");
            System.out.println("Enter the URL you wish to crawl..");
            System.out.print("> ");
            String myUrl = new Scanner(System.in).nextLine();

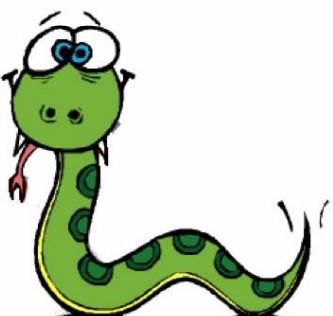
            String response = getContentByUrl(myUrl);

            Matcher matcher = Pattern.compile("href=['\"][^'\"]+['\"]").matcher(response);
            while (matcher.find()) {
                String url = matcher.group(1);
                System.out.println(url);
                textfile.println(url);
            }
        } finally {
            if(textfile != null) {
                textfile.close();
            }
        }
    }

    private static String getContentByUrl(String myUrl)
        throws IOException {
        URL url = new URL(myUrl);
        URLConnection urlConnection = url.openConnection();
        BufferedReader in = null;
        StringBuilder response = new StringBuilder();
        try {
            in = new BufferedReader(new InputStreamReader(
                urlConnection.getInputStream()));
            String inputLine;
            while ((inputLine = in.readLine()) != null) {
                response.append(inputLine);
            }
        } finally {
            if(in != null) {
                in.close();
            }
        }
        return response.toString();
    }
}
```

**Python**

```
if __name__ == '__main__':
    with open("result.txt", "wt") as textFile:
        print("Enter the URL you wish to crawl..")
        myUrl = input("> ")
        for i in re.findall("href=['\"][^'\"]+['\"]", myUrl):
            urllib.request.urlopen(myUrl).read().decode(), re.I):
                print(i)
                textFile.write(i+'\n')
```



**Being fast**  
be slow

Python, /itowski

on can

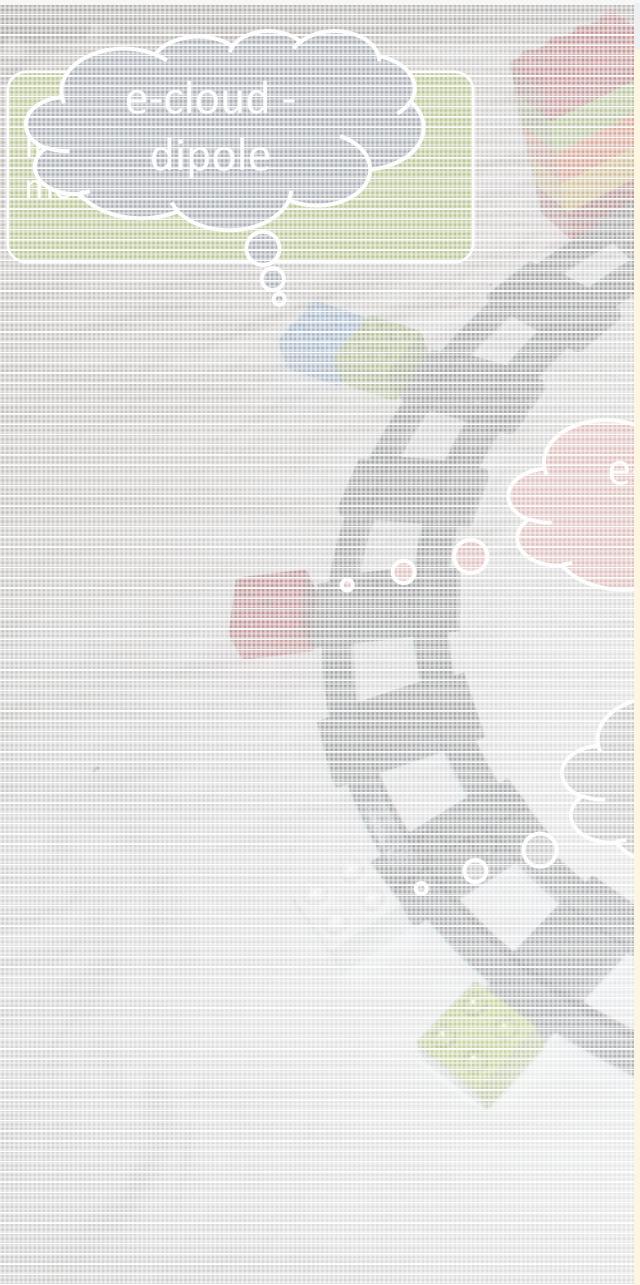
ng

ICFA

06/06/2016

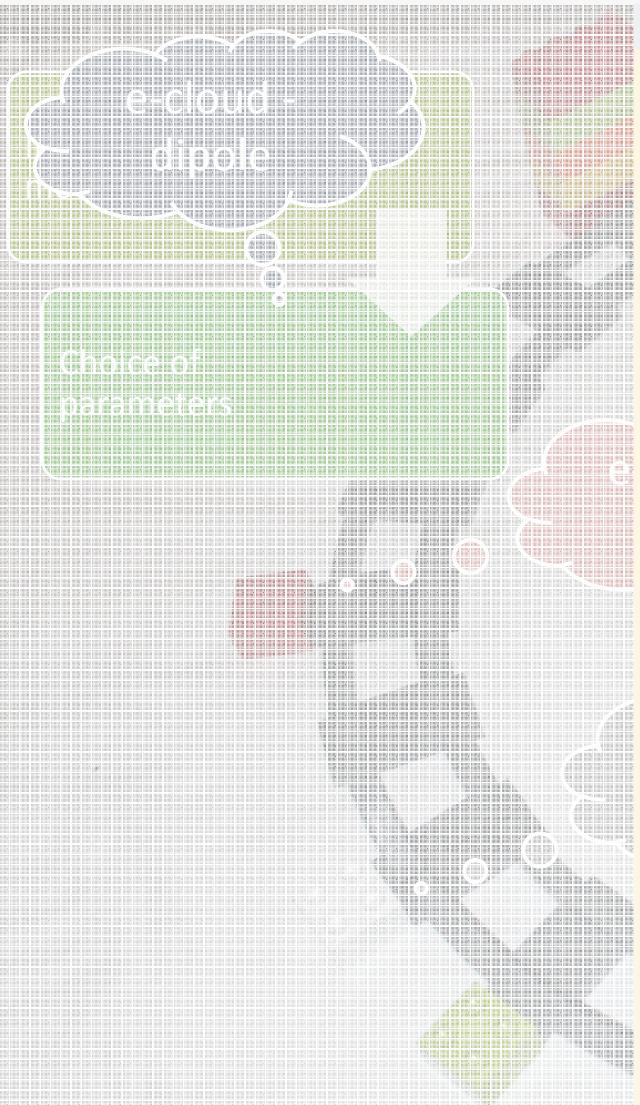
60/40

# Building the simulation



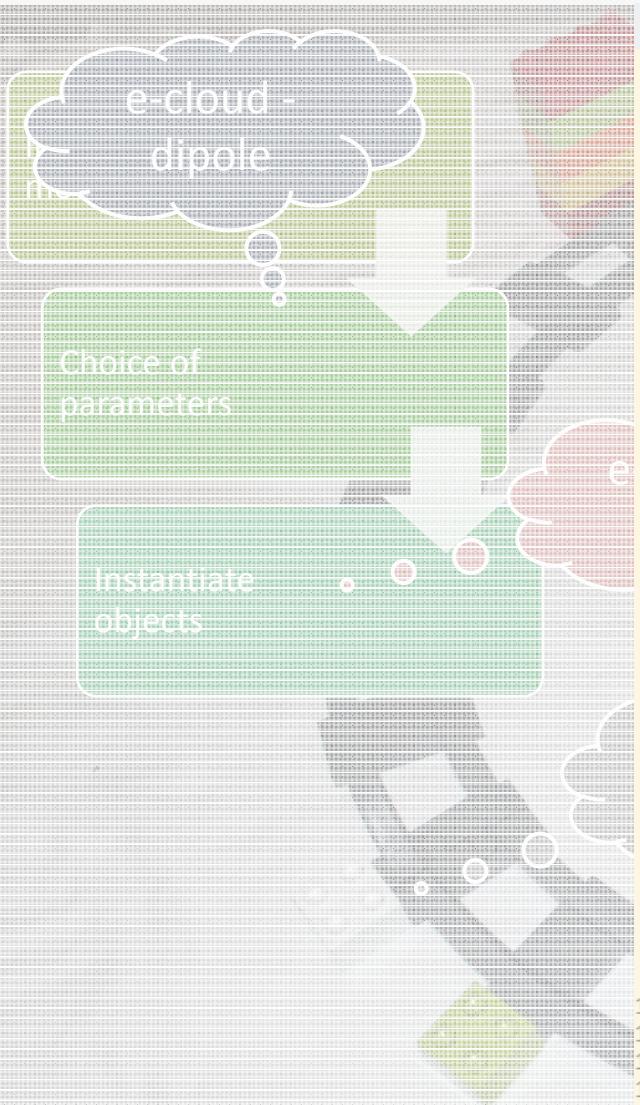
```
File Edit Options Buffers Tools Python Virtual Envs Elpy YASnippet Help
1 from __future__ import division
2
3 import time
4 import numpy as np
5 import seaborn as sns
6 import matplotlib.pyplot as plt
7 from scipy.constants import c, e, m_p
8
9 from PyHEADTAIL.trackers.rf_bucket import RFBucket
10 from PyHEADTAIL.particles.generators import ParticleGenerator
11 from PyHEADTAIL.particles.generators import gaussian2D, RF_bucket_distribution
12
13 from PyHEADTAIL.trackers.transverse_tracking import TransverseMap
14 from PyHEADTAIL.trackers.detuners import Chromaticity, AmplitudeDetuning
15
16 from PyHEADTAIL.trackers.simple_long_tracking import RFSystems
17
18 from PyHEADTAIL.particles.slicing import UniformBinSlicer
19 from PyHEADTAIL.impedances.wakes import CircularResonator, WakeField
20
21 from PyHEADTAIL.feedback.transverse_damper import TransverseDamper
22
23 from PyHEADTAIL.monitors.monitors import BunchMonitor, SliceMonitor
24
25
26 plt.switch_backend('TkAgg')
27 sns.set_context('talk', font_scale=1.5,
28                 rc={'lines.markeredgewidth': 1})
29 sns.set_style('darkgrid', {
30     'axes.linewidth': 2,
31     'legend.fancybox': True})
32
33
34 # PARAMETERS
35 # =====
36 p0 = 7000e9 * e/c
37 E0 = p0*c
38 gamma = np.sqrt((p0/(m_p*c))**2 + 1)
39 beta = np.sqrt(1 - gamma**-2)
40 betagamma = np.sqrt(gamma**2 - 1)
41
42 C = 26658.883
43 R = C/(2*np.pi)
44 T0 = C/(beta*c)
45 omega0 = 2*np.pi/T0
```

# Building the simulation



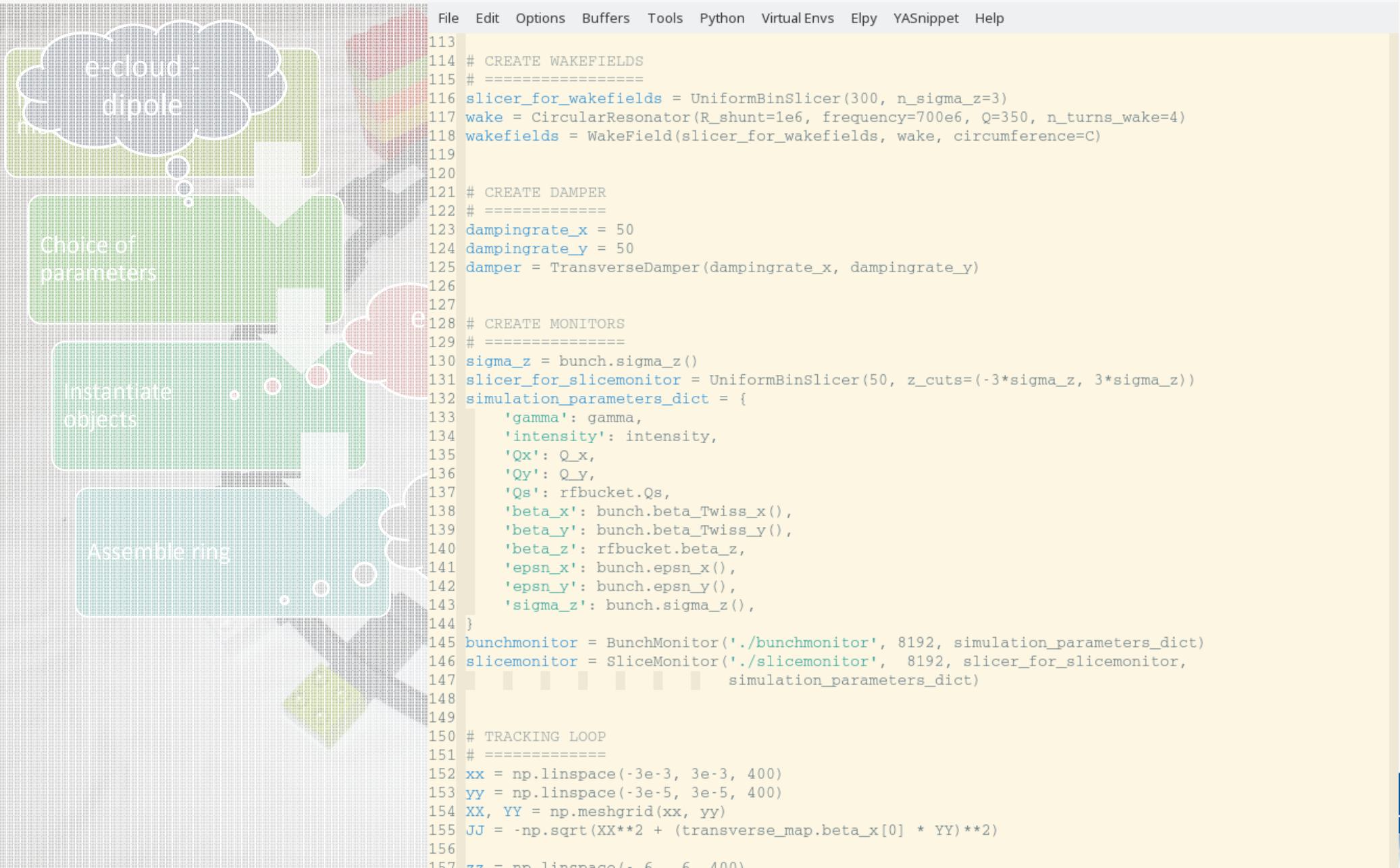
```
File Edit Options Buffers Tools Python Virtual Envs Elpy YASnippet Help
33
34 # PARAMETERS
35 # =====
36 p0 = 7000e9 * e/c
37 E0 = p0*c
38 gamma = np.sqrt((p0/(m_p*c))**2 + 1)
39 beta = np.sqrt(1 - gamma**-2)
40 betagamma = np.sqrt(gamma**2 - 1)
41
42 c = 26658.883
43 R = c/(2*np.pi)
44 T0 = c/(beta*c)
45 omega0 = 2*np.pi/T0
46 alpha = 53.86**-2
47 eta = alpha - gamma**-2
48
49 V_RF = [16e6, 0*8e6]
50 h_RF = [35640, 71280]
51 dphi_RF = [0, 0*np.pi]
52
53 macroparticlenumber = 50000
54 intensity = 1.3e11
55 epsn_x = 2.2e-6
56 epsn_y = 2.2e-6
57 epsn_z = 2.5
58
59 Q_x = 62.31
60 Q_y = 60.32
61 Qp_x = 0
62 Qp_y = 0
63 beta_x = R/Q_x
64 beta_y = R/Q_y
65
66
67 # PARTICLE DISTRIBUTION
68 # =====
69 rfbucket = RFBucket(
70     circumference=C, charge=e, mass=m_p, gamma=gamma,
71     alpha_array=[alpha], p_increment=0,
72     harmonic_list=h_RF, voltage_list=V_RF, phi_offset_list=dphi_RF)
73
74 bunch = ParticleGenerator(
75     macroparticlenumber=macroparticlenumber, intensity=intensity,
76     charge=e, mass=m_p, gamma=gamma, circumference=C,
77     distribution_x=gaussian2D(sigma_x/betagamma), beta_x=beta_x,
```

# Building the simulation

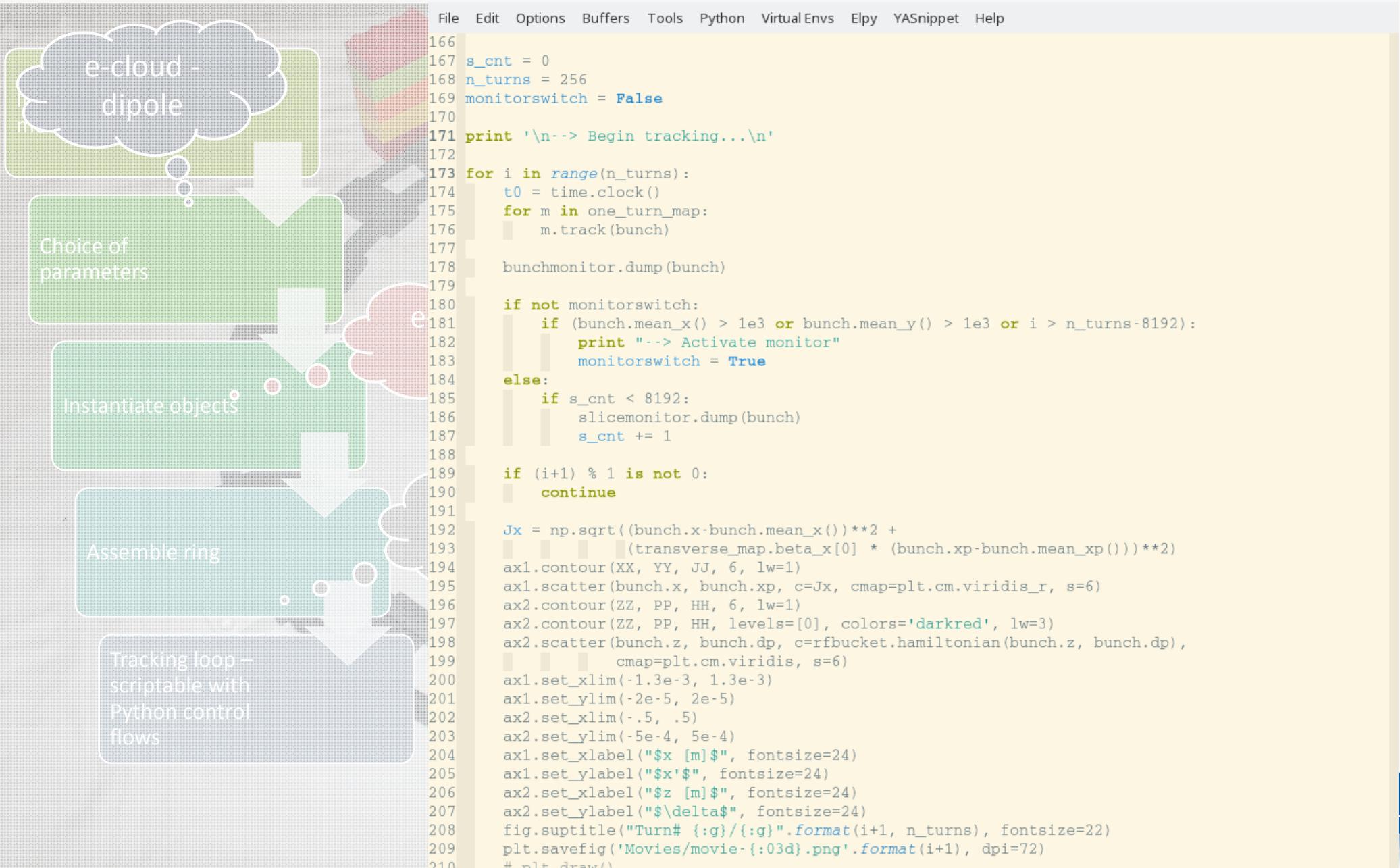


```
File Edit Options Buffers Tools Python Virtual Envs Elpy YASnippet Help
66
67 # PARTICLE DISTRIBUTION
68 # =====
69 rfbucket = RFBucket(
70     circumference=C, charge=e, mass=m_p, gamma=gamma,
71     alpha_array=[alpha], p_increment=0,
72     harmonic_list=h_RF, voltage_list=V_RF, phi_offset_list=dphi_RF)
73
74 bunch = ParticleGenerator(
75     macroparticlenumber=macroparticlenumber, intensity=intensity,
76     charge=e, mass=m_p, gamma=gamma, circumference=C,
77     distribution_x=gaussian2D(epsn_x/betagamma), beta_x=beta_x,
78     distribution_y=gaussian2D(epsn_y/betagamma), beta_y=beta_y,
79     distribution_z=RF_bucket_distribution(rfbucket, epsn_z=epsn_z)).generate()
80 bunch.x += 3.5e-4
81
82
83 # TRANSVERSE MAP
84 # =====
85 n_segments = 3
86
87 s = np.array([i * C/n_segments for i in range(n_segments + 1)])
88 alpha_x = np.zeros(n_segments + 1)
89 beta_x = np.ones(n_segments + 1) * beta_x
90 D_x = np.zeros(n_segments + 1)
91 alpha_y = np.zeros(n_segments + 1)
92 beta_y = np.ones(n_segments + 1) * beta_y
93 D_y = np.zeros(n_segments + 1)
94
95 detuners = [Chromaticity(Qp_x, Qp_y),
96               AmplitudeDetuning(-4e-9, 4e-9, -2e-10)]
97
98 transverse_map = TransverseMap(
99     s=s,
100     alpha_x=alpha_x, beta_x=beta_x, D_x=D_x,
101     alpha_y=alpha_y, beta_y=beta_y, D_y=D_y,
102     accQ_x=Q_x, accQ_y=Q_y,
103     detuners=detuners)
104 one_turn_map = [m for m in transverse_map]
105
106
107 # LONGITUDINAL MAP
108 # =====
109 longitudinal_map = RFSystems(
110     C, h_RF, V_RF, dphi_RF, [alpha], gamma, charge=e, mass=m_p)
```

# Building the simulation



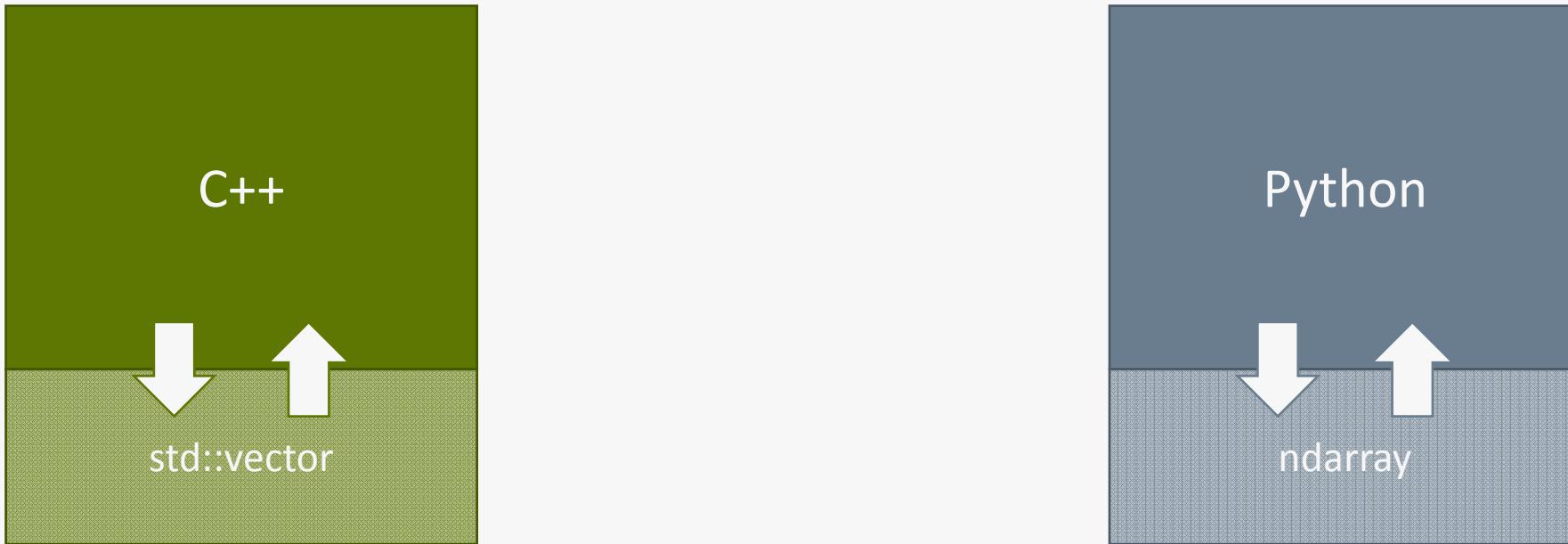
# Building the simulation



## Outline:

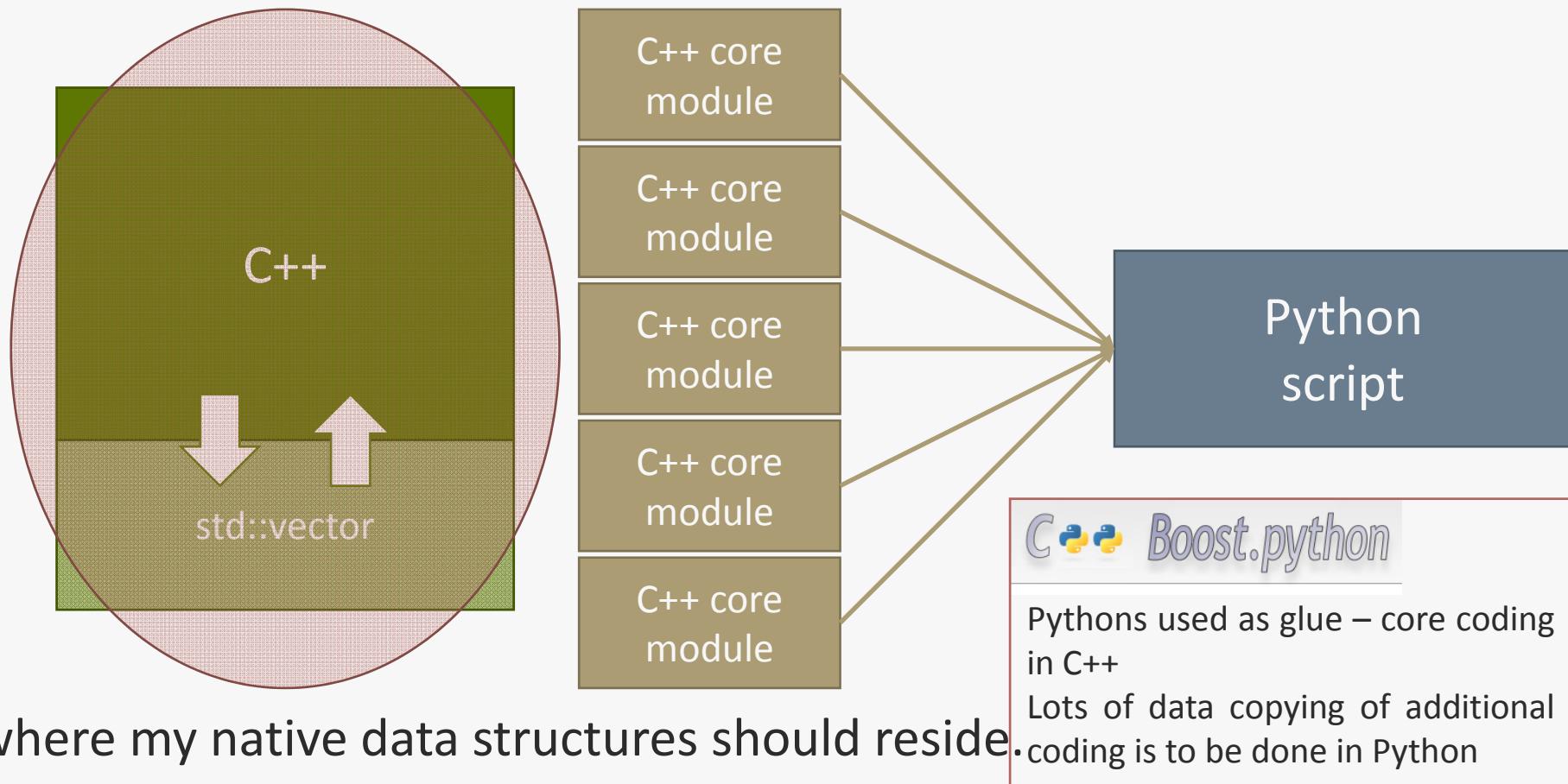
1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. **Performance considerations**
5. Applications, present status and perspectives

Where do I want to spend most of my time coding in – in which world do I want to live?



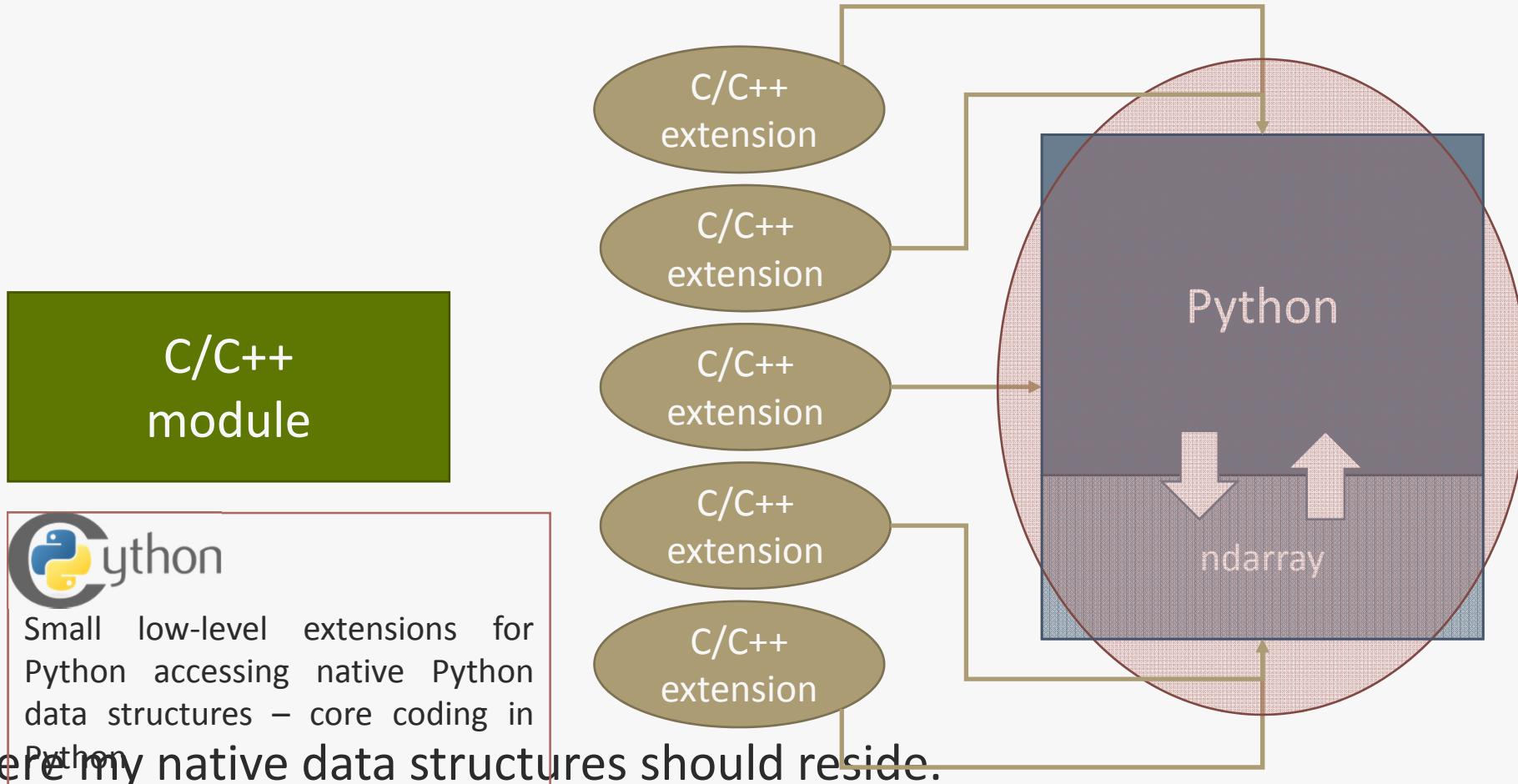
This is where my native data structures should reside.

Where do I want to spend most of my time coding in – in which world do I want to live?



This is where my native data structures should reside.

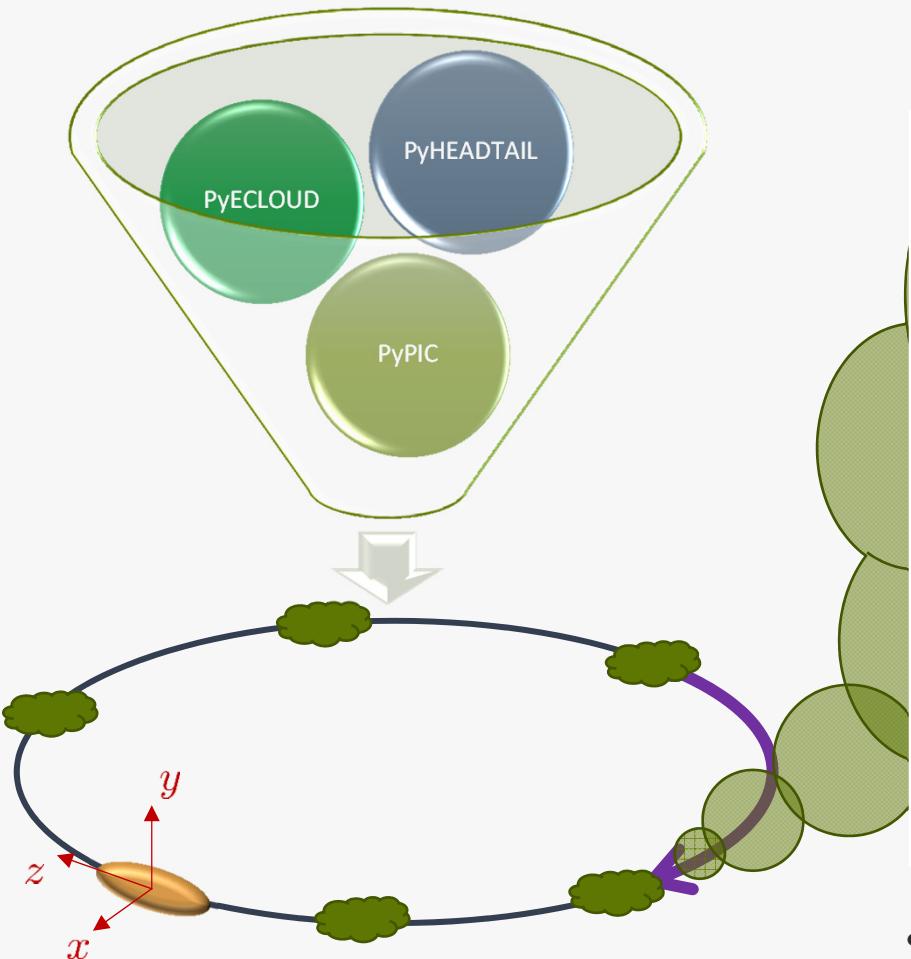
Where do I want to spend most of my time coding in – in which world do I want to live?



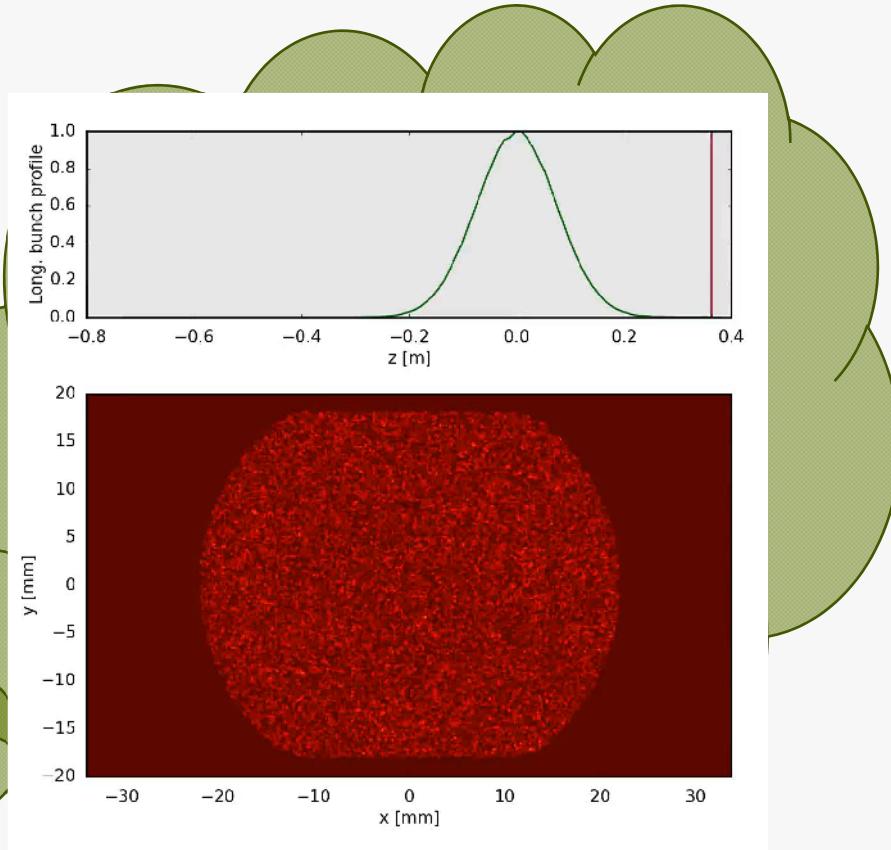
## Outline:

1. Introduction
2. Basic model of the accelerator-beam system
3. Modern approaches and program architectures
4. Performance considerations
5. Applications, present status and perspectives

# Electron clouds in a bending magnet



- 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

# Results: Benchmark Study

Typical application:

LHC@injection instability,  
impedance + transverse damper

CPU Time: ~ 1day  
GPU Time: 5x less

**Two lines of code added to script**

Benchmark for CPU  
**Results agree**

