

# **Xsuite code**

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With contributions from

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A. Oeftiger, M. Schwinzerl, G. Sterbini

https://xsuite.readthedocs.io



#### Introduction to Xsuite

- Motivation
- Requirements
- Design choices
- Architecture
- Development status
- Documentation and developer's resources

- Single-particle tracking
- Collective elements
- Interface to other codes
- Checks and first applications
- Summary

# **Outline**

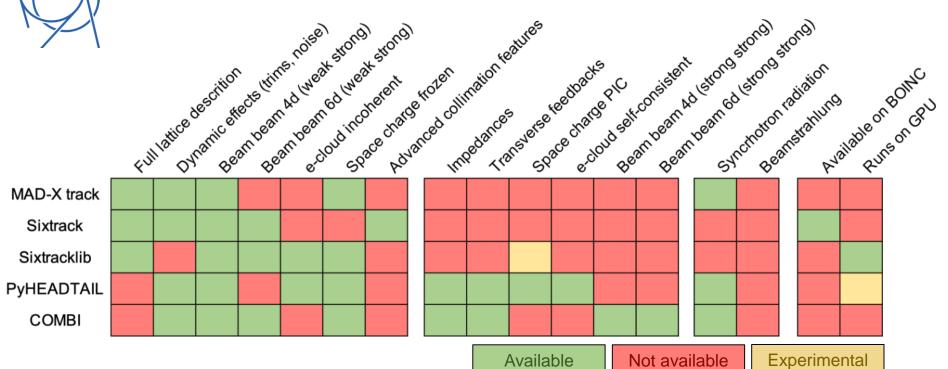


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# CERN-developed multiparticle codes



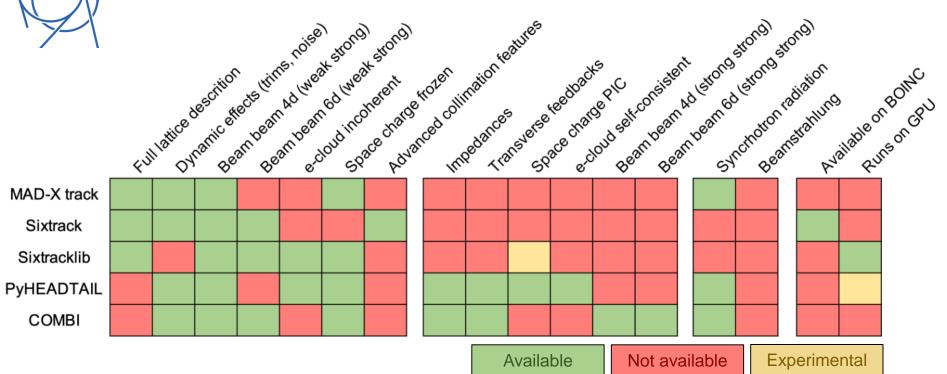
We currently have at least **five CERN-developed multiparticle codes** that are **used in production** studies for CERN synchrotrons (+ need to use PyORBIT-PTC for Particle-In-Cell space charge studies)

#### This has multiple **drawbacks**:

- **Simulation capabilities are limited** (e.g. full-lattice + impedance is not possible)
- Expensive to maintain and further develop (duplicated efforts)
- Long and very specific learning curve for new-comers (know-how is not transferrable)
- Difficult to define a consistent strategy to tackle **future challenges**, FCC-ee, muon collider, PBC<sup>4</sup>

# CERN

# **CERN-developed multiparticle codes**



#### Adapting one of the existing codes to fulfil all the needs would be very difficult

- → Opted to start a **new design (Xsuite) considering all requirements**
- → No need to reinvent the wheel → reused experience from existing codes, notably sixtracklib and pyheadtail

# **Xsuite: requirements**



#### The following main **requirements** were identified:

- Sustainability: development/maintainance compatible with ABP's available manpower and knowhow
  - Favor mainstream technologies (e.g. python) to:
    - profit from existing knowhow in ABP
    - have a short learning curve for newcomers
    - "guarantee" sufficient long life of the code
  - Code simple and slim: introduction of new features should be "student friendly"
- Code should easy and flexible to use (scriptable)
- It should be **easy to interface** with many existing physics tools:
  - MAD-X via cpymad, PyHEADTAIL, pymask, COMBI/PyPLINE, FCC-EPFL framework
- Speed matters
  - Performance should stay in line with Sixtrack on CPU and with Sixtracklib on GPU
- Need to run on CPUs and GPUs from different vendors



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#### Design choice #1:

The code is provided in the form of a set of
 Python packages (Xobjects, Xtrack, Xpart, ...)





#### This has several advantages:

- Profit of ABP know-how and experience with python (OMC tools, pytimber, PyHEADTAIL, PyECLOUD, harpy, lumi modeling and followup tools, ...)
- Newcomers typically have been already exposed to Python + learning-curve is common many tools used in ABP and at CERN for simulation, data analysis, operation...
- Python can be used as glue among Xsuite modules and with several CERN and generalpurpose Python packages (plotting, fft, optimization, data storage, ML, ...)
- Python is easy to extend with C, C++ and FORTRAN code for performance-critical parts

# **Xsuite – Support of GPUs**



#### Support of Graphics Processing Units (GPUs) is a necessary requirement

→ applications like incoherent effects studies of space-charge or e-cloud are feasible only with GPUs

#### Market situation is somewhat complicated

- → there is no accepted standard for GPU programming
- → Different vendors have different languages, frameworks, etc.
- → Picture not expected to change on the short term

#### **Design choice #2**: same code should work on **multiple platforms**

- Usable on conventional CPUs (including multithreading support) and on GPUs from major vendors (NVIDIA, AMD, Intel)
- It is ready to be extended to new standards that are likely to come in the near future

Leveraged on available **open-source packages** for compiling/launching CPU and GPU code **through Python** 









**PyOpenCL** 





#### Xsuite is made of **five python modules**:

- One **low-level module (xobjects)** managing memory and code compilation at runtime on CPUs and GPUs
- Four **physics modules** which interact with the underlying computing platforms (CPU or GPU) through Xobjects

# Physics modules

#### **Xtrack**

single particle tracking engine

#### **Xpart**

generation of particles distributions

#### **Xfields**

computation of EM fields from particle ensembles

#### **Xobjects**

interface to different computing plaforms (CPUs and GPUs of different vendors)

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# **Xsuite development status**



- Several colleagues could already contribute to the development (many thanks!)
  - → Demonstrated **short learning curve for developers**
  - → Greatly helped to achieve a **quick progress of the project** (Xsuite is now being used for first production studies)



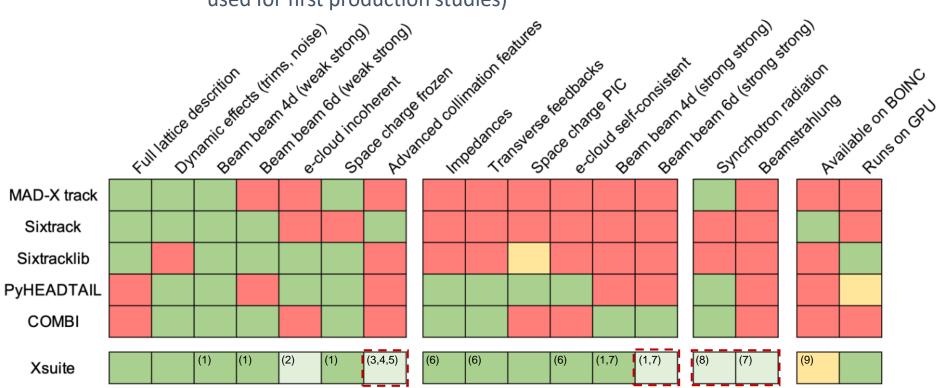
- (1) Uses optimized implementation of Faddeeva function providing x10 speedup on GPU (M.Schwinzerl)
- (2) To be ported from Sixrtacklib (straightforward)
- (3) Electron lens implemented (P. Hermes)
- (4) Geant4 interface working (A. Abramov)
- (5) Porting K2 scattering and Fluka coupling is under development (F. Van Der Veken, P. Hermes)

- (6) Through PyHEADTAIL interface (X. Buffat) Only CPU for now
- (7) Under development (P. Kicsiny, X. Buffat)
- (8) Under development (A. Latina)
- (9) Under study

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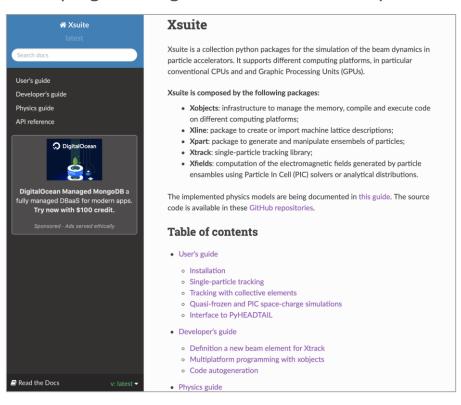


→ Include developments dedicated to **FCC-ee** (EPFL/Chart collaboration)

# User's guide



- Documentation pages available at <a href="https://xsuite.readthedocs.io">https://xsuite.readthedocs.io</a> and <a href="mailto:integrated-by-sets-of-examples">integrated by sets of examples</a> available in the repository
  - → So far **experience was very positive**: users with some python experience were able to get started with little or no tutoring
- Xsuite is intended as an open-source community project:
  - User community is encouraged to contribute
  - Documentation includes developer's guide on how to extend the code
  - Aiming at keeping learning curve for new developers as short as possible



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Simulations are configured and launched with a **Python script** (or Jupyter notebook)

```
import xobjects as xo
import xtrack as xt
import xpart as xp
```

We import the Xsuite modules that we need

```
## Generate a simple beamline
line = xt.Line(
    elements=[xt.Drift(length=1.), xt.Multipole(knl=[0, 1.], ksl=[0,0]),
              xt.Drift(length=1.), xt.Multipole(knl=[0, -1.], ksl=[0,0])],
    element names=['drift 0', 'quad 0', 'drift 1', 'quad 1'])
## Choose a context
context = xo.ContextCpu() # For CPU
## Transfer lattice on context and compile tracking code
tracker = xt.Tracker( context=context, line=line)
## Build particle object on context
n part = 200
import numpy as np
particles = xp.Particles( context=context, p0c=6500e9,
    x=np.random.uniform(-1e-3, 1e-3, n part),
    zeta=np.random.uniform(-1e-2, 1e-2, n_part),
    delta=np.random.uniform(-1e-4, 1e-4, n part))
## Track (saving turn-by-turn data)
tracker.track(particles, num turns=100, turn by turn monitor=True)
## The particle is changed in place and turn-by-turn data is available at:
tracker.record last track.x, tracker.record last track.px # etc...
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We use Xtrack to create a simple sequence (a FODO)

→ can import more complex lattice from MAD-X



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```

We choose the computing platform on which we want to run (CPU or GPU)



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```

We build a tracker object, which can track particles in our beam line on the chosen computing platform



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## Choose a context
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## Build particle object on context
                                                                             We generate a set of
n part = 200
                                                                             I particles (in this case
import numpy as np
                                                                              using a standard
particles = xp.Particles( context=context, p0c=6500e9,
    x=np.random.uniform(-1e-3, 1e-3, n part),
                                                                              python random
    zeta=np.random.uniform(-1e-2, 1e-2, n_part),
                                                                             generator)
    delta=np.random.uniform(-1e-4, 1e-4, n_part))
## Track (saving turn-by-turn data)
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```

## The particle is changed in place and turn-by-turn data is available at:
tracker.record last track.x, tracker.record last track.px # etc...

## Track (saving turn-by-turn data)

We launch the tracking (particles are updated as tracking progresses)



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```

## The particle is changed in place and turn-by-turn data is available at:
tracker.record\_last\_track.x, tracker.record\_last\_track.px # etc...

Access to the recorded particles coordinates



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To run on GPU all we

change the context



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    element names=['drift 0', 'quad 0', 'drift 1', 'quad 1'])
## Choose a context
context = xo.ContextCupy() # For NVIDIA GPUs
## Transfer lattice on context and compile tracking code
tracker = xt.Tracker( context=context, line=line)
## Build particle object on context
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    element names=['drift 0', 'quad 0', 'drift 1', 'quad 1'])
## Choose a context
                                                                              need to do is to
context = xo.ContextPyopencl() # For AMD GPUs and other hardware
## Transfer lattice on context and compile tracking code
tracker = xt.Tracker( context=context, line=line)
## Build particle object on context
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# **Collective beam elements**



Xsuite can handle **collective elements**, i.e. elements for which the action on a particle depends on the coordinates of other particles

→ it means that the tracking of different particles cannot happen asynchronously

No special action is required by the user. Collective elements are handled automatically by the the Xtrack tracker

```
# [Imports, contexts, particles as for single-particle simulations]
## Build a collective element (e.g. space-charge interaction)
import xfields as xf
spcharge = xf.SpaceCharge3D(_context=context, update_on_track=True,
    x_range=(-5e-3, 5e-3), y_range=(-4e-3, 4e-3), z_range=(-4e-3, 4e-3),
    length=1, nx=256, ny=256, nz=100, solver='FFTSolver2p5D')
## Build a simple beamline including the space-charge element
line = xt.Line(
    elements = [xt.Multipole(knl=[0, 1.]), xt.Drift(length=1.),
                spcharge,
                xt.Multipole(knl=[0, -1.]), xt.Drift(length=1.)]
    element names = ['qf1', 'drift1', 'spcharge' 'qd1', 'drift2', '])
## Transfer lattice on context and compile tracking code
## as for single particle simulations
tracker = xt.Tracker( context=context, line=line)
```

A PIC space-charge element is a collective element

# **Collective beam elements**



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## Build a simple beamline including the space-charge element
                                                                               It can be included in a
line = xt.Line(
                                                                               Xtrack line together
    elements = [xt.Multipole(knl=[0, 1.]), xt.Drift(length=1.),
                spcharge,
                                                                                with single-particle
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```

The tracker can be built as seen for single-particle simulations

The tracker takes care of **cutting the sequence** at the collective elements

- Tracking between the collective elements is performed asynchronously (better performance)
- Simulation of collective interactions is performed synchronously

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# Interface to other codes

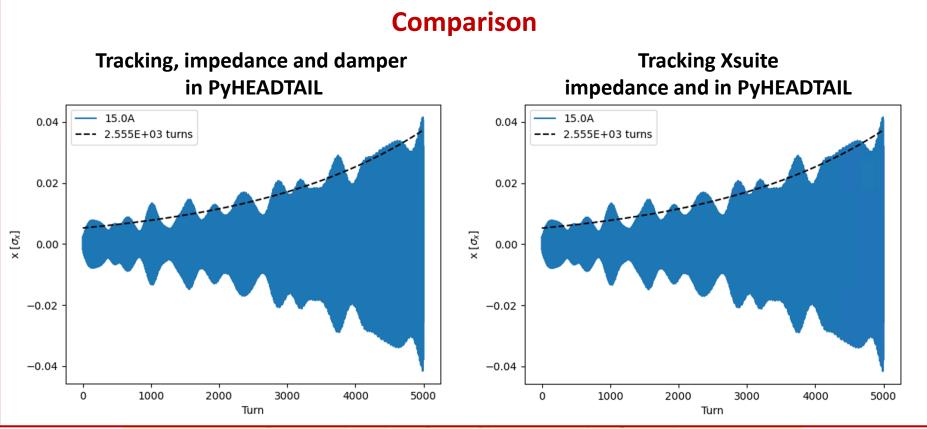


Xsuite is conceived to be interfaced to other Python modules

- Any python object provideing a "el.track(particles)" method can be insterted in a Xsuite lattice (assumes convention on particle coordinates naming and data structure)
- For example PyHEADTAIL can be used to intruduce collective beam elements (impedances, dampers, e-cloud) in Xsuite simulation
  - For this purpose we built a "PyHEADTAIL-compatiblity mode" in Xtrack as PyHEADTAIL uses a slightly different naming convention



X. Buffat



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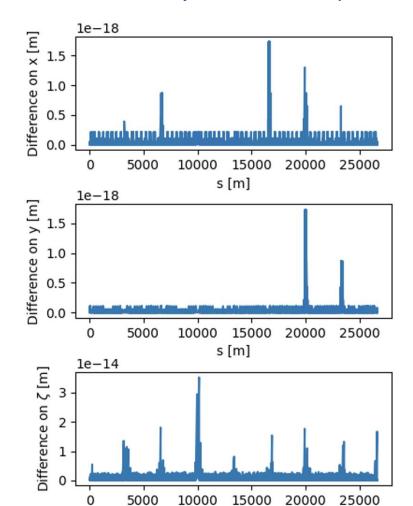
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# Single-particle tracking – benchmarks and performance

- Single-particle tracking has been successfully benchmarked against SixTrack
  - → Checks performed for protons and ions
- Computation time very similar to Sixtrack on CPU and to sixtracklib on GPU



s [m]

Platform	Computing time
CPU	190 (μs/part./turn)
<b>GPU</b> (Titan V, cupy)	0.80 (μs/part./turn)
<b>GPU</b> (Titan V, pyopencl)	0.85 (μs/part./turn)

<sup>(\*)</sup> tests made on ABP GPU server

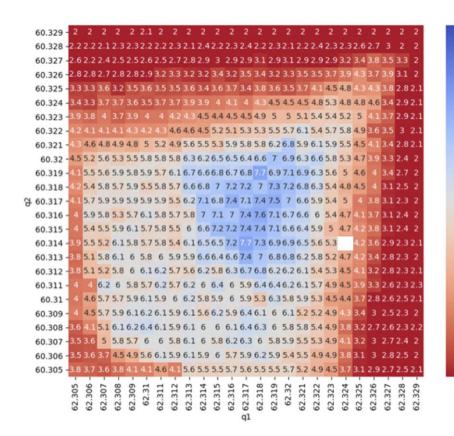


# **HL-LHC Dynamic Aperture scan**

G. Sterbini, K. Paraschou, S. Kostoglou

Example of integration with other Pythonic tools in a complex workflow

- Pymask used to prepare the machine configurations
- Generation of matched particle distribution using python module from pysixtrack
- Job management using a new Python package (TreeMaker)
- Tracking performed with Xsuite (parquet files used for data storage)
- **Dynamic Aperture computation** in Python using **Pandas**



#### Parameters of pilot study

Full HL-LHC lattice (20k elements) Weak strong Beam-beam

N. tune configurations = 625

N. tracked particles/conf. = 1780

N. turns =  $10^6$ 

N. jobs =  $^{\sim}10'000$ 

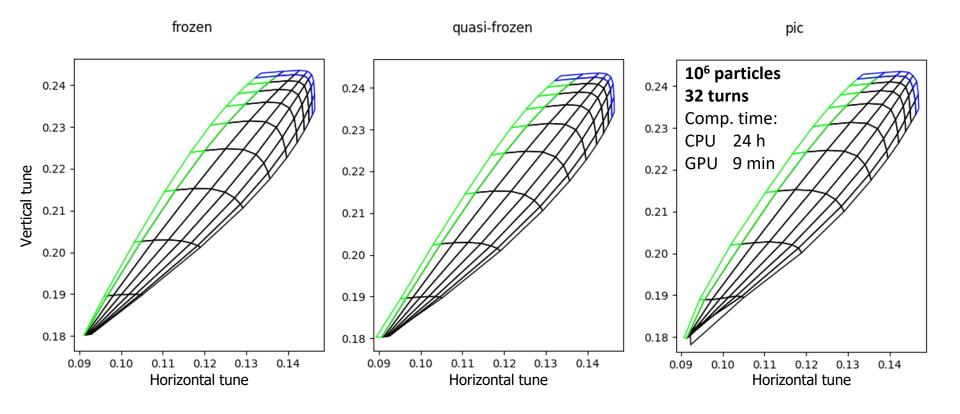
Comp. time ~48h on INFN- CNAF cluster



# **Space-charge – benchmarks and performance**

Xsuite allows **different kinds of space-charge simulations** (frozen, quasi-frozen, Particle In Cell - switching from one to the other is straightforward)

- Tested in the realistic case of the full SPS lattice with 540 space-charge interactions
- Example of application where the usage of GPUs is practically mandatory



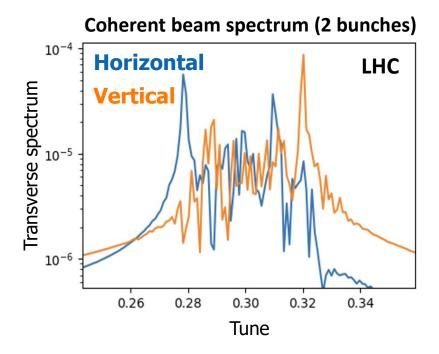




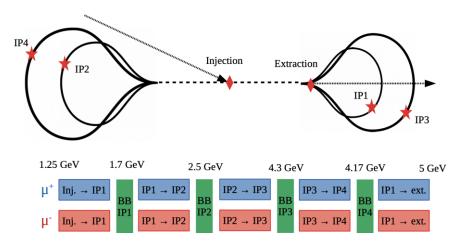
X. Buffat

### Xsuite used to simulate **strong-strong beam beam effects**

- Additional package (PyPLINE) is under development to provides multi-node parallelization and simulate many bunches
  - → Provides two-level parallelization in combination with Xsuite multithreading
- Tested and routinely used on CERN HPC cluster



Xsuite used for first studies on **beam-beam effects** in recirculating linac for **muon collider** 



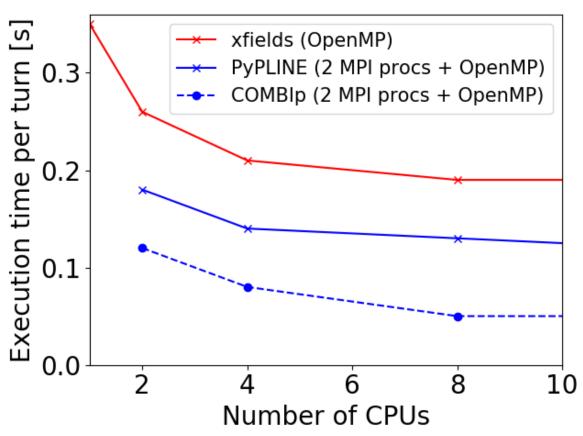




X. Buffat

## Xsuite used to simulate **strong-strong beam beam effects**

- Additional package (PyPLINE) is under development to provides multi-node parallelization and simulate many bunches
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# Performance optimization is ongoing

 Speed getting close to COMBIP (heavily optimized in the past)

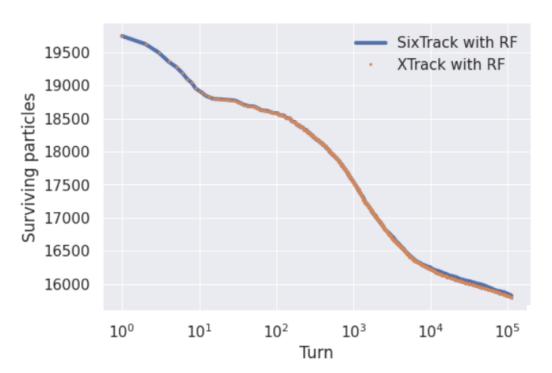
# **Hollow electron lens studies**



P. Hermes

Xsuite is being used to study halo depletion with hollow electron lenses for HL-LHC

- Implemented hollow e-lens in Xtrack
- Benchmarked against Sixtrack
- Performed first realistic studies (parametric scans)
- → Showed significant advantage of using GPUs



## Test run (10 turns)

Setup	Tracking time [s]
SixTrack without K2	40
XTrack without K2 (GPU)	0.3

# Realistic study (parametric scan)

	Simulated time interval	Number of jobs	Time needed*
Xtrack (GPU)	10s	400	~ 24 h
SixTrack	1s	40000	~ 7 days

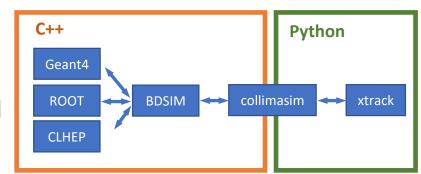
<sup>\*</sup> CPUs and GPUs in HTCondor

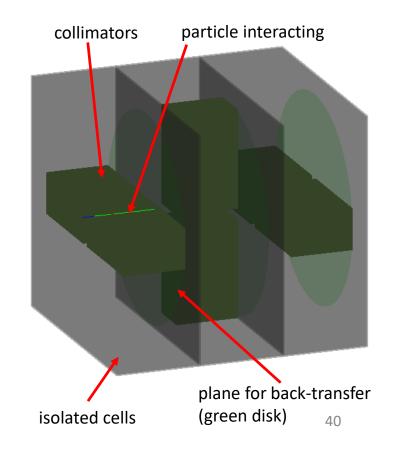
# **Xsuite-Geant4 simulations**

A. Abramov



- - Needed for **FCC-ee collimation studies**
  - Using a C++ framework based on BDSIM (L. Nevay):
    - Geant4 radiation transport model with collimators in individual cells
    - Particles exchanged between the tracking code and the Geant4 model
    - Similar mechanism to the SixTrack-FLUKA coupling
  - Dedicated C++ Python interface implemented (collimasim)
  - The first integration with Xtrack is available:
    - Supports collimator definition, beamline integration, and particle transfer
    - Tests ongoing





# **Outline**



#### Introduction to Xsuite

- Motivation
- Requirements
- Design choices
- Architecture
- Development status
- Documentation and developer's resources

# Usage examples

- Single-particle tracking
- Collective elements
- Interface to other codes
- Checks and first applications
- Final remarks and summary



# And the ecosystem is growing...

Already a few **spin-offs** from the community (some at early stages):

- PyPLINE: multilevel parallelization for strong-strong beam beam simulations)
- Xdeps: equivalent of MAD-X deferred expressions in python
- Xsequence: sequence manager for different codes (including knobs via xdeps), smart slicing, etc. (driven by EPFL collaborators for FCC-ee dev. efforts)
- **Xcollimation:** setup and post-processing of collimation simulations

Physics modules

#### **Xtrack**

single particle tracking engine

#### **Xpart**

generation of particles distributions

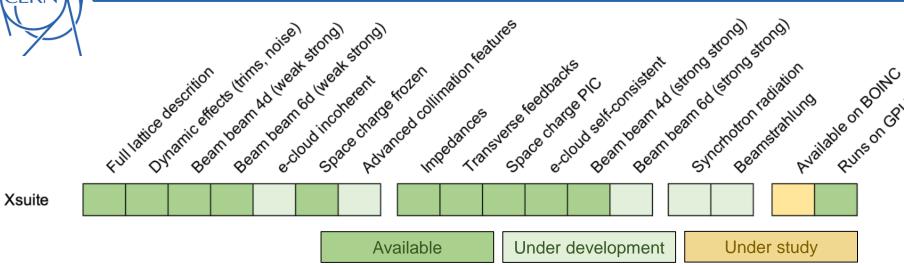
#### **Xfields**

computation of EM fields from particle ensembles

### **Xobjects**

interface to different computing plaforms (CPUs and GPUs of different vendors)





# Xsuite development **experience so far**:

- Shows **feasibility of integrated modular code** covering the application of our interest
- Demonstrates a convenient approach to handle multiple computing platform while keeping compact and readable physics code
- Already **being used for production runs**  $\rightarrow$  gradually becoming our workhorse for tracking simulations
- Very positive response from external collaborators (EPFL team working on FCC-ee software, Gamma factory collaboration, GSI, SEEIIST)

You are very welcome to give it a try, give us feedback and contribute more features!



Thanks for your attention!

# **Test suite**



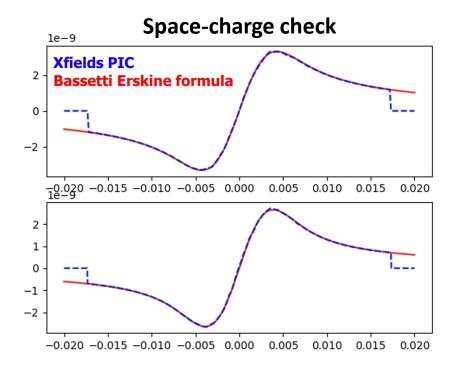
- To verify that new modifications don't affect the functionality and correctness of existing features, test suites are implemented for all modules
  - Notably they include check of tracking results for LHC, HL-LHC and SPS
- Before releasing new versions of the code, the tests are run on different computing platforms (CPU and GPU)

```
platform linux -- Python 3.8.5, pytest-6.2.4, py-1.10.0, pluggy-0.13.1
rootdir: /home/giadarol/Desktop/20210303 xfields gpudev/xobjects
plugins: cov-2.12.1
collected 58 items
tests/test_align.py
tests/test array.py
tests/test buffer.py ......
tests/test capi.py ......
tests/test_chunk.py
tests/test_kernel.py ...
tests/test_nplike_arrays.py ...
tests/test ref.py ...
tests/test scalars.py ...
tests/test_strides.py ...
tests/test_string.py .....
tests/test_struct.py ......
tests/test_unionref.py ...
        ------ test session starts ------
platform linux -- Python 3.8.5, pytest-6.2.4, py-1.10.0, pluggy-0.13.1
rootdir: /home/giadarol/Desktop/20210303_xfields_gpudev/xfields
plugins: cov-2.12.1
collected 7 items
tests/test beambeam.py
tests/test_cerrf.py
tests/test mean std.py
tests/test profiles.py
tests/test spacecharge.py ...
       ==================== test session starts ============
platform linux -- Python 3.8.5, pytest-6.2.4, py-1.10.0, pluggy-0.13.1
rootdir: /home/giadarol/Desktop/20210303_xfields_gpudev/xtrack
plugins: cov-2.12.1
collected 11 items
tests/test_aperture_turn_ele_and_monitor.py ...
tests/test collective tracker.py
tests/test collimation infrastructure.py .
tests/test dress.py ...
tests/test_elements.py ...
tests/test_full_rings.py
tests/test_pyht_interface.py .
                                                                        90%
tests/test_random_gen.py
```



# **Space-charge – benchmarks and performance**

- Different methods crosschecked against each other
- Particular care in optimizing performance on GPU



Platform	Computing time
CPU	5.5 s
GPU (Titan V, cupy)	20 ms
GPU (Titan V, via pyopencl)	38 ms

(\*) tests made on ABP GPU server for typical SPS space-charge interaction (PIC)

# **Xsuite foundations**



We did not start from scratch, instead we could learn and inherit features from the following existing tools:

#### sixtraklib-pysixtrack

- Clean, tested and documented implementation of machine elements (basically reused without changes, physics from SixTrack)
- Particle description with redundant energy variables for better precision and speed (from sixtrack experience)
- Experience with **multiplatform code** (CPU/GPU)
- Tools for importing machine model from MAD-X or sixtrack input

#### **PyHEADTAIL**

- Driving a multiparticle simulation through Python
- Usage of vectorization through numpy to speed up parts of the simulation directly in Python

#### **PyPIC**

- 2D and 3D FFT Particle In Cell with integrated Green functions
- Experience with CPU and GPU

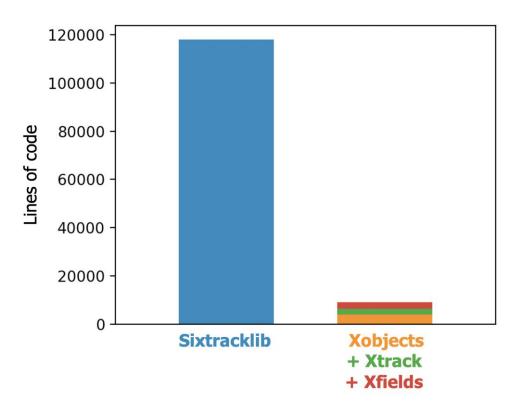
# Don't reinvent the wheel...



# **Xsuite: code complexity**



- Xsuite leverages Python's flexibility (introspection) and massive code autogeneration to minimize code complexity
  - Code is compact and readable (significant step forward w.r.t. Sixtracklib, where we had achieved multiplatform compatibility using pre-compiler macros)
  - A developer who knows the basics of Python and C can easily contribute code (e.g. introduce new beam elements)
- → Fundamental to guarantee future development and maintenance with available manpower!



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  - Multiplatform programming with Xobjects
- Summary

# CERN

# **Xobjects – data manipulation in python**

The main features of Xobjects can be illustrated with a simple **example** (Xsuite physics packages are largely based on the features illustrated here)

A **Xobjects Class** can be defined as follows:

```
import xobjects as xo

class DataStructure(xo.Struct):
    a = xo.Float64[:] # Array
    b = xo.Float64[:] # Array
    c = xo.Float64[:] # Array
    s = xo.Float64 # Scalar
```

An **instance of our class** can be instantiated on CPU or GPU by passing the appropriate context

Independently on the context, the **object is accessible in read/write directly from Python**. For example:

```
print(obj.a[2]) # gives: 3
obj.a[2] = 10
print(obj.a[2]) # gives: 10
```

# **Xobjects – data access from C**



The definition of a Xobject class in Python, automatically triggers the generation of a set of functions (C-API) that can be used in C code to access the data.

They can be inspected by:

```
print(DataStructure._gen_c_decl(conf={}))
```

which gives (without the comments):

```
// ...
// Get the Length of the array DataStructure.a
int64 t DataStructure len a(DataStructure obj);
// Get a pointer to the array DataStructure.a
ArrNFloat64 DataStructure_getp_a(DataStructure obj);
// Get an element of the array DataStructure.a
double DataStructure get a(const DataStructure obj, int64 t i0);
// Set an element of the array DataStructure.a
void DataStructure set a(DataStructure obj, int64 t i0, double value);
// get a pointer to an element of the array DataStructure.a
double DataStructure getp1 a(const DataStructure obj, int64 t i0);
// ... similarly for b, c and s
```



# **Xobjects – writing cross-platform C code**

# A **C** function that can be parallelized when running on GPU is called "Kernel".

**Example**: C function that computes obj.c = obj.a \* obj.b

```
src = '''
/*gpukern*/
void myprod(DataStructure ob, int nelem){
   for (int ii=0; ii<nelem; ii++){ //vectorize_over ii nelem
        double a_ii = DataStructure_get_a(ob, ii);
        double b_ii = DataStructure_get_b(ob, ii);
        double c_ii = a_ii * b_ii;
        DataStructure_set_c(ob, ii, c_ii);
    }//end_vectorize
}</pre>
```

# CERN

# **Xobjects – writing cross-platform C code**

# A **C** function that can be parallelized when running on GPU is called "Kernel".

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        double b_ii = DataStructure_get_b(ob, ii);
        double c_ii = a_ii * b_ii;
        DataStructure_set_c(ob, ii, c_ii);
   }//end_vectorize
}</pre>
```

(Comments in red are Xobjects annotation, defining how to parallelize the code on GPU)

The Xobjects context compiles the function from python:

The kernel can be easily called from Python and is executed on CPU or GPU based on the context:

```
# obj.a contains [3., 4., 5.] , obj.b contains [4., 5., 6.]
ctx.kernels.myprod(ob=obj, nelem=len(obj.a))
# obj.c contains [12., 20., 30.]
```



# **Xobjects – code specialization**

Before compiling, Xobjects specializes the code for the chosen computing platform.

 Specialization and compilation of the C code are done at runtime through Python, right before starting the simulation → gives a lot of flexibility

#### Code written by the user

#### **Code specialized for CPU**

```
void myprod(DataStructure ob, int nelem){
  for (int ii=0; ii<nelem; ii++){ //autovectorized

    double a_ii = DataStructure_get_a(ob, ii);
    double b_ii = DataStructure_get_b(ob, ii);
    double c_ii = a_ii * b_ii;
    DataStructure_set_c(ob, ii, c_ii);

}//end autovectorized
}</pre>
```

#### **Code specialized for GPU (OpenCL)**

```
__kernel void myprod(DataStructure ob, int nelem){
  int ii; //autovectorized
  ii=get_global_id(0); //autovectorized

  double a_ii = DataStructure_get_a(ob, ii);
  double b_ii = DataStructure_get_b(ob, ii);
  double c_ii = a_ii * b_ii;
  DataStructure_set_c(ob, ii, c_ii);

//end autovectorized
}
```



# **Xobjects – code specialization**

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 Specialization and compilation of the C code are done at runtime through Python, right before starting the simulation → gives a lot of flexibility

#### Code written by the user

#### **Code specialized for CPU**

```
void myprod(DataStructure ob, int nelem){
  for (int ii=0; ii<nelem; ii++){ //autovectorized}

    double a_ii = DataStructure_get_a(ob, ii);
    double b_ii = DataStructure_get_b(ob, ii);
    double c_ii = a_ii * b_ii;
    DataStructure_set_c(ob, ii, c_ii);

}//end autovectorized
}</pre>
```

### **Code specialized for GPU (Cuda)**

```
__global___ void myprod(DataStructure ob, int nelem){
   int ii; //autovectorized
   ii=blockDim.x * blockIdx.x + threadIdx.x; //au
   if (ii<nelem){

        double a_ii = DataStructure_get_a(ob, ii);
        double b_ii = DataStructure_get_b(ob, ii);
        double c_ii = a_ii * b_ii;
        DataStructure_set_c(ob, ii, c_ii);

}//end autovectorized
}</pre>
```



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