An Integrated Beam Physics Simulation Framework

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Work supported by: CHART

https://xsuite.web.cern.ch

Outline

- **Introduction**
  - Motivation
  - Design goals and constraints
  - Architecture
  - Agile development
- **Lattice modeling, simulation and optimization**
  - Lattice modeling
  - Single-particle tracking
  - Dynamic parameter control
  - Multi-objective optimizer
- **Simulation of specific processes**
  - Particle-matter interaction
  - Synchrotron radiation
  - Handling of collective effects
  - Space-charge
  - Beam-beam
  - Electron clouds
- **Final remarks**

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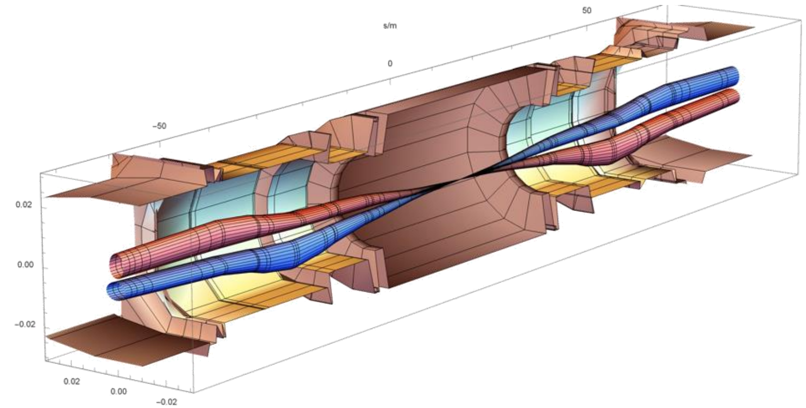
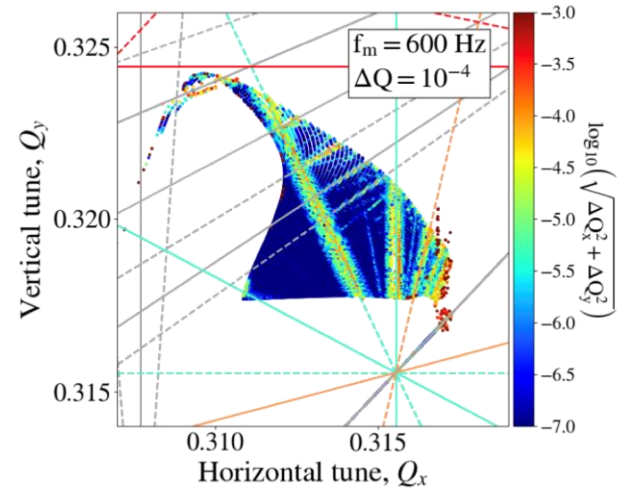
CERN has a **long tradition** in the **development of software tools for beam physics**

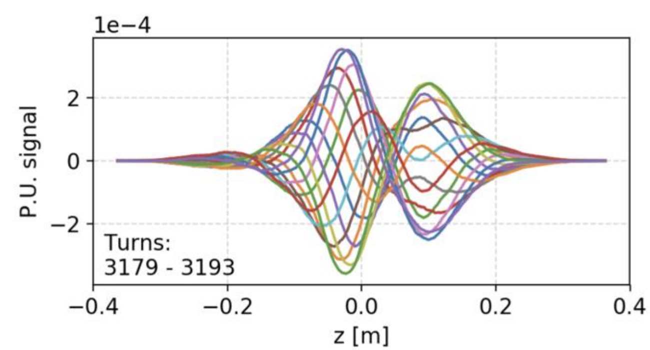
Powerful **tools** provided to the user community:

- **MAD-X**, standard for lattice description, optics calculation and design, tracking
- **Sixtrack**, a **fast-tracking program** used mainly for long **single-particle simulations**
- **Sixtracklib**, a **C/C++library for single-particle tracking** compatible with Graphics Processing Units (GPUs)
- **COMBI**, for the simulation of **beam-beam** effects using **strong-strong modelling**
- **PyHEADTAIL**, a **Python** toolkit for **collective effects** (impedance, feedbacks, space charge, and e-cloud).

Developed over decades, providing **advanced features** in their respective domains



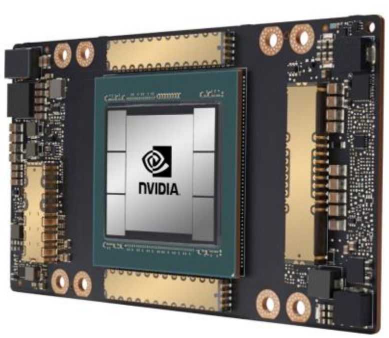




Motivation

Over the years we started to **face needs that could not be easily fulfilled with legacy tools**:

- **Integration**: difficult to combine features from different codes to simulate complex heterogeneous effects
- **User interface**: need to move away from custom interfaces (text files / ad-hoc scripting) towards standard **Python packages**
    - Present **de-facto standard in scientific computing**
    - **Easy to combine** in notebooks and or in more complex Python codes
    - Allows **leveraging an ever-growing arsenal of general-purpose Python libraries** (statistics, linear algebra, frequency analysis, optimization, plot, etc.)
        - Boosted by **substantial investments from general industry** (big data, AI)
- **GPU acceleration**: mandatory for several applications but cumbersome to retrofit in the existing codes



Xsuite

This led to the **launch of the Xsuite project** in **2021**

- **Main goal:** bring into a **modern Python toolkit** the know-how built in developing and exploiting MAD, Sixtrack, COMBI, PyHEADTAIL etc.,
- Designed for **seamless integration** among the different components and for **extendability**
- Designed to support **different computing platforms**, including **multicore CPUs and GPUs** from different vendors

Design constraints:

- Need to cover **a large spectrum of phenomena and applications** (flexibility!)
- Need **developer learning curve** to be short as possible

  → Features developed **directly by field experts**
- Need **to grow the code in a "sustainable" way**, being managed and maintained by a **small core team experts** integrating (in a clean way!) contributions by a wide developer community

Xsuite – architecture

Physics modules

Xpart
generation of particles distributions

Xtrack
single particle tracking engine

Xfields
computation of EM fields from particle ensembles

Xdeps
Dependency manager, deferred expressions

Xcoll
Particle-matter interaction and collimation

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

CFFI PyOpenCL CuPy

Lower level libraries (external, open source)

intel AMD NVIDIA

Hardware

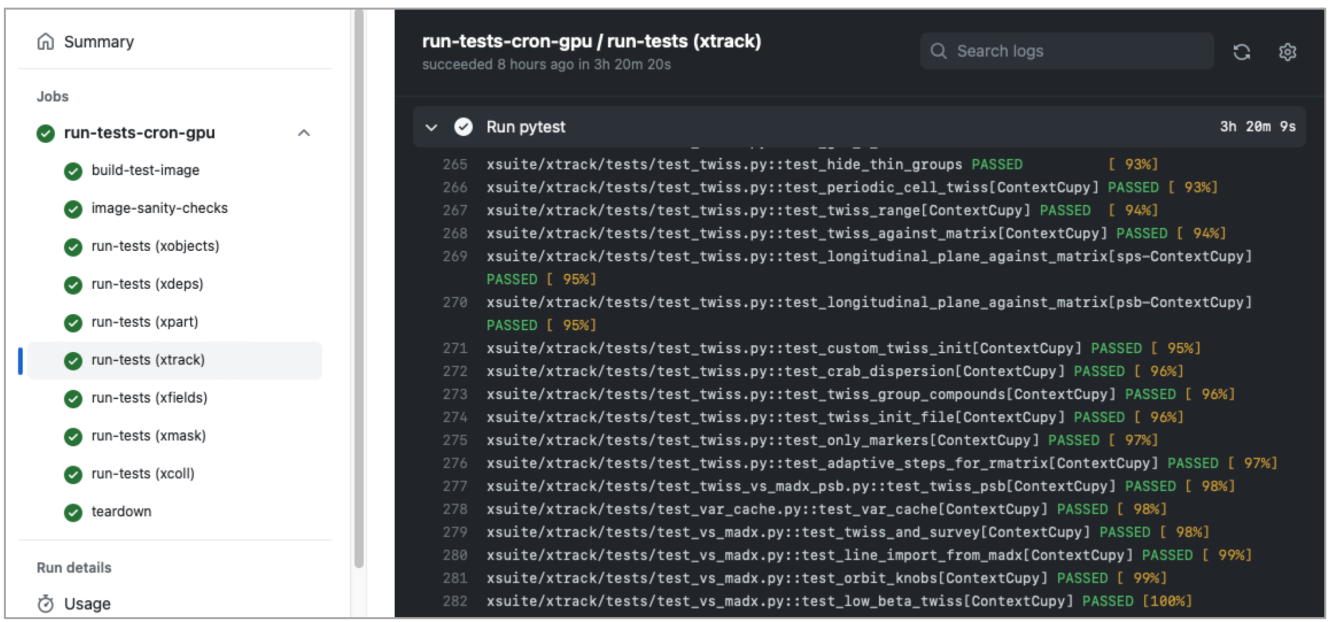
Orthogonal design

Project employs an **“orthogonal” design strategy**:

- Ensure that **each functional block** remains **well-isolated** and interacts with the others through **clearly defined interfaces**
- This approach has two key **advantages**:
    - Enables **contributors** to **modify or expand** specific components **without full knowledge of other parts** nor of underlying software infrastructure
    - **Minimize codebase complexity**, ensuring that it **increases linearly rather than exponentially** as new features are added

Our development follows the **agile principles**:

- Since early states **we engaged with the user community**, encouraging and **supporting users** to **test and exploit** available features in **full-scale studies**
- Code **evolves incrementally**, promptly applying needed fixes and improvements
- **Rely on fast release cycle** (new versions released multiple times per month) while ensuring **no disruption due to version changes** on the user's side.
- Made possible by large investment **automatic testing**: each version of Xsuite undergoing over a **thousand automatic checks** (on CPU and GPU)



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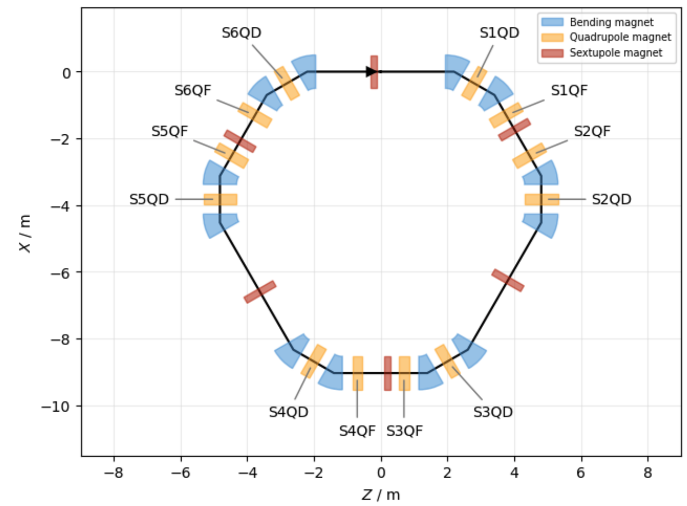
Lattice modelling

- The **beam line** is represented as a **sequence of Python objects**, each corresponding to an accelerator element or to other physical processes (e.g. magnets, cavities, aperture restrictions, etc.).
  - Can be **defined manually** or **imported from MAD-X**
    - Including **tilts**, **misalignments** and **multipolar errors**

Xsuite model of a ring
(represented with the Xplt package)

```
survey = tracker.survey()
```

```
plot = xplt.FloorPlot(survey, line, labels="S.Q.")
plot.legend()
```



We provide:

- **"Thin" lattice integration**, largely based on the Sixtrack and Sixtracklib experience
- **"Thick" maps** for bending and quadrupole magnets are also available:
  - For bends, we provide a **"full" map** (appropriate for small rings), and an **"expanded" map** (for large rings and small bending angles).
- **Dipole edge effects** including **fringe fields** can be modeled either in their **linearized form** or as **full non-linear maps** (same fringe model as in MAD-NG and PTC).

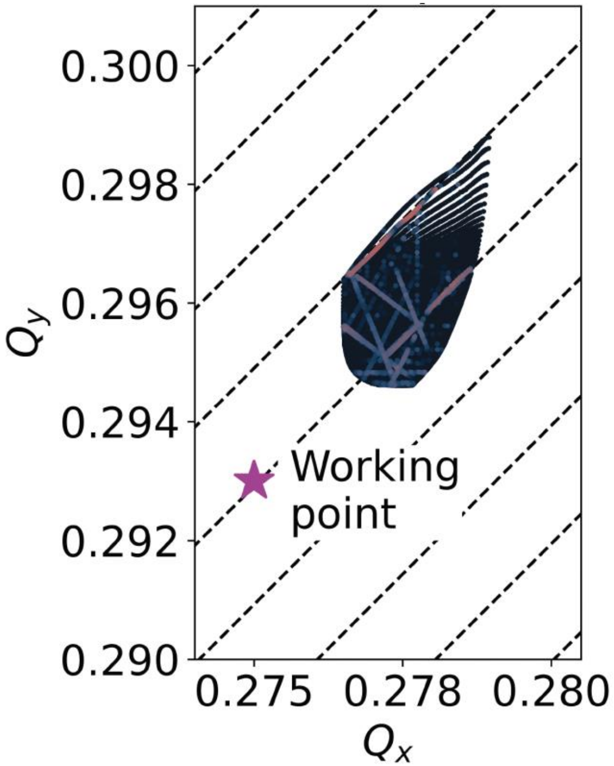
Single particle tracking

- To **speed up tracking simulations**, Xsuite assembles and compiles a **C kernel** (callable from Python) **optimized for the given beamline** and **specialized for the chosen platform** (CPU or GPU)
  - The **tracking speed** is found to be **similar to Sixtrack** for single-core CPU and **about two orders of magnitudes faster than that on high-end GPUs**
  - Developments are well advanced to deploy Xsuite on the **LHC@Home** volunteer computing platform

Tracking time for a typical LHC simulation

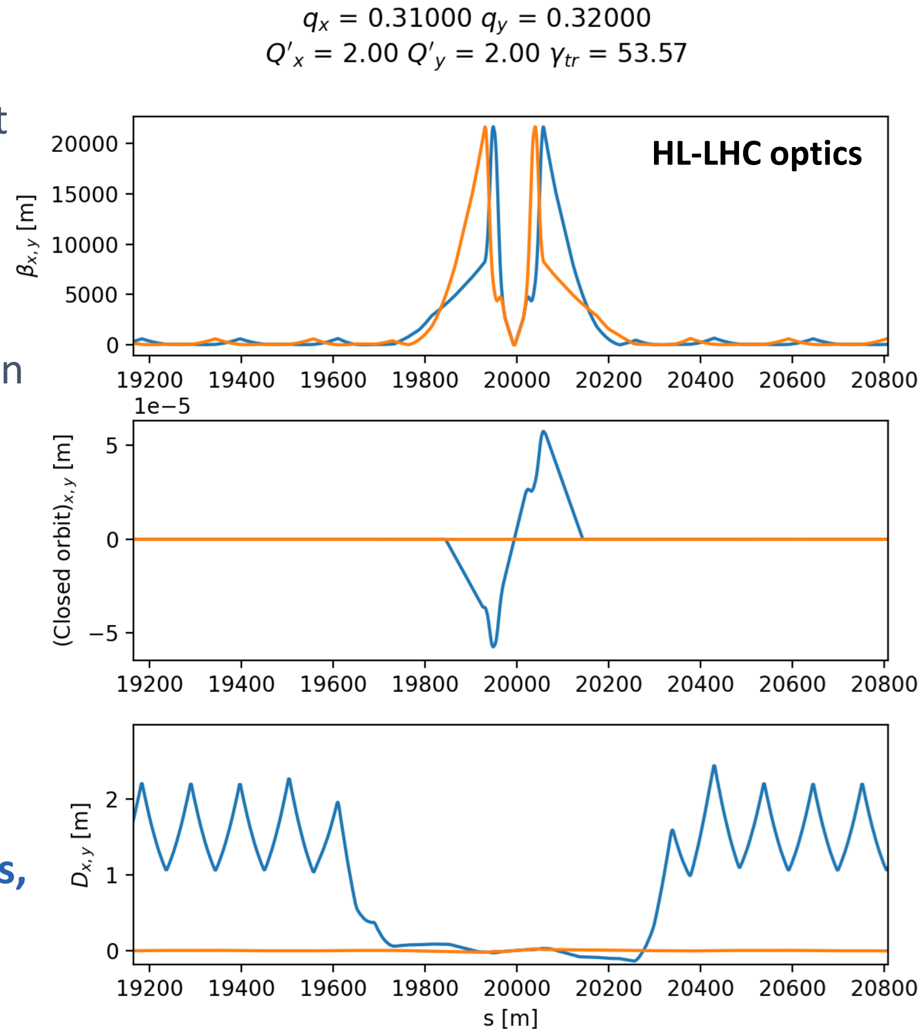
Platform	Computing time
CPU (single core)	190 (μs/part./turn)
GPU (NVIDIA V100, cupy)	0.80 (μs/part./turn)
GPU (NVIDIA V100 pyopencl)	0.85 (μs/part./turn)

FMA produced with Xsuite



Twiss module

- The **Xsuite Twiss** module can be used to extract **lattice functions** of a ring or a beamline
- The calculation **probes the lattice <u>simply by tracking particles</u>**:
  - **Closed orbit** obtained by applying a Python root finder on the tracking
  - The **Jacobian** matrix obtained by **tracking (central differences)**
  - Compute **"Linear Normal Form"** of the Jacobian matrix (diagonalization)
  - **Propagate eigenvectors** by **tracking**
  - Obtain from the eigenvectors **Twiss parameters (α, β, γ) , dispersion functions, phase advances, coupling coefficients**
- Computation can be done with **assigned beam momentum** to get **off-momentum beta-beating**, **non-linear chromaticity** etc.



Accuracy compared to MAD-X: $\Delta\beta / \beta << 10^{-4}$
Computation time is very similar

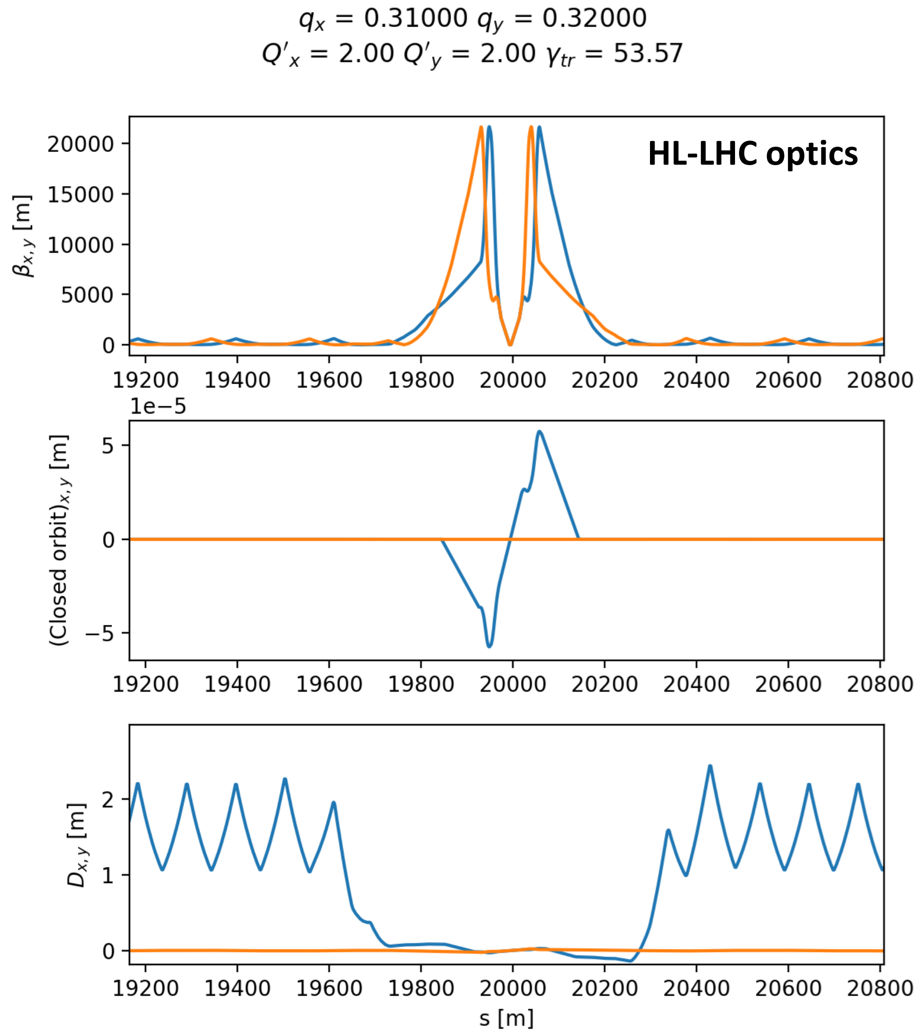
```
In [37]: tw.bety[0] # xsuite
Out[37]: 149.4305507849305

In [38]: mad.table.twiss.bety[0] # madx
Out[38]: 149.43055000962505

In [39]: t_mad_ms
Out[39]: 202.0

In [40]: t_xsuite_ms
Out[40]: 185.0
```

Example

Twiss module

Computation of **Twiss parameters based on the tracking** has **two main advantages**:

- Any **physical model included in the tracking** is **automatically usable in Twiss**
  - Without additional development effort
- Twiss becomes a **powerful diagnostics tool** on the built **tracking model**
  - Allows **measuring directly on the tracking model** tunes, chromaticities, closed orbit, beta functions, etc.
  - Can be done **effortlessly** and **without exporting or manipulating the model**.
  - **Used daily** to for validating simulation models, catching mistakes, investigating issues



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Example

Dynamic control of beam line parameters

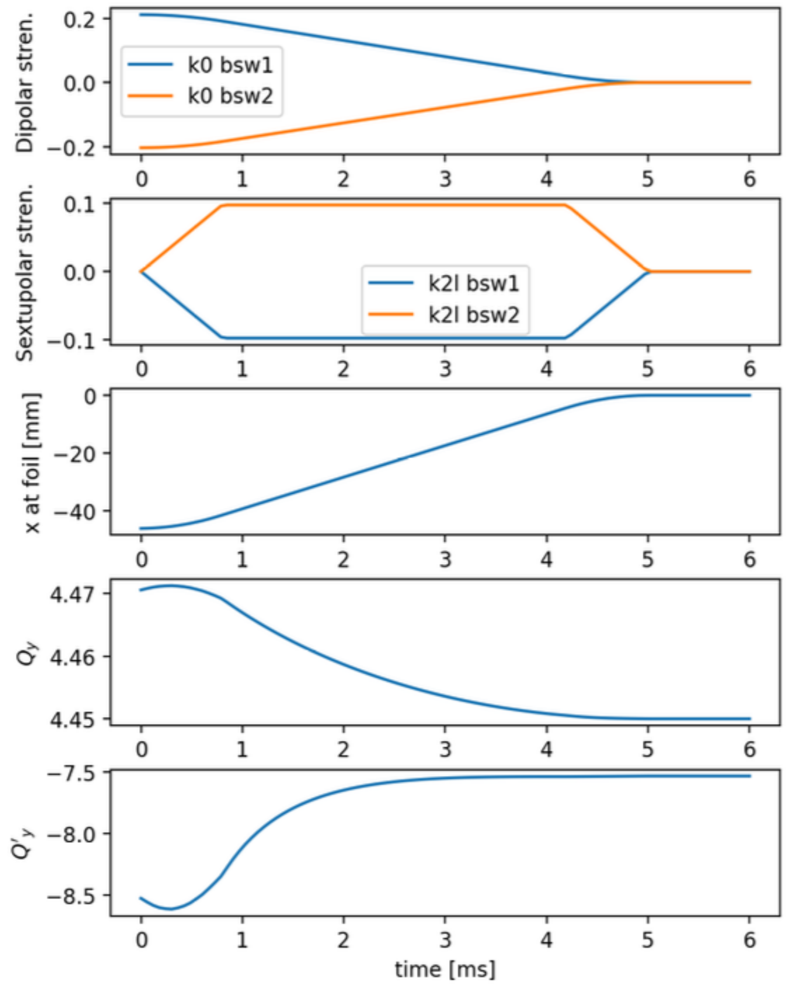
- In accelerators often a single **high-level parameter** can be used to control **groups of components** with complex dependency relations. (e.g. magnets in series, groups of RF cavities, etc.)
- The **Xdeps module** provides the capability to include such dependencies in the simulation model (as done by MAD-X deferred expressions)
- **Example**, LHC crossing angle knob:

  At any time, the user can set:

  ```
  lhc.vars['on_x1'] = 160 # murad
  ```

  which **automatically changes the strength of 40 dipole correctors** to get the required crossing angle
- User can also use **"Time functions"**, i.e. **time dependent knobs** that are updated automatically during the simulation

Simulation of a fast orbit bump used for the H^- injection into the CERN PS Booster



Optimizer

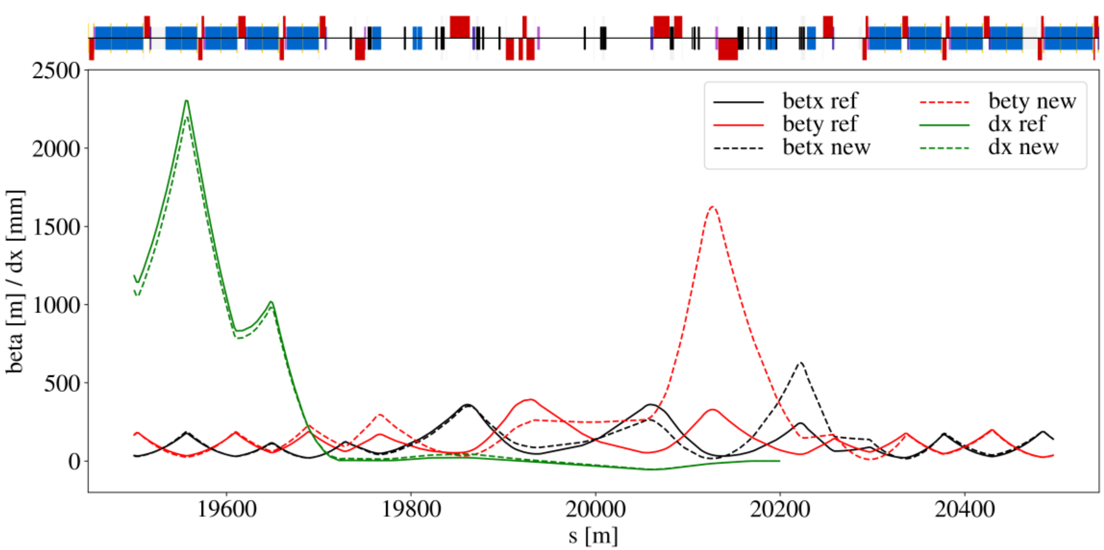
Xsuite provides a **multi-objective optimizer** to "match" model parameters to assigned constraints (e.g. control tunes, chromaticity, build orbit bumps, modify the optics)

- Based on the **extensive experience of MAD-X** → Uses the **same optimization algorithm** (Jacobian, proven robustness)
- The optimizer can be used to **synthesize knobs**
- Optimizations can involve **targets and knobs from multiple beam lines** (colliders)
- Interface **designed for usage flexibility**. User can **intervene in the optimization** by:
    - Enabling/disabling targets or knobs
    - Rolling back optimization steps
    - Changing knob limits, target values, convergence tolerances

Used for **optics matching of the LHC and of FCC-ee colliders**

→ Proved capability of handling **large problems** with several constraints and degrees of freedom.

Optimized optics for the LHC collimation area (designed with Xsuite)



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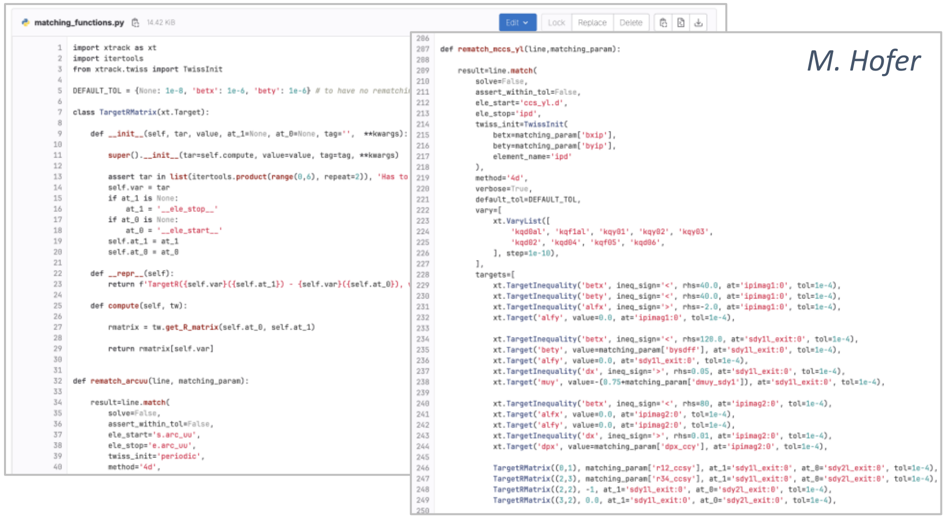
Full optics desing for FCC-ee HFD lattice ported to Xsuite (from MAD8)

https://gitlab.cern.ch/mihofer/xample_hfd_matching



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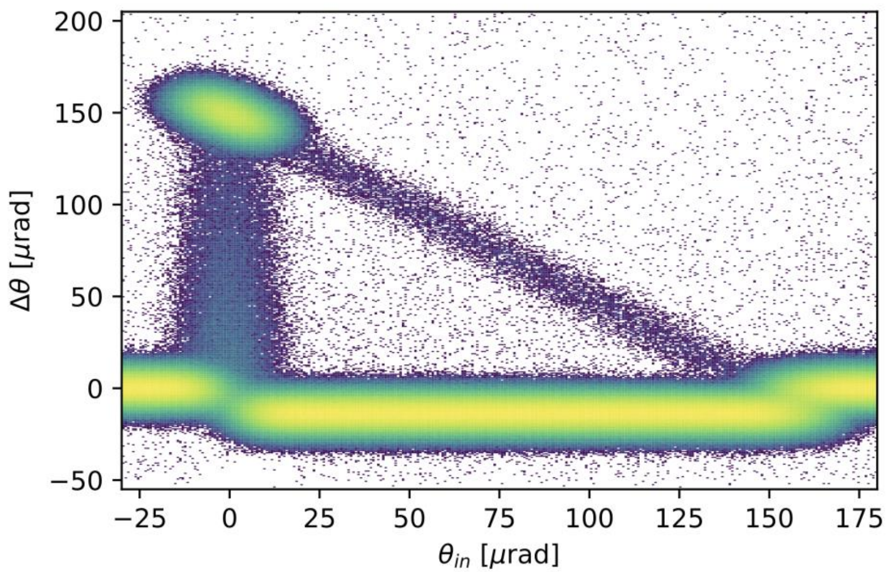
For collimation studies, the **Xcoll module** provides **three engines** to simulate **particle-matter interactions:**

- The **"Everest" engine** embedded in Xcoll (evolution of K2 module from Sixtrack)
- The **"Geant 4" engine**, based on an **interface Xsuite-BDSIM-Geant4**
- The **"FLUKA" engine**, based on an interface with the **FLUKA** Monte Carlo code

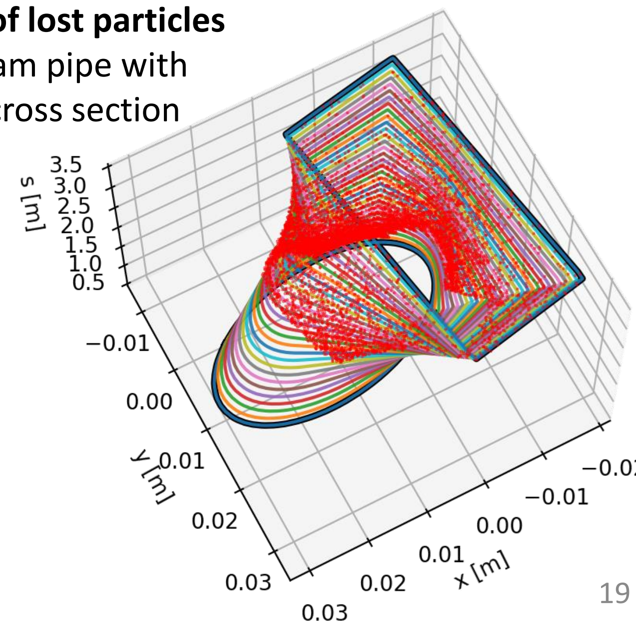
To support collimation studies, Xsuite provides:

- Tools to **automatically install and set collimators** in the simulation model
- Support for **complex aperture modelling** and **accurate localization of the lost particles along** the beam line (typically within 1-10 cm)

Particle deflection from a bent crystal (Everest engine)

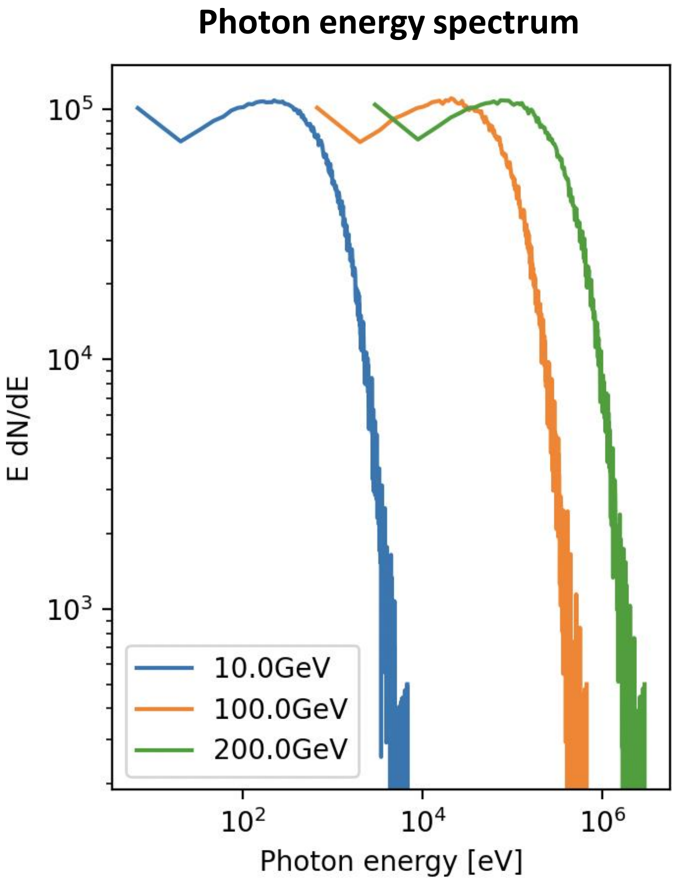


Localization of lost particles along a beam pipe with changing cross section



The effect of **synchrotron radiation** can be included in Xsuite tracking simulations. Two models available:

- The **"mean" model**, for which the energy loss from the radiation is applied particle by particle without accounting for quantum fluctuations;
- The **"quantum" model** for which the actual photon emission is simulated(1).



Plots courtesy Leon Van Riesen-Haupt, EPFL

(1) *Based on H. Burkhardt, "Monte Carlo generator for synchrotron radiation", 1990. Implementation ported from PLACET (A. Latina)*

(2) *E. Forest, From tracking code to analysis: generalised Courant-Snyder theory for any accelerator model. Springer, 2016*

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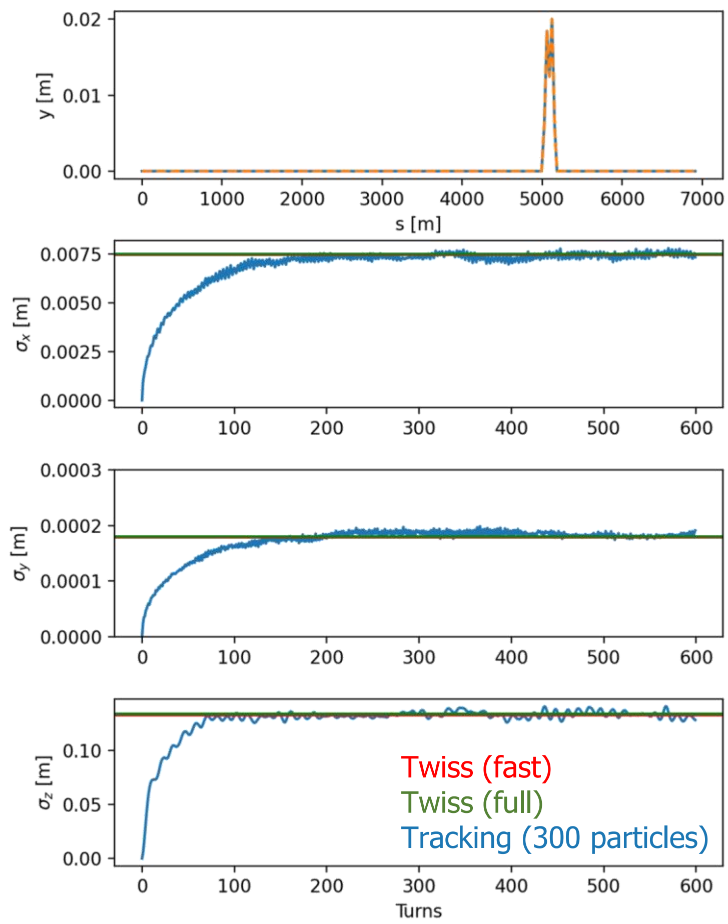
The **Xsuite Twiss** also includes:

- Dedicated algorithm for **non-symplectic one-turn map**[2]
- Computation of **radiation energy loss, damping times and equilibrium emittances**

An **automatic tool** is provided for **phasing the RF cavities** and **adjusting magnet strengths** to **compensate the radiation energy loss ("tapering")**

Equilibrium emittance (twiss vs track)



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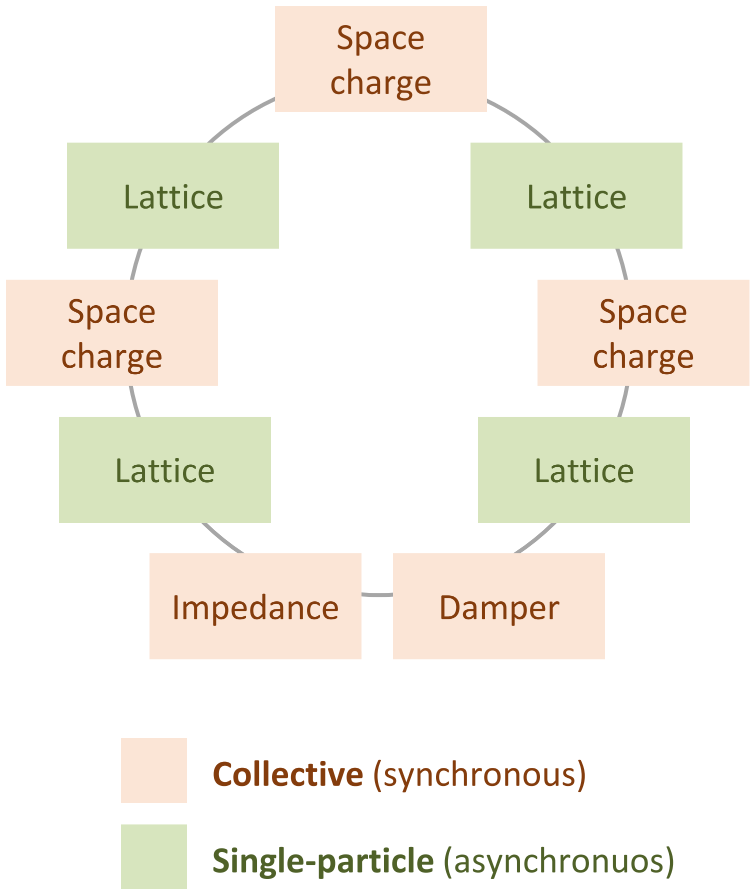
Collective effects



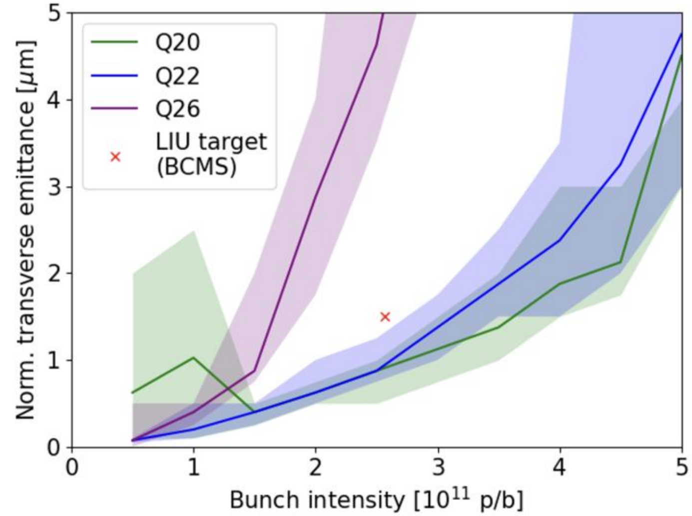
- Xsuite is designed to include **collective effects** in the simulations
- Handling of collective elements is **fully automatic** → The Xtrack module identifies the collective elements and **splits the sequence**:
    - The **non-collective** parts are handled **asynchronously** to **gain speed**
    - The simulation of the **collective effects** is **performed synchronously**
- **If requested** by the collective element, the particles' data is **automatically transferred from GPU to CPU and back**
- **Space-charge**, **beam-beam**, **e-cloud** (weak-strong) are handled **natively**
- **Impedances** and **feedback systems** are handled through an interface with **PyHEADTAIL**
- An automatic tool for the **computation of stability diagrams** from amplitude detuning is also provided

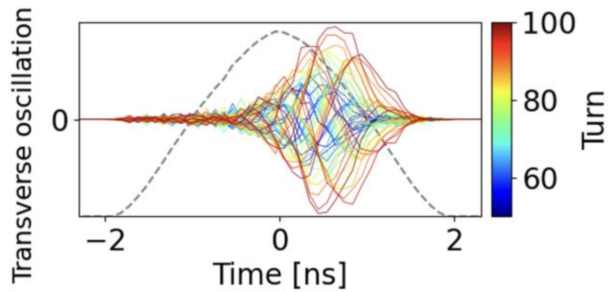
The implementation is largely based on **PyHEADTAIL-PyPIC**

Different **space-charge models** are implemented:

- The **“frozen” model**, in which particles interact with fixed charge distributions
- The **“quasi frozen”** model, in which the **beam intensity and beam sizes are recomputed at each interaction**
- The **“Particle In Cell (PIC)”** model:
  - Charge of tracked particles distributed on a **rectangular grid**
  - **Fast Poisson solver** based on **FFT** method with Integrated Green Functions
- Space charge simulations **strongly profiting from GPU acceleration**

Simulation campaign for the CERN SPS including full non-linear lattice, space charge and wakefields

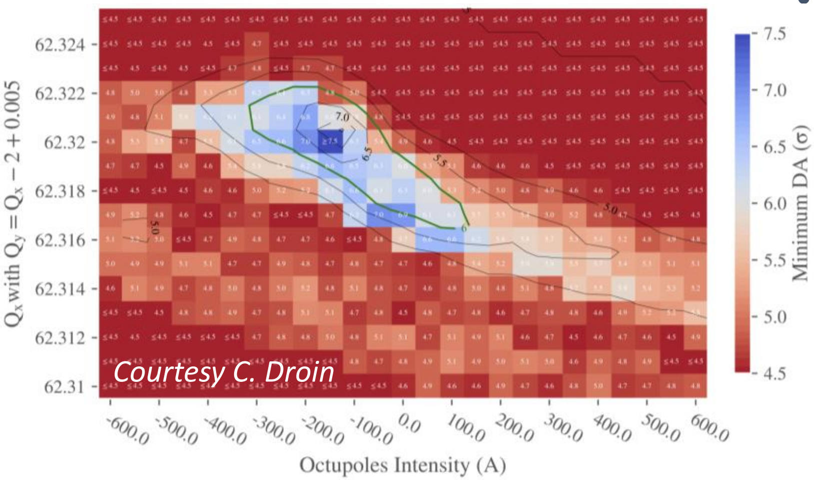




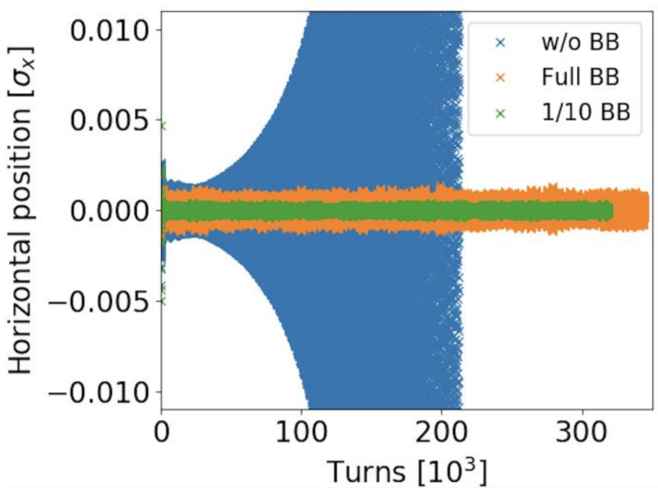
N. simulations	400
Number of PIC calculations per turn	540
Number of turns per simulation	40’000
Computing time per sim. (GPU)	~3 days
Computing time per sim. (CPU serial)	> 12 months

Courtesy X. Buffat

Dynamic aperture optimization study for HL-LHC (weak-strong modelling)



Wakefield + beam-beam simulations for HL-LHC (strong-strong modelling)



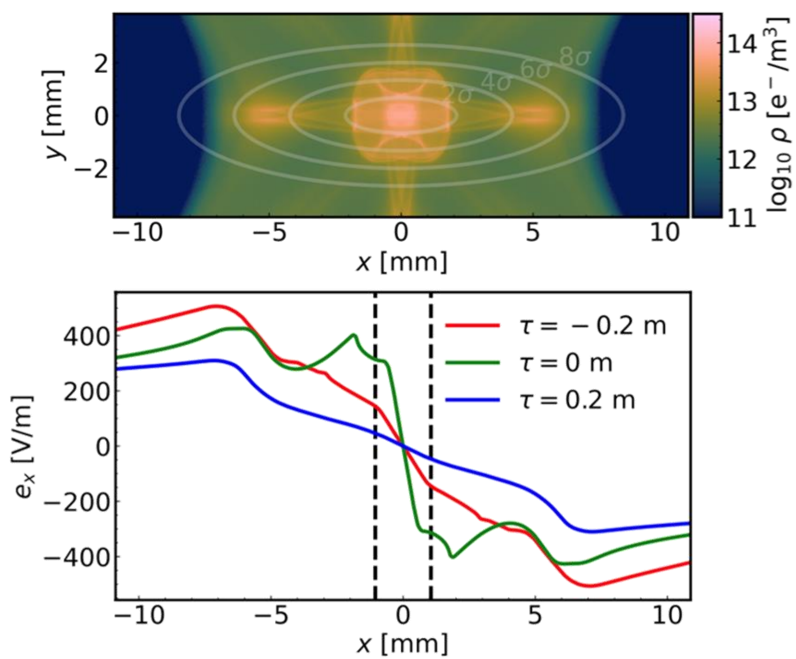
- Xsuite implementation based on experience from **Sixtrack** and **COMBI**
- Two models are provided:
  - The **"4D" model**, which applies **only transverse** forces **independent on the longitudinal motion**
  - The **"6D" model**, which applies **longitudinal and transverse** forces accounting for the synchrotron motion (method by Hirata et al.)

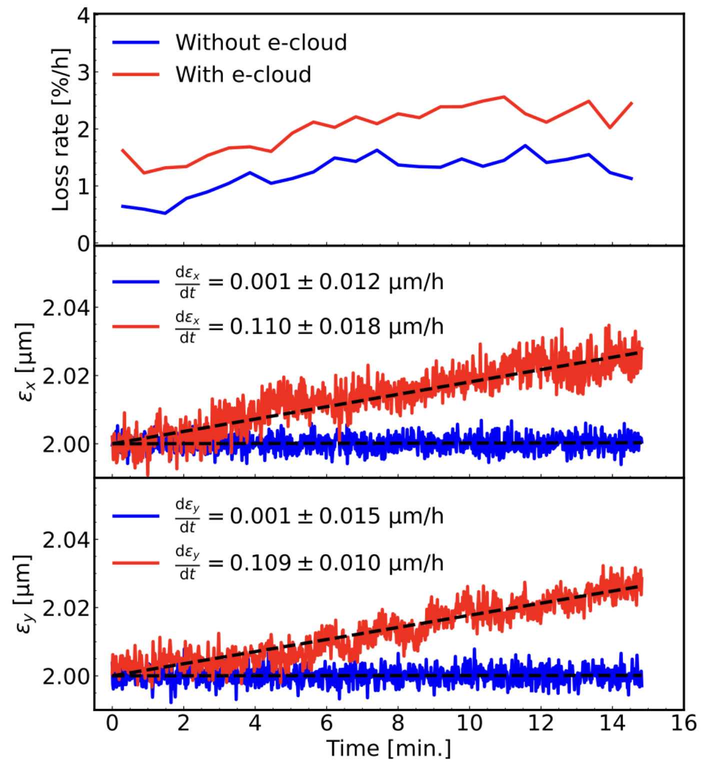
  Both models can be used either in **"weak-strong" mode** (fixed assigned distribution for the other beam) or in **"strong-strong" mode** (self-consistent two-beam simulation)
- For the simulation of lepton colliders, the code can also simulate for **beamstrahlung** and **Bhabha scattering**
- **Strong-strong simulations** are accelerated by **parallel computing on HPC clusters** (based on MPI)
  - **"Pipeline" algorithm**[1] used to optimize workload distribution across the nodes

[1] *S. Furuseth and X. Buffat, Comput. Phys. Commun. 244 (2019)*

Xsuite has been exploited to study the **effect of electron cloud** on **slow beam degradation** (emittance growth, lifetime degradation).

- Done by applying a **high-order interpolation scheme** to the **e-cloud potential imported** from a dedicated multipacting simulator.
  - Scheme designed to **preserve the symplecticity of the resulting map** by ensuring the global continuity of the potential and required derivatives.
- **Use of GPUs is mandatory** to simulate the required long time scales (>10^6 turns).





See also: K. Paraschou, THBP16

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Who uses Xsuite and for which applications?

[Activities that are already in production, or for which testing work is ongoing]

LHC and HL-LHC

- **Tracking for DA** - lattice only (M. Le Garrec, E. Maclean, C. E. Montanari , T. Pugnat, D. Veres)
- **Crab-cavity noise studies**(A. Fornara, Uni. Manchester)
- **Beam-beam weak-strong** (G. Sterbini, S. Kostoglou, C. Droin, E. Lamb, D. Christie Uni. Manchester)
- **Beam-beam strong-strong** (X. Buffat)
- **Wire compensation studies** (P. Belanger, D. Kalchev TRIUMF)
- **Collimation studies** (F. Van Der Veken, N. Triantafillou, B. Lindstrom, M. D'Andrea, P. Hermes)
- **Optics/orbit matching, including RDT matching** (B. Lindstrom, K. Paraschou, C. Droin, S. Kostoglou, Y. Angelis)
- **Non-linear corrections calculation** (J. Dilly)
- **Hollow e-lens studies** (P. Hermes + students)
- **Incoherent e-cloud effects** (K. Paraschou)
- **Beam instrumentation studies** (D. Alves, K. Lasocha, SY-BI)

Injector complex (PSB, PS, SPS, LEAR, AD, ELENA)

- **Space-charge studies** (F. Asvesta, T. Prebibaj)
- **Cooling studies** (D. Gamba, P. Kruyt)
- **Instabilities with wakes and space-charge** (X. Buffat)
- **Slow extraction studies at PS and SPS** (P. Arrutia Sota, T. Bass, F. Velotti, SY-ABT)
- **Ion studies** (E. Waagaard)
- **Beam transfer simulations** (F. Velotti, SY-ABT)
- **MTE simulations**, optics+tracking (A. Huschauer, starting)

Light sources (Petra IV, Elettra, Bessy III)

- **Tracking and DA**

FCC

- **FCC-ee optics matching, tapering + RF phasing** (M. Hofer, J. Keintzel, P. Kicsiny (L. Van Riesen-Haupt)
- **FCC-ee DA studies** (M. Hofer, L. Van Riesen-Haupt, EPFL)
- **FCC-ee and FCC-hh beam-beam-SS&WS** (P. Kicsiny, D. Di Croce, EPFL)
- **Beamstrahlung, Bhabha** (P. Kicsiny)
- **FCC-ee and FCC-hh collimation studies** (A. Abramov, G. Broggi)
- **FCC-ee vibration studies** (J.P. Salvesen, M.Hofer, LAPP Annecy collab.)
- **Compton scattering studies** (A. Abramov, I. Debrot, M. Hofer)
- **Collective effects** (M. Migliorati, A. Ghribi - Uni Sapienza, A. Rajabi – Desy)

GSI/FAIR

- **Space-charge** simulations (A. Oeftiger and team)
- **Slow extraction** simulations - SIS18 and SIS100 (P. Niedermayer, C. Cortes)
- **BTF studies** (C. Cortes)

Medical accelerators

- **Slow-extraction for PIMMS** (R. Tailor)
- **Slow-extraction for MedAustron** (F. Kuehteubl, E. Renner, et al.)

BNL - RHIC and EIC

- **Optics calculations and tracking**
- **Collimation studies**

Fermilab – Main Injector, Recycler, IOTA

- **Tracking studies**
- **Impedance + space-charge** simulations

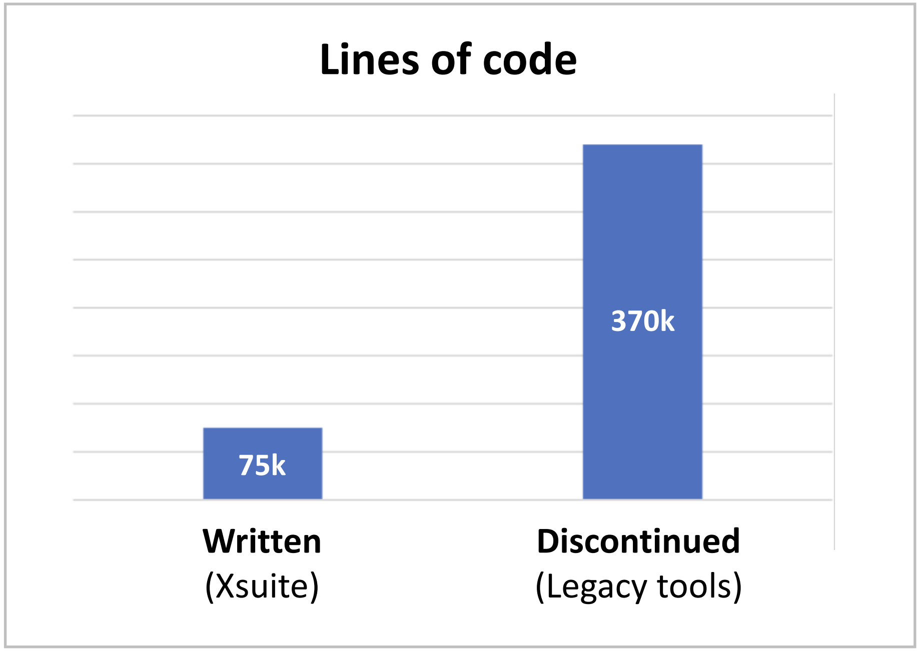
Training (Universiy of Rome and EPFL)

Discontinuation of legacy tools

In 2022-23 we have **essentially discontinued** the development and, to a very large extent, the usage of the following tools:

- Sixtrack
- Sixdesk
- Sixtracklib
- COMBI
- PySSD
- DistLib

This led to a **massive simplification** of our code base.



Some numbers and next steps

Some numbers:

Core team	**3** persons
Contributing developers	**16** persons
User community	**~80** users
Publications including Xsuite simulations (in 2022-23):	**25** papers

What next:

- **Most importantly:** user support, fixes and improvements based on user feedback, keep good quality documentation and testing
- **Additional features** (coming in 2024):
  - Equilibrium emittances in twiss in the presence of element shifts and tilts
  - Handling energy ramp functions
  - Faster reload of deferred expressions (cython)
  - Native implementation of wakefields (with MPI parallelization)
  - RFTrack interface for tracking in fieldmaps
  - Intra-beam scattering model
  - Approximated 2D PIC (pyorbit style, good compromise accuracy/speed)
  - Strong-strong beam-beam with PIC
  - Native save/load of sequence in ascii format (now done through cpymad)

Thanks for your attention!