



An Integrated Beam Physics Simulation Framework

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Work supported by:





- 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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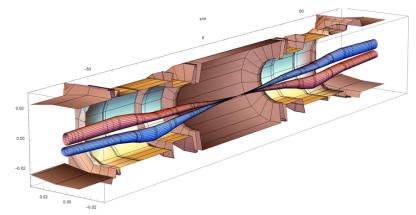


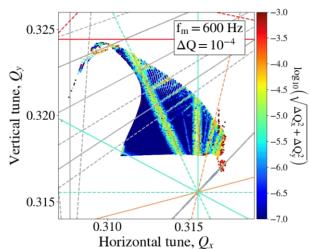
CERN has a **long tradition** in the **development of software tools for beam physics**

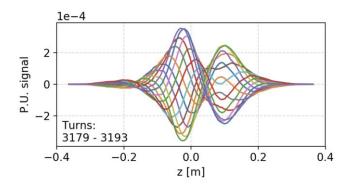
Powerful tools provided to the user community:

- 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















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

- <u>Integration</u>: difficult to combine features from different codes to simulate complex heterogeneous effects
- <u>User interface</u>: need to move away from custom interfaces (text files / ad-hoc scripting) towards standard <u>Python packages</u>
 - 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)
- <u>GPU acceleration</u>: mandatory for several applications but cumbersome to retrofit in the existing codes





This led to the launch of the Xsuite project in 2021

- Main goal: bring into a modern Python toolkit the knowhow 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
- 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



Physics modules

Xpart

generation of particles distributions

Xfields

computation of EM fields from particle ensembles

Xtrack

single particle tracking engine

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



Lower level libraries (external, open source)





Hardware

Orthogonal design



Project employs an "orthogonal" design strategy:

- Ensure that each functional block remains wellisolated 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

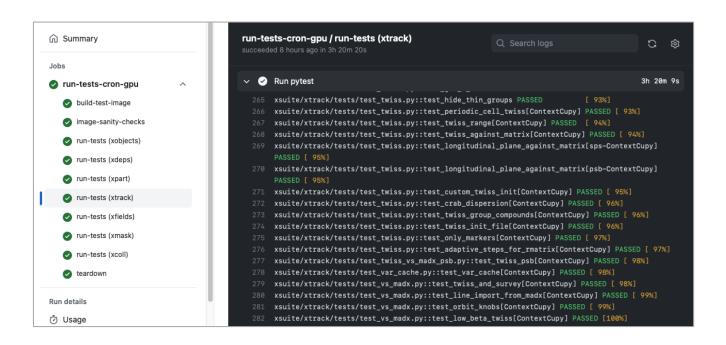


Agile development



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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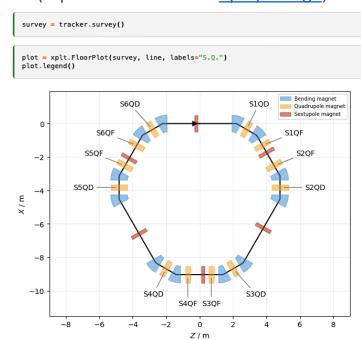
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Lattice modelling



- 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)



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).

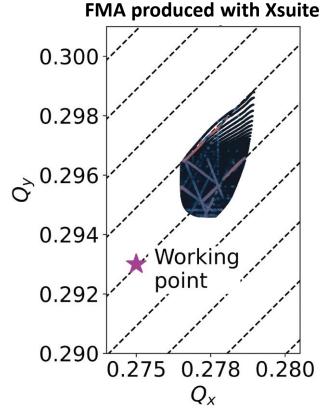
Single particle tracking



- 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

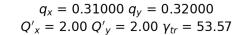
Platform	Computing time
CPU (single core)	190 (μs/part./turn)
GPU (NVIDIA V100, cupy)	0.80 (μs/part./turn)
GPU (NVIDIA V100 pyopencl)	0.85 (μs/part./turn)

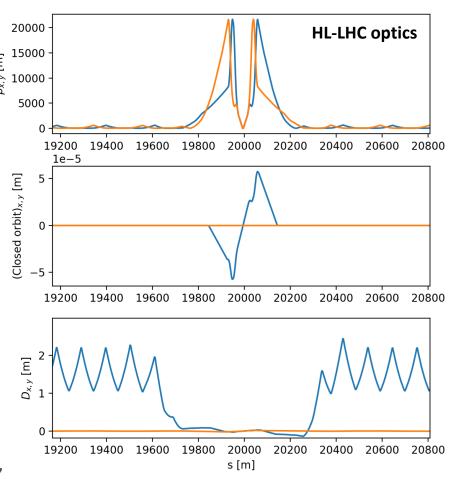


Twiss module



- The Xsuite Twiss module can be used to extract lattice functions of a ring or a beamline
- The calculation probes the lattice simply by tracking particles:
 - 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.



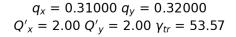


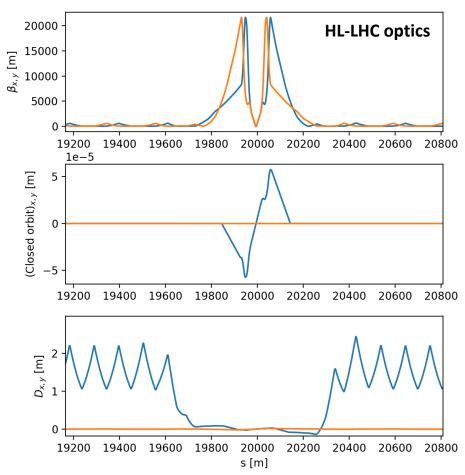
Accuracy compared to MAD-X: $\Delta\beta$ / β << 10⁻³ Computation time is very similar

Twiss module



- 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





Accuracy compared to MAD-X: $\Delta\beta$ / β << 10⁻³ Computation time is very similar

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:

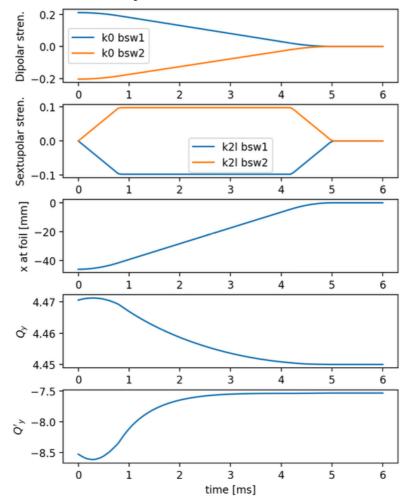
At any time, the user can set:

$$lhc.vars['on x1'] = 160 \# murad$$

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



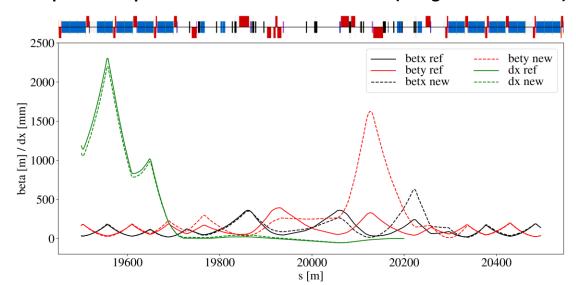
Xsuite provides a **multi-objective optimizer** to "match" model parameters to assigned constraints (e.g. control tunes, chromaticity, build orbit bumps, modify the optics)

- 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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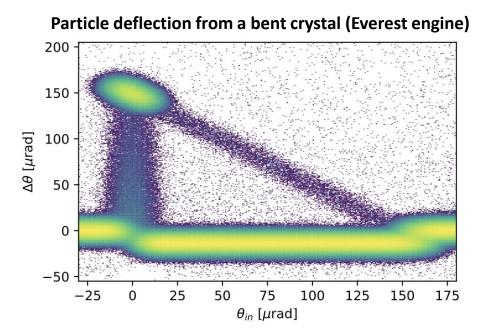
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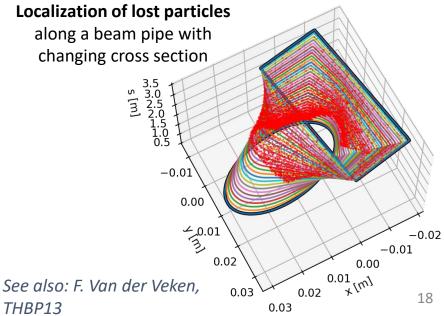
Particle-matter interaction



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)





Synchrotron radiation



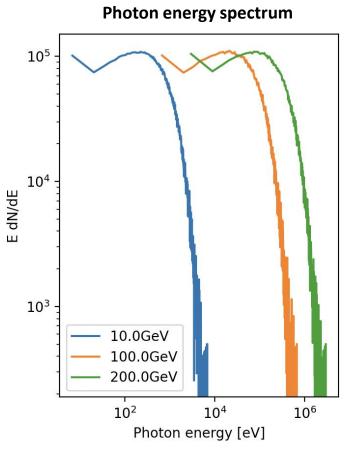
The effect of **synchrotron radiation** can be included in Xsuite tracking simulations. Two models available:

- 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⁾.

The **Xsuite Twiss** also includes:

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

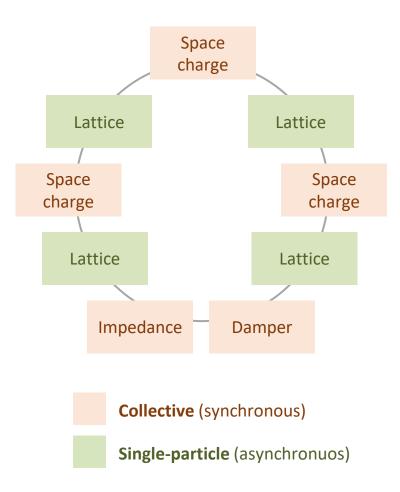
An automatic tool is provided for phasing the RF cavities and adjusting magnet strengths to compensate the radiation energy loss ("tapering")



Plots courtesy Leon Van Riesen-Haupt, EPFL

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 (weakstrong) 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



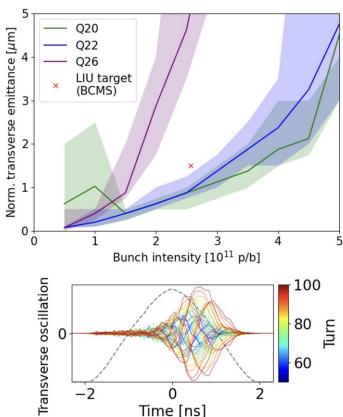


The implementation is largely based on **PyHEADTAIL-PyPIC**

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

- The "frozen" model, in which particles interact with fixed charge distributions
- The "quasi frozen" model that is a variant of the 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

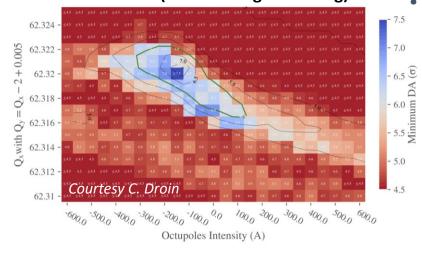


N. simulations	400
Number of PIC calculations per turn	540
Number of turns per simulation	40′000
Computing time per sim. (GPU)	~3 days
Computing time per sim. (CPU serial)	> 12 months

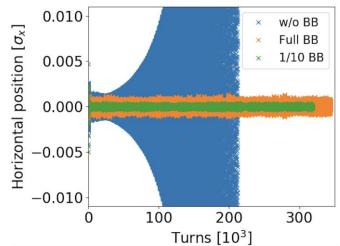
Beam beam effects



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)

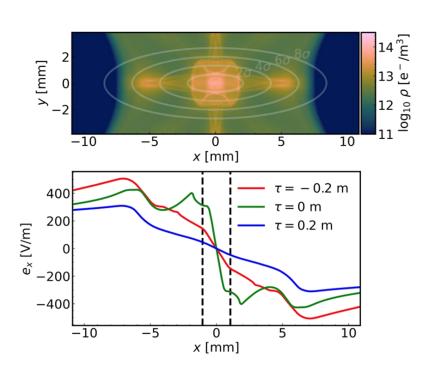
- For the simulation of lepton colliders, the code can also simulate for beamstrahlung and Bhabha scattering
- Strong-strong simulations are accelerated by parallel computing on HPC clusters (based on MPI)
 - "Pipeline" algorithm⁽¹⁾ used to optimize workload distribution across the nodes

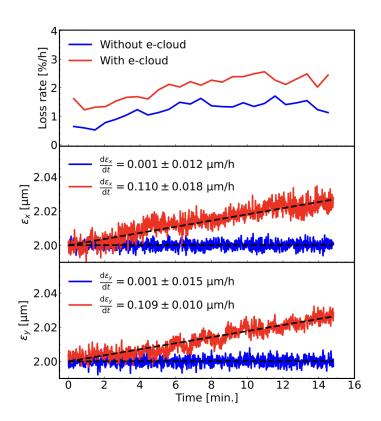
Electron cloud modeling



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 (>10⁶ turns).







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 Xsuite has by now reached a mature stage of development and has already been adopted as "production tool" by a quite large user community

In numbers:

Core team	3 persons
Contributing developers	15 persons
User community	~80 users
Publications including Xsuite simulations (in 2022-23):	21 papers

Xsuite **tested** and/or **exploited** for the simulation of several rings:

- CERN hadron rings: PSB, PS, SPS, LHC, ELENA
- FCC-ee lepton collider
- Fermilab rings (Main Injector, Recycler)
- FAIR SIS100
- BNL Electron-Ion Collider (hadron ring)
- Medical accelerators: PIMMS, Med-Austron, Heidelberg Ion Beam Therapy Center (HIT)
- Light sources: ELETTRA, Petra IV, [+ CLIC DRs]

The **input and feedback from the community** has been **fundamental** in improving the **quality**, **usability** and **robustness** of the code

Xsuite is **openly available** → You are very welcome to **test it on your applications**, give us **feedback**, **contribute** new features!



Thanks for your attention!