



## **Integrated Beam Physics Simulation Framework**

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Work supported by:



https://xsuite.web.cern.ch





#### Introduction

- $\circ$  Motivation
- o Design goals and constraints
- $\circ$  Architecture
- Agile development
- Lattice modeling, simulation and optimization
  - $\circ$  Lattice modeling
  - Single-particle tracking
  - o Dynamic parameter control
  - o Multi-objective optimizer
- Simulation of specific processes
  - Particle-matter interaction
  - Synchrotron radiation
  - Collective effects
- Final remarks



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## Introduction



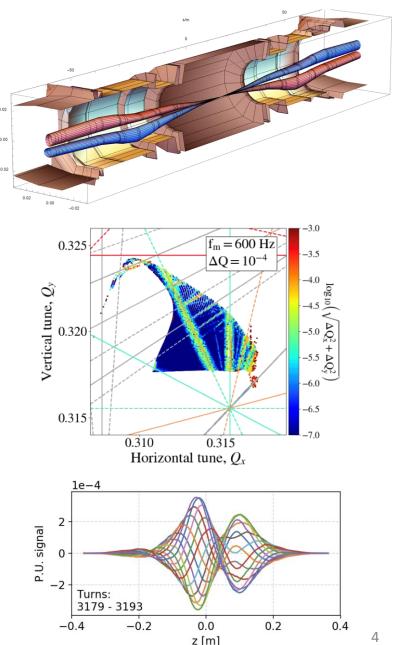
Coming from long tradition in the development of software tools for beam physics

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 **powerful features** in their respective domains

• Nevertheless, limitations also became apparent...









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

- <u>Integration</u>: very difficult to combine features from different codes to simulate complex heterogeneous effects
- <u>Extendability</u>: difficult to extend to present needs (notably those coming from FCC-ee)
- <u>User interface</u>: need to move away from custom interfaces (text files / ad-hoc scripting) towards standard Python packages
  - Present de-facto standard in scientific computing
  - Allows leveraging an ever-growing arsenal of general-purpose Python libraries (statistics, linear algebra, frequency analysis, optimization, plot, etc.)
    - Boosted by large investments from 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 MAD, Sixtrack, COMBI...
  - Cover with one toolkit applications ranging from lowenergy hadron rings to high-energy lepton colliders
- Designed for seamless integration of components and for extendibility
- Support different computing platforms, including multicore CPUs and GPUs from different vendors

#### **Design constraints:**

- Need to grow the code in a "sustainable" way, being managed and maintained by a small core team integrating (in a clean way!) contributions by a wide developer community
- Need **developer learning curve** to be short as possible
  - ightarrow Field specific features developed **directly by field experts**





# Physics modules

<b>Xpart</b>	Xtrack
generation of particles	single particle
distributions	tracking engine
<b>Xfields</b>	Xdeps
computation of EM fields	Dependency manager,
from particle ensembles	deferred expressions
X	

Xcoll Particle-matter interaction and collimation

## **Xobjects**

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



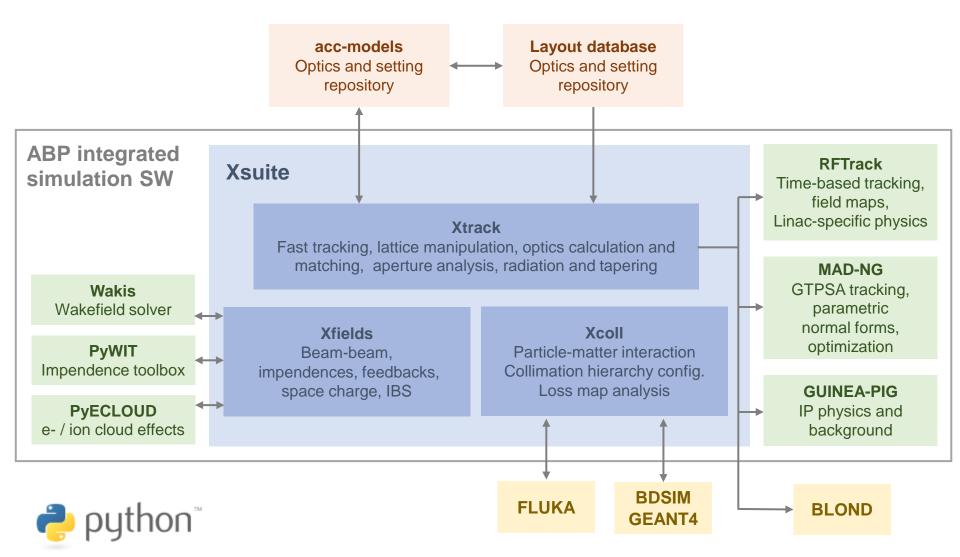
Lower level libraries (external, open source)

# intel AMD 🕽 📀 nvidia 🛛

Hardware



Xsuite working as aggregation point of a wider Python ecosystem (under development)





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





Our development follows the agile principles:

- We engaged with the user community, encouraging and supporting users to test and exploit available features in full-scale studies since early development stages
- 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)

G Summary	run-tests-cron-gpu / run-tests (xtrack)       Q. Search logs         succeeded 8 hours ago in 3h 20m 20s	\$ \$	
Jobs	✓ Ø Run pytest	3h 20m 9s	
🕑 run-tests-cron-gpu 🛛 🔿			
build-test-image	265 xsuite/xtrack/tests/test_twiss.py::test_hide_thin_groups PASSED 266 xsuite/xtrack/tests/test_twiss.py::test_periodic_cell_twiss[ContextCL	[ 93%]	
image-sanity-checks	267 xsuite/xtrack/tests/test_twiss.py::test_twiss_range[ContextCupy] PASS		
	268 xsuite/xtrack/tests/test_twiss.py::test_twiss_against_matrix[ContextCupy] PASSED [ 94%]		
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	271 xsuite/xtrack/tests/test_twiss.py::test_custom_twiss_init[ContextCupy	] PASSED [ 95%]	
run-tests (xtrack)	272 xsuite/xtrack/tests/test_twiss.py::test_crab_dispersion[ContextCupy]		
🖉 run-tests (xfields)	<pre>273 xsuite/xtrack/tests/test_twiss.py::test_twiss_group_compounds[ContextCupy] PASSED [ 96%]</pre>		
run-tests (xmask)	274 xsuite/xtrack/tests/test_twiss.py::test_twiss_init_file[ContextCupy] PASSED [ 96%]		
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run-tests (xcoll)	277 xsuite/xtrack/tests/test_twiss_vs_madx_psb.py::test_twiss_ps[Context		
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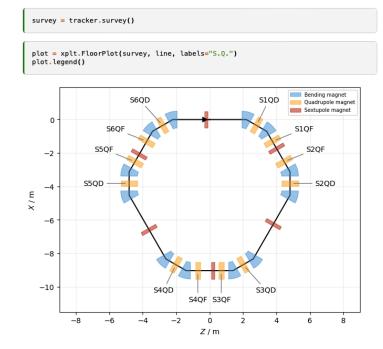
## • Lattice modeling, simulation and optimization

- Lattice modeling
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- o Dynamic parameter control
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- 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 <u>Xplt package</u>)



We provide:

- "Thin" lattice integration, largely based on the Sixtrack and Sixtracklib experience
- **"Thick" maps** for bending and quadrupole magnets
- **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).

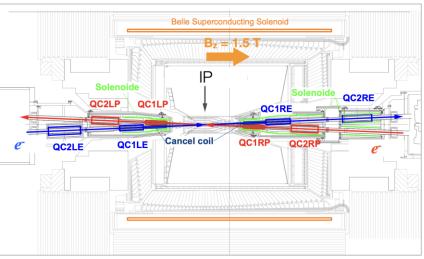
## Solenoids and overlapping elements

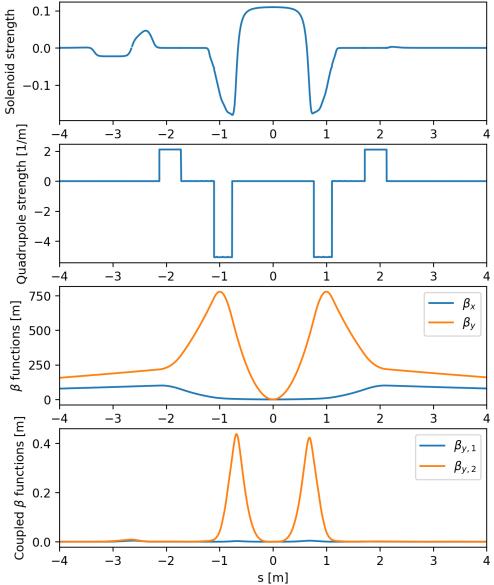
CERN

Recent developments allow modelling of **experimental solenoids** of lepton colliders also in the presence of **overlapping multipole fields** 

 Tested on FCC-ee and SuperKEKb models







SuperKEKb interaction region

Many thanks to G. Broggi, J. P. Salvesen, KEK experts

## Single particle tracking

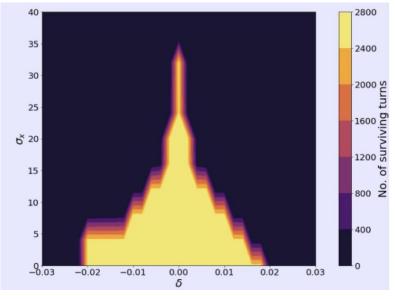


- Multiturn element-by-element tracking speed is critical for several application
- To **speed up tracking simulations**, Xsuite assembles and compiles a **C kernel** (callable from Python) **optimized for the given beamline** and **specialized for the chosen platform** (CPU or GPU)
  - The tracking 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 (collaboration with EPFL)

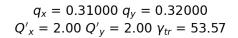
hacking time for a typical life simulation		
Platform	Computing time	
CPU (single core)	190 (µs/part./turn)	
GPU (NVIDIA V100, cupy)	0.80 (µs/part./turn)	
GPU (NVIDIA V100 pyopencl)	0.85 (µs/part./turn)	

#### Tracking time for a typical LHC simulation

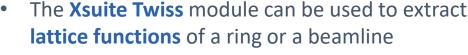
#### Example: Xsuite simulations used to study FCC-ee DA and momentum acceptance



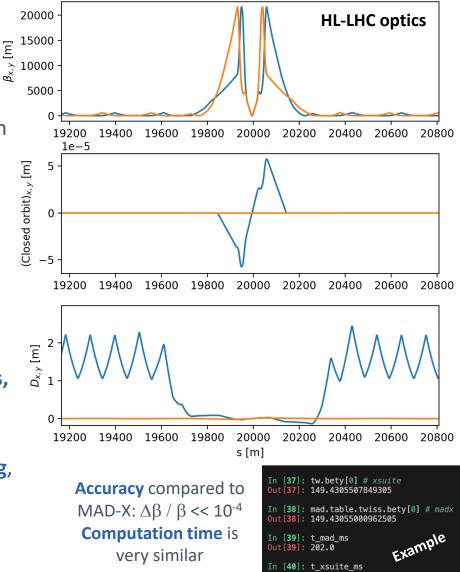
Courtesy M. Hofer







- 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 ( $\alpha$ ,  $\beta$ ,  $\gamma$ ), dispersion functions, phase advances, coupling coefficients
- Computation can be done with assigned beam momentum to get off-momentum beta-beating, non-linear chromaticity, non-linear dispersion, etc.





- In accelerators often a single high-level parameter can be used to control groups of components with complex dependency relations. (e.g. circuits with multiple magnets, 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:

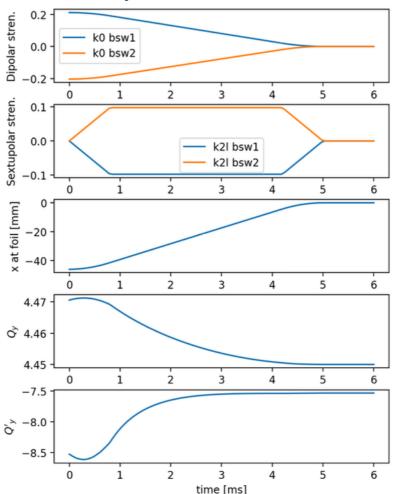
At any time, the user can set:

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<sup>-</sup> injection into the CERN PS Booster

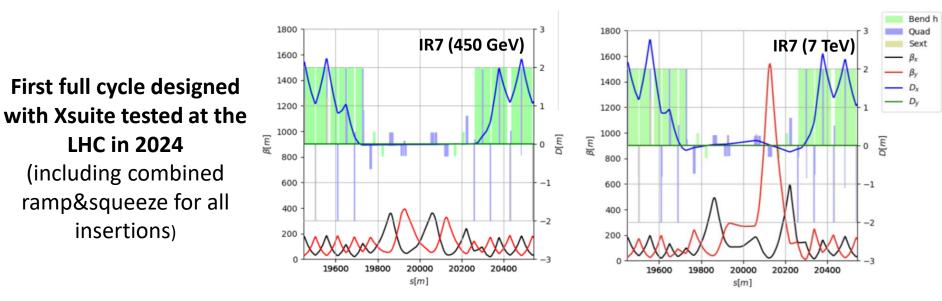






Xsuite provides a **multi-objective optimizer** to "match" model parameters to assigned constraints (e.g. control tunes, chromaticity, build orbit bumps, design the optics)

- Based on the extensive experience of MAD-X → Uses the same optimization algorithm (Jacobian, proven robustness)
- 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



Courtesy R. De Maria and B. Lindstrom

## Outline



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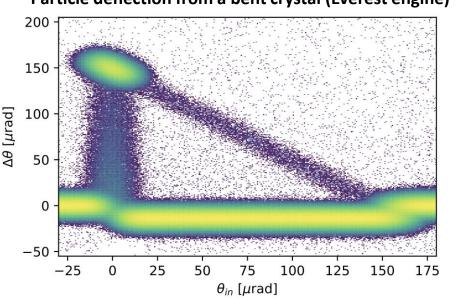
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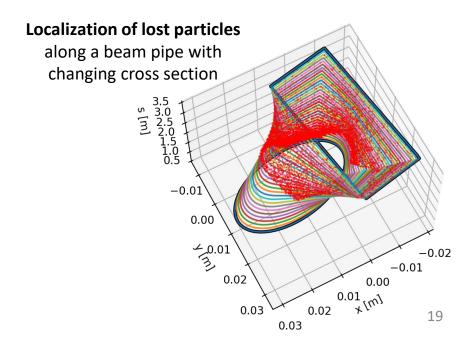


## **Particle-matter interaction**

For collimation studies, the Xcoll module provides three particle-matter sim. engines:

- The **"Everest" engine** embedded in Xcoll (evolution of K2 module from Sixtrack)
- The "Geant 4" engine, based on an interface with BDSIM-Geant4
  - Used for FCC-ee collimation studies (see presentation by G. Broggi)
- 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)





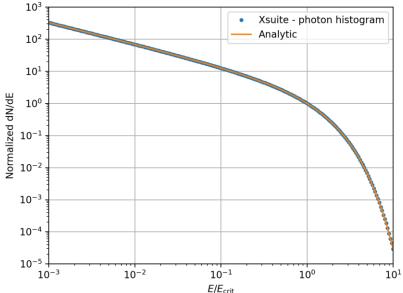
#### Particle deflection from a bent crystal (Everest engine)

## **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<sup>(1)</sup>.

#### Validation against analytical photon spectrum





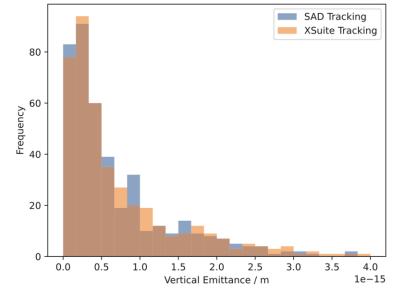
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## Benchmark of equilibrium emittaces from tracking (with lattice errors)



L. Van van Riesen-Haupt, T. Pieloni, et al., EPFL



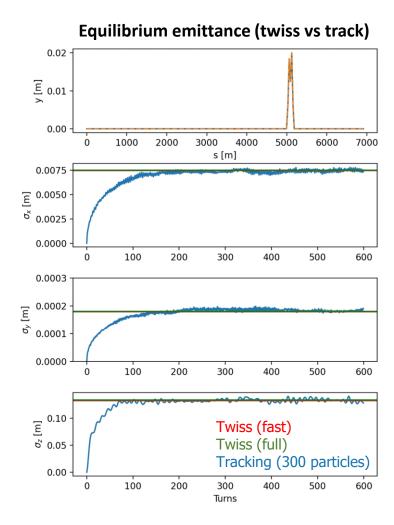
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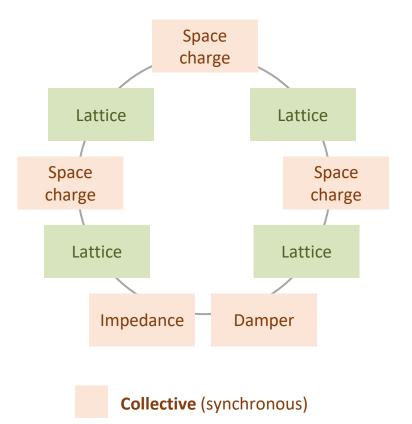
The Xsuite Twiss also includes:

- Dedicated algorithm for non-symplectic one-turn map<sup>(2)</sup>
- 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")



<sup>(1)</sup> Based on H. Burkhardt, "Monte Carlo generator for synchrotron radiation", 1990. Implementation ported from PLACET (A. Latina) <sup>(2)</sup> E. Forest, From tracking code to analysis: generalised Courant-Snyder theory for any accelerator model. Springer, 2016

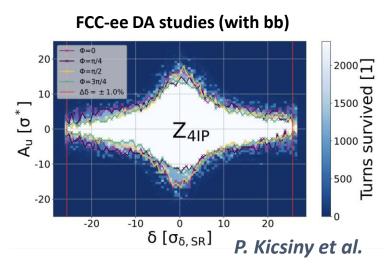


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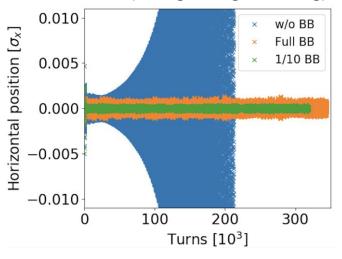
Single-particle (asynchronuos)

- 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
- 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

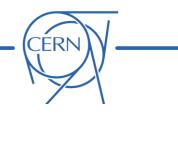


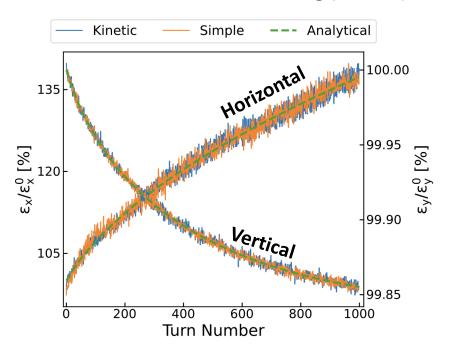


Wakefield + beam-beam simulations for HL-LHC (strong-strong modelling)



- 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, "soft Gaussian")
- For the simulation of lepton colliders, the code can also simulate for **beamstrahlung** and **Bhabha** scattering (developed in collaboration with EPFL)
- Strong-strong simulations are accelerated by parallel computing on HPC clusters (based on MPI)
  - "Pipeline" algorithm<sup>(1)</sup> used to optimize workload distribution across the nodes
  - (1) S. Furuseth and X. Buffat, Comput. Phys. Commun. 244 (2019)
    (2) For more details, see presentation by P. Kicsiny





#### Benchmark case for the SPS ring (Pb ions)

**Intra Beam Scattering (IBS)** simulation capabilities have been recently introduced:

- **IBS growth rates computation** from beam parameters and optics. Two methods available:
  - <u>Nagaitsev</u> (very fast, vertical dispersion neglected)
  - <u>Bjorken-Mtingwa</u> (slower, *D<sub>y</sub>* correctly accounted)
  - Effect of IBS can be included in multiparticle simulations in combination with all other effects available in Xsuite. Two methods available:
    - o <u>Effective kick</u>
    - o Kinetic formalism

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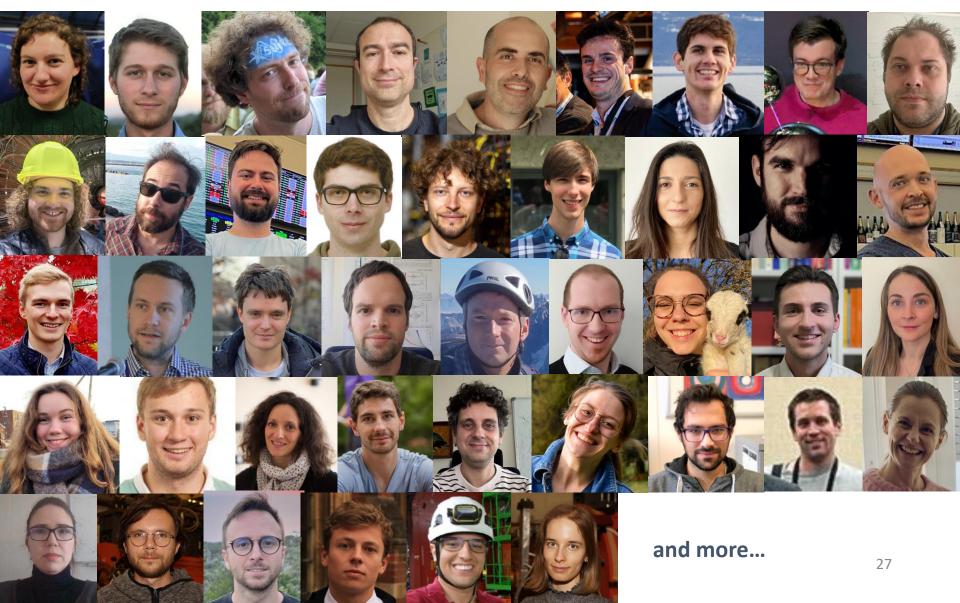
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## **Final remarks**



After three years the software has grown very rapidly, thanks to many people contributing code and expertise...



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#### Response went well beyond our expectation:

FR

- >30 colleagues from CERN and other labs contributed by developing new features and debugging issues
  - Leveraging their python skills and the short tool-specific learning curve
- Xsuite was adopted by a large and diverse user community (>100 users!!!)
  - Very lively community providing mutual support, advice, lots of feedback to developers (very precious!)
  - For first time at CERN we are using the same software tool for optics, dynamic aperture studies, collimation, beam-beam, space-charge, instabilities, lepton machines, extraction and beam transfer studies and more...
    - Already profited from lots of synergies
  - Adopted for many FCC studies (counted ~10 talks in this workshop presenting work based on Xsuite)



and more...



## Xsuite simulations have been already used for **studies covering a variety of rings**:

## CERN

- ELENA
- LEIR
- PSB
- PS
- SPS, TI2, TI8
- LHC
- Muon collider
- LEP

- GSI
- SIS-18
- SIS-100

## **Medical facilities**

- HIT (Heidelberg) •
- FCC-ee, FCC-hh MEDAUSTRON
  - PIMMS
  - NIMMS

## **BNL**

- RHIC
- Booster
- EIC

#### **Fermilab**

- Main injector •
- Recycler
- Booster
- IOTA

- Light sources and damping rings:
- PETRA
- DESY injector ring
- **ELETTRA**
- **BESSY III**
- CLIC-DR
- ... and more

Each of these tought us something and contributed to extend and improve the software!



- CERN Accelerator and Beam Physics group is **committed to maintain Xsuite** and support its users for the years to come
  - For other legacy tools (e.g. MAD-X, PyHEADTAIL) we will keep present level of functionality and support for as long as needed, while focusing resources on the development of this stack.
- Xsuite development continues:
  - Next items on our plate include 3D PIC for beam-beam, spin tracking, insertion devices, quadrupole fringes, and more...
- The code is **publicly available** on GitHub and can be installed through pip
  - You are **vey welcome to give it a try** for your use case
  - Installation instructions and many examples available in the documentation pages
  - We are very interested in getting your **feedback** (don't hesitate to contact us for issues, questions, suggestions)
- Code is **open-source** and is open to **developments from the community** 
  - Get in touch if you are interested in contributing to the development



# **Thanks for your attention!**

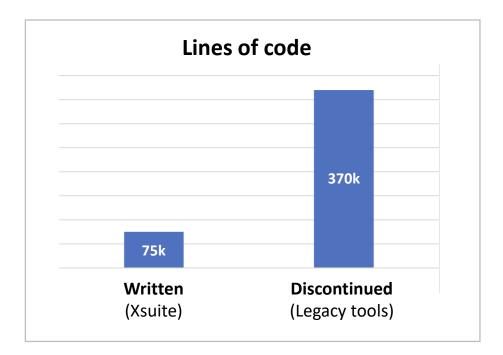


In 2022-23 we have **essentially discontinued** the development and, to a very large extent, the usage of the following tools:

- Sixtrack
   COMBI
- Sixdesk
   PySSD
- Sixtracklib

• DistLib

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



## Space charge

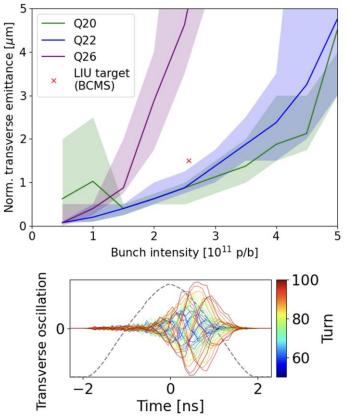


# The implementation is largely based on **PyHEADTAIL-PyPIC**

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

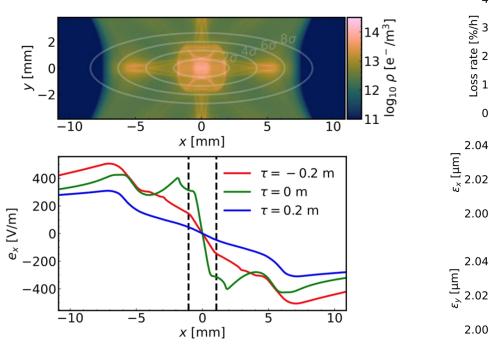


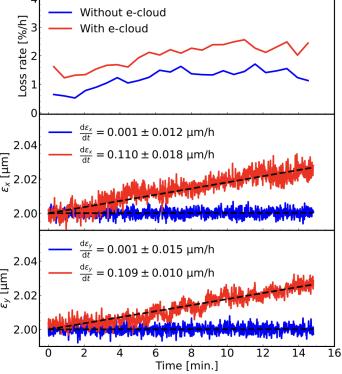
N. simulations	400
Number of PIC calculations per turn	540
Number of turns per simulation	40'000
Computing time per sim. (GPU)	~3 days
Computing time per sim. (CPU serial)	> 12 months
Courtesy X. Buffat	



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<sup>6</sup> turns).





See also: K. Paraschou, THBP16



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

- Any physical model included in the tracking is automatically usable in Twiss
  - o 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

