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SIXTRACK VERSION 5: STATUS AND NEW DEVELOPMENTS*

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Abstract

SixTrack Version 5 is a major SixTrack release that introduces new features, with improved integration of the existing ones, and extensive code restructuring. New features include dynamic-memory management, scattering-routine integration, a new initial-condition module, and reviewed post-processing methods. Existing features like on-line aperture checking and Fluka-coupling are now enabled by default. Extensive performance regression tests have been developed and deployed as part of the new-release generation. The new features of the tracking environment developed for the massive numerical simulations will be discussed as well.

MAIN FEATURES

SixTrack [1] is a 6D single-particle symplectic tracking code for studying dynamic aperture (DA) or evaluating the performance of beam-intercepting devices like collimators [2]. SixTrack is licensed as GNU Lesser General Public License software and is under very active development in the GitHub repository [3]. Extensive restructuring and new features have been added in the last years. The SixDesk runtime environment manages SixTrack simulations from input generation, job queue management (using HTCondor [4] in the CERN BATCH service [5] and customised software in the CERN BOINC server [6]), to collecting and post-processing results. This paper presents a summary of the existing features in the last SixTrack and SixDesk releases and focuses on some of the most recent developments.

SixTrack computes very efficiently the trajectories of individual relativistic charged particles in circular accelerators by using explicitly 6D symplectic maps (see [7] and references therein), or scattering elements. The set of coordinates used internally is larger than the minimum needed to describe the motion. Additional variables are used to store energy-related quantities and are updated only on energy changes, which do not occur very frequently in synchrotrons in the absence of radiation effects, to save computational time. Thick maps for dipoles and quadrupoles also reuse the energy-dependent factors of the first- and second-order polynomials of the map that are recalculated at each energy change. Furthermore, different ion species can be tracked at the same time using an extension of the usual symplectic formalism (see later).

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SixTrack tracking maps are optimised for speed and numerical reproducibility. Scattering maps are being refactored to be numerically reproducible, thus increasing the type of simulations that can be ported to LHC@Home [8]. SixTrack can also be linked with the BOINC library [6] to use the volunteer computing project LHC@Home.

SixTrack can compute linear and non-linear optical functions using a 5D matrix code and a 6D truncated power series algebra (TPSA) tracking code. Coupled Twiss parameters, using the Mais-Ripken formalism [9], can be extracted along the lattice. The optical parameters are optionally used in the beam-beam elements for self-consistent simulations.

Differently from other codes, SixTrack uses ($\sigma = s - \beta_0\, c\, t$) as the longitudinal coordinate during tracking to avoid rounding errors associated to the relativistic β when updating time delays in drifts and $\left(\zeta = \frac{\beta}{\beta_0}\sigma,\ \delta = \frac{P-P_0}{P_0}\right)$ as conjugate canonical variables in 6D optics calculations.

Table 1: Physical Elements Implemented in SixTrack

Drift expanded	Drift exact [10]
Single thin multipole	Thin multiple block
Thick dipole-quadrupole	Thin solenoid
Accelerating cavities	RF-multipoles [11]
4D-6D beam-beam [12]	Wire [13]
Electron lens [14]	Fringe fields [15–17]

Table 1 shows the different types of beam-line elements implemented in SixTrack. Thin multipoles are used in conjunction with the `MAKETHIN` and `SIXTRACK` commands in MAD-X [18] to implement symplectic integrators of thick maps. Thin multipoles include the effect of the curvature, when present, up to second order. Recently, a model of s-dependent fringe fields has been merged and is being used to study the impact on the dynamic aperture of the field quality of the new triplet quadrupoles foreseen in the HL-LHC [19].

SixTrack allows setting turn-varying functions for most of the beam elements and simulation parameters (see `DYNK` module [20] and references therein), including multipoles, RF amplitude and phase, reference energy, and beam-beam elements. These functions are specified using a flexible language that allows combining functions to achieve the required effect.

Initial conditions can be given in normalised-amplitude steps or taken from an external file. A general distribution module is under development to generate matched or

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mismatched distributions in both physical and normalised coordinates so to enable more flexible coordinates' scans.

A dump module offers multiple ways to extract tracking data both in terms of type of observable, such as physical, canonical, or normalised coordinates, averages and second-order momenta distribution, over a selection of turns and observation points. Data are written in ASCII and, in a few cases, a binary option is also available. Support for output of simulation data to HDF5 [21] files and ROOT [22] is also currently being developed. SixTrack includes a general interface `BDEX` for interfacing to external codes using Unix pipes [23]. This enables, for instance, tracking of multiple bunches or coupling to cavity-simulation codes.

SixTrack implements a set of methods to extract chaos indicators, which are used, in conjunction with the SixDesk environment, to study the dynamic aperture of a lattice. A collection of routines (from PLATO [24] and NaffLib [25]) for frequency analysis have been linked in SixTrack.

A CMake/CTest-based build and test system has recently been added [23] and integrated in the GitHub workflow. It allows building and testing executables under an extensive set of operating systems, CPU architectures, and compilers.

Thanks to the recent re-factoring, the internal particle arrays are fully dynamic, therefore the number of particles that can be tracked in parallel is only limited by the system memory and not by a build-time flag. As an example, an LHC lattice model (made of about 18k elements and 4.6k high-order multipole blocks), needs about 220μs per particle per turn on a single-CPU core at 3.4 GHz. The dynamic allocation introduced an overhead of only 5% to 10% with respect to the static version, after careful evaluation and re factoring of CPU-sensitive code.

SCATTERING

SixTrack is widely used for simulating the performance of a collimation system in circular machines [26–29], which considers the physics of scattering events undergone by particles in beam-intercepting devices on a turn-by-turn basis. The `K2` scattering engine [30, 31] was initially embedded in SixTrack [32] and used for the design of existing cleaning systems [33, 34].

In the coupling [35] between FLUKA [36] and SixTrack, the two codes exchange particles at run-time. Tracked particles are handled by either of the codes depending on whether the tracking takes place in the accelerator lattice or in a beam-intercepting device. Contrary to `K2`, FLUKA is a full Monte Carlo code for particle-matter interactions. It allows dealing with any hadron, lepton, and ion species interacting with any elemental or composite material with arbitrarily complicated geometries, greatly increasing the accuracy of results and the range of potential applications. In addition, the same collimator geometries and material definitions used for subsequent energy-deposition calculations can be deployed, thus increasing the degree of consistency of results.

The SixTrack scatter module was added recently to generate scattering events at the interaction points for medium- and long-term tracking simulations. The scattering point is inserted as a marker in the lattice, and elastic or diffractive events are generated on the fly [37]. The scattering probability can be scaled on a turn-by-turn basis via the `DYNK` module.

At present, one internal event generator is provided by SixTrack. This generator provides elastic events by Monte Carlo sampling of a fit to data published by the TOTEM Collaboration [38]. Pythia8 [39] is also available as an event generator, but must be included via a compiler flag when SixTrack is built. When the Pythia integration is available, access to the SoftQCD event generator is provided via the scatter configuration section of the SixTrack input file, as well as a separate Pythia configuration block.

TRACKING OF ARBITRARY CHARGE-TO-MASS RATIO PARTICLES

Previous work on tracking of ions [40], and by extension, any generic particle with any charge-to-mass ratio, has been implemented in SixTrack. This allows tracking of particles other than protons, such as heavy ions, and even electrons (synchrotron radiation effects are yet to be included).

In conjunction with the updates to the scattering code described in the previous section, this allows the tracking of all charged particle types exiting a collimator as a result of the interaction of a primary charged particle with the collimator jaw. These secondary particles can interact further with downstream collimators. In order to account for a potentially large number of secondary particles generated by a collimator interaction, all SixTrack internal particle arrays are dynamically allocated, and will be expanded automatically as required when the number of tracked particles changes within a simulation run.

ON-LINE APERTURE CHECKING

SixTrack can verify that particles fall onto the mechanical aperture of the machine during tracking. The implementation extends what was set up in the past [32] by adding new shapes. Transverse offsets (horizontal and vertical) and angles about the longitudinal axis can be specified as well. A smooth, linear interpolation between all supported aperture markers ensures that the aperture is well defined at any location along the ring. The bisection method, faster than the original one, is used to determine the location of the final loss point, down to any desired accuracy. For the time being, the feature is available only for thin-lens tracking, where back-tracking is comfortably performed along a drift, but extension to thick-lens linear elements is in plan.

ELECTRON LENSES

Electron lenses can be used to deplete over-populated beam tails in a controlled manner or to compensate beam-beam effects [41]. The former application is currently being investigated in the framework of the HL-LHC project [42]. The original implementation [14, 43] has been greatly extended, e.g. to ion tracking, relevant for benchmarking recent

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measurements at RHIC [44]; to model measured radial profiles of electron beams; to model Gaussian electron-beam profiles for beam-beam compensation. The code is compatible with LHC@Home, relevant for evaluating long-term effects on dynamic aperture. All new features are also compatible with the time-varying module DYNK. The extension of the module to lenses made of arbitrary charged particles is on-going.

ELECTRIC-POTENTIAL MAPS AND CHEBYSHEV POLYNOMIALS

SixTrack has been extended to deal with electric-potential maps described by means of Chebyshev polynomials of the first kind. These are univariate polynomials in x and y, defined recursively by means of linear operations. Their product describes a 2D electric-potential field, integrated longitudinally; the kicks are computed by SixTrack as derivatives of the potential map. There is no upper limit to the deployed order. The user can also define an offset and a rotation angle about the longitudinal axis to be applied to the map to enhance flexibility.

Chebyshev polynomials are extremely valuable for describing non-linear systems and their dynamics. Maps derived from a 2D potential expressed with Chebyshev polynomials are 4D-symplectic by construction. In the current implementation, the longitudinal coordinates are not modified. The development is especially promising for simulating effects on beam dynamics from the injection of the electron-lens beam into the beam pipe or to simulate the effect from non-ideal electron distributions in the electron lens [45].

TRACKING ENVIRONMENT

The SixDesk runtime environment [46] allows the large amount of information necessary for SixTrack studies of dynamic aperture to be managed. These studies are based on massive simulation campaigns, where the beam phase space is scanned and different machine configurations, e.g. tune, chromaticity, octupole current, beam intensity, crossing bump conditions, etc., are sampled. Each SixTrack job covers a little portion of the whole space spanned, dedicating CPU time to tracking for a large number of turns (typically 10^5–10^6), such that the onset of chaotic motion can be detected.

SixDesk currently supports both the CERN batch system [5] as well as the BOINC platform for volunteer computing [6], available at the LHC@Home project since 2004. The former, based on HTCondor [4], provides users with a responsive computing resource. The latter provides additional computing power for CPU-intensive applications with small data sets on as many operating systems, architectures, and CPU instruction sets as possible, with important requirements on code structure, build system and test suite.

LHC@home is capable of handling 1×10^5 tasks on average, with peaks of 3.5×10^5 tasks simultaneously running on 2.4×10^4 hosts observed during SixTrack massive simulation campaigns. Task redundancy is deployed to eliminate random host errors and minimise the impact of a failing host. The LHC@Home capacity available for SixTrack can be compared to the average of 2.5×10^5 running tasks on 1.4×10^5 processor cores in the CERN computer centre, which is fully loaded with tasks from analysis of collisions recorded by LHC experiments, and has limited spare capacity for beam dynamics simulations.

The SixDeskDB post-processing tool collects data from SixDesk, performs post-processing analysis, and prepares reports and plots. It also offers a Python application programming interface (API) for interactive analysis.

Similarly to the SixTrack code, the SixDesk environment and SixDeskDB are continuously updated, extending the coverage of the studies and keeping the environment up to date with the latest developments in the CERN IT infrastructure. In particular, a relevant effort is on-going to port the present system fully under Python 3.7, including all the tool suites for collimation studies.

CONCLUSIONS

SixTrack is actively developed and used in production studies in particular for CERN accelerators, existing, under upgrade or future. In recent years it gained flexibility, additional features, and a robust development framework, while maintaining backward compatibility and excellent performance. New features like generic distributions, refined post-processing, and GPU offloading are planned to be implemented in the future.

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