RECENT DEVELOPMENTS WITH THE NEW TOOLS FOR COLLIMATION SIMULATIONS IN Xsuite

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Abstract

Simulations of single-particle tracking involving collimation systems need dedicated tools to perform the different tasks needed. These include the accurate description of particle-matter interactions when a tracked particle impacts a collimator jaw; a detailed aperture model to identify the longitudinal location of losses; and others. One such tool is the K2 code in SixTrack, which describes the scattering of high-energy protons in matter. This code has recently been ported into the Xsuite tracking code that is being developed at CERN. Another approach is to couple the tracking with existing tools, such as FLUKA or Geant4, that offer better descriptions of particle-matter interactions and can treat lepton and ion beams. This includes the generation of secondary particles and fragmentation when tracking ions. In addition to the development of coupling with Geant4, the SixTrack-FLUKA coupling has recently been translated and integrated into the Xsuite environment as well. In this paper, we present the ongoing development of these tools. A thorough testing of the new implementation was performed, using as case studies various collimation layout configurations for the LHC Run 3.

INTRODUCTION

Xsuite is a modern Python toolkit developed at CERN to simulate particle behaviour in an accelerator [1, 2]. It aims at integrating existing tools for different applications into one framework, and as such currently consists of 6 individual Python packages: Xobjects, Xdeps, Xpart, Xtrack, Xfields, and Xcoll. The focus of this paper lies on the latter, which is dedicated to integrating collimation simulations featuring particle-matter interactions into this new framework [3].

Simulations that study how beam-intercepting devices like collimators influence the performance of an accelerator make use of two different types of software, namely a dedicated tool to track the 6D motion of a charged particle in an accelerator lattice, and a Monte Carlo simulation package for the interaction and transport of particles (including leptons and nuclei) in matter. For the former, SixTrack [4–12] has been the standard at CERN for many years, while for the latter two tools are principally used at CERN, namely FLUKA [13–19] and Geant4 [20–22]. Next, one needs to construct a communication that guarantees the adequate exchange of particles from the tracking code to the material interaction code and back. In the case of FLUKA this is managed by the FlukaIO coupling [23–26] which uses a network protocol for reliable transmission, while in the case of Geant4, this communication is handled by the BDSIM interface [27–30] which acts as a dedicated API to the Geant4 engine. Additionally, for simulations involving only protons without fragmentation, SixTrack has a built-in scattering engine called K2 to simulate proton-matter interactions [4, 31–33]. It greatly simplifies both the initial setup and final post-processing, while vastly reducing the necessary computation time, with excellent results when its output is used as input to FLUKA for energy deposition. All three scattering engines have been thoroughly benchmarked against experiment and each other.

A NEW APPROACH

With the advent of Xsuite and its move to Python and its modular approach, adapting the collimation code to the same environment is a logical step. Due to the complicated nature of this type of simulation, in particular the internal scattering engine and the coupling to external tools, this migration is quite challenging. Significant progress has been made, and we are nearing a complete integration into Xsuite. Furthermore, thanks to its design based on JIT (just-in-time) compilation to C, Xsuite is constructed to be compatible with many different architectures including GPUs [34]. The migration to Xsuite hence opens the road to high-performance computing for collimation as well.

Most tools needed to perform collimation studies in Xsuite are collected into the Xcoll Python package [3]. These include, but are not limited to:

- The management of collimator settings in a lattice via a database on file or in memory, and the automatic conversion of the collimator jaw openings in units of the transverse beam size into physical units;
- The generation of matched particle distributions, such as an annular halo or a pencil beam [35] at a given location, for a CPU-efficient simulation of the first particle encounters with the collimators (Xpart);
- An interpolation of losses on the aperture, to precisely define their location along the lattice (Xtrack);
- The logging of particles that are scattered by and absorbed in collimators and the aperture, in order to create a longitudinal histogram of losses (a loss map);
- The inclusion of and connection to adequate scattering engines to describe particle-matter interactions.

These capabilities were already present in the SixTrack environment, however, due to the modular nature of Python they become much more flexible in use and are easily expandable.

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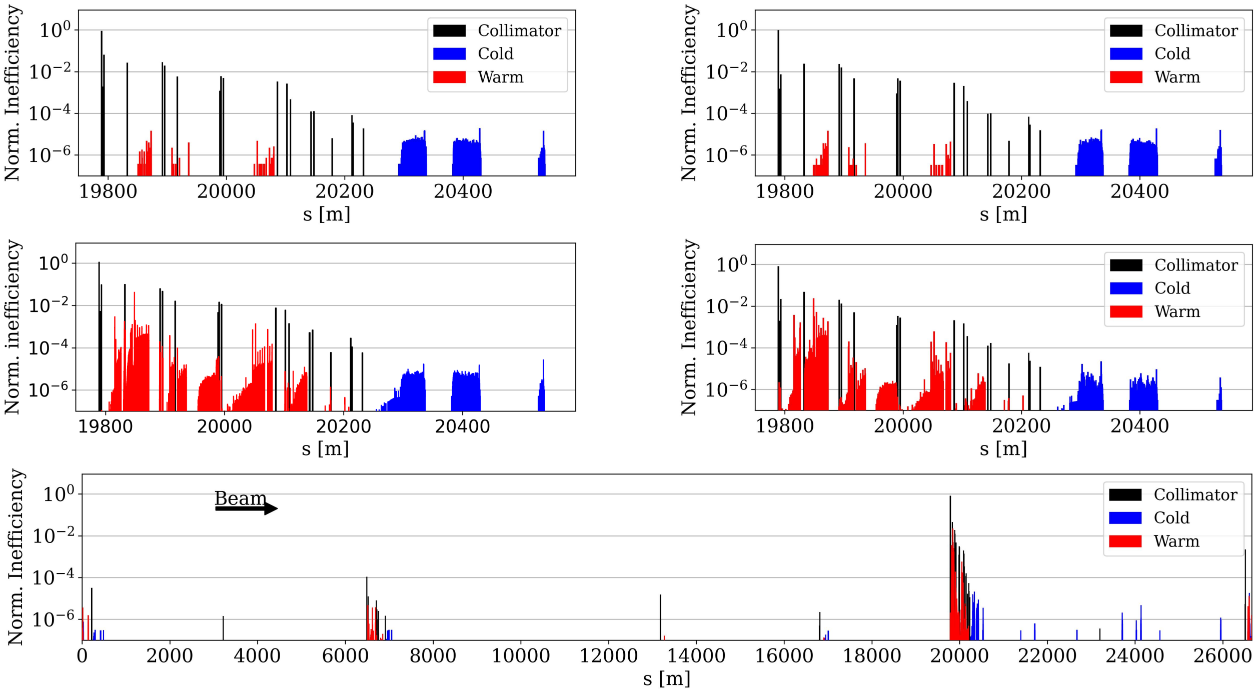

Figure 1: Comparison between simulated B1V loss maps for the LHC in SixTrack K2 (top left), Xcoll Everest (top right), Xcoll+Geant4 (mid left), and Xcoll+FLUKA (mid right). Shown is a zoom on the IR7 insertion containing the collimators for betatron cleaning (top and mid) and a full ring overview (bottom, Xcoll + FLUKA). Red and blue lines represent aperture losses in warm resp. cold regions and black lines represent losses on the collimators. The values are scaled by length and normalised by the losses on the primary collimator.

Recently, two more tools were added to Xcoll, inspired by existing possibilities in SixTrack and expanded upon:

- The logging of a detailed impact table, which registers the coordinates of each hit on a collimator and every type of physical interaction that has occurred inside;
- The implementation of an RF sweep, which adiabatically sweeps the frequency of the accelerating cavities.

The impact table has been very helpful in the development of the updated crystal routine (see next section), allowing us to trace and understand the chain of the multiple interactions that a particle can undergo in a long crystal. The RF sweep allows one to simulate in a realistic way an off-momentum loss map performed over several seconds, where one can see the losses shift from purely betatronic to dominantly off-momentum (see Refs. [3, 36] for more information).

EVEREST AND ITS CRYSTALS

The original FORTRAN implementation of the K2 routine, the scattering engine within SixTrack, was translated from its original implementation in FORTRAN into Xsuite-style C using Xobjects [34]. The new routine is renamed “Everest” [3], and encompasses nearly all functionalities present in the original K2 code, with the addition of several new features, such as user-definable collimator materials and the possibility to define precise collimator tilts. Comprehensive testing was conducted on the code to ensure statistical reproducibility against K2. In addition to the enhanced flexibility, a gain of a factor of two or more in computational speed has been observed. See the top line of Fig. 1 for a comparison between a loss map simulation performed in SixTrack K2 and Xcoll Everest (the other plots are simulated with Geant4 and FLUKA and will be discussed below).

In recent months, the subsequent phase of Everest’s development involved a substantial overhaul of the crystal scattering engine. The original implementation was limited to a single interaction at the midpoint of the crystal. While this approach is certainly justified for short crystals such as those employed in the LHC (~4 mm), for longer crystals such as envisioned for the Physics Beyond Colliders project (several cm) [38], a more suitable iteration of the code was essential. This necessitated an extensive refactoring of the source code, which, incidentally, significantly enhanced its readability.

A particle travelling inside a crystal can experience different interactions, depending on the direction of its movement with respect to the alignment of the crystal planes [39–42]. This is depicted in the top left plot of Fig. 2, where the different angular regions are as follows:

1. Amorphous: Interactions as in any other material, dominated by multiple-Coulomb scattering;
2. Channeling: A particle is captured between two crystal planes (and deflected by the curvature of the crystal);
3. Dechanneling: A channeled particle has a probability to lose channeling and continue amorphously;
4. Volume reflection: A particle travelling amorphously can reflect off the crystal planes;

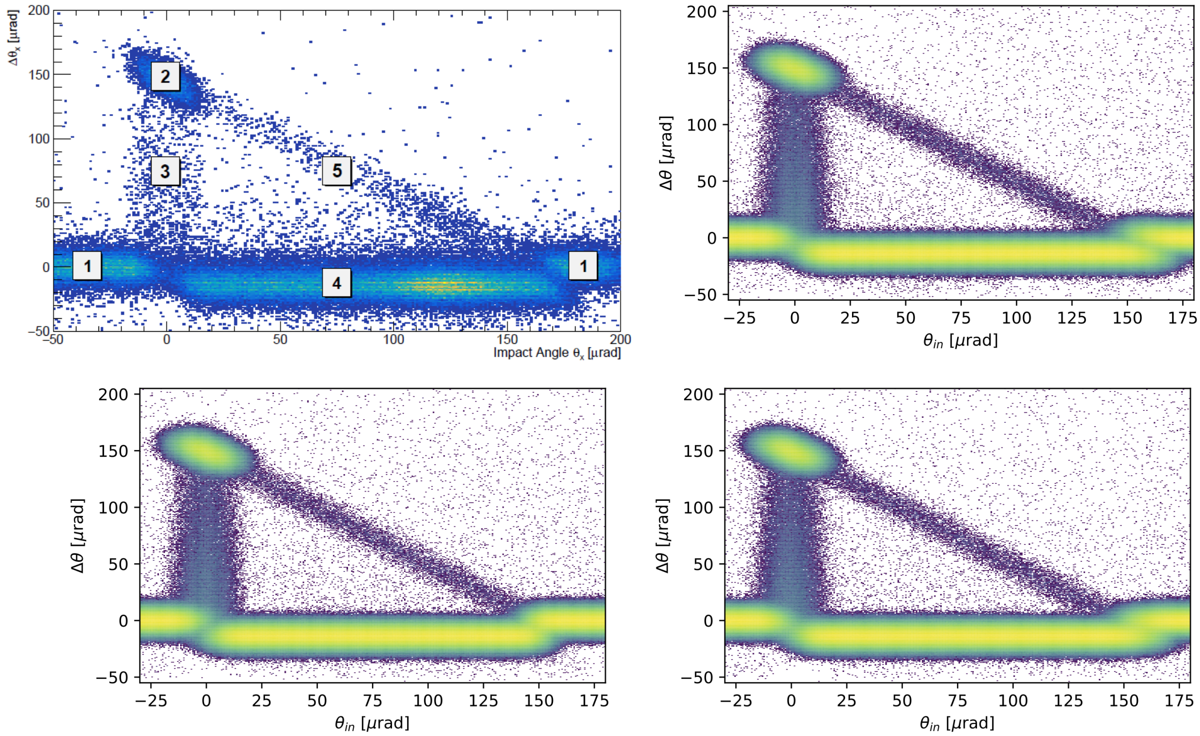

Figure 2: Deflected angle in function of the initial angle. Measurement data from Ref. [37] (top left). Simulation performed with SixTrack K2 (top right), with Xcoll Everest without transition effects (bottom left), and with Xcoll Everest with transition regions included (bottom right). All simulations include an angular smear of 2.8 μrad to account for the detector resolution.

5. Volume capture: A particle travelling amorphously can start channeling;

Amidst the process of code revision, a few inconsistencies were found and adapted. One of these was related to the channeling probability being artificially saturated, and another one to the longitudinal location of volume reflection and volume capture. These and other inconsistencies will be elaborated upon in a forthcoming follow-up paper.

A final observation on the crystal physics pertains to the transition from volume reflection to the amorphous regions (from region 4 to 1 in the top left plot of Fig. 2) which have a dedicated implementation in SixTrack. After having adapted the aforementioned inconsistencies, these transition regions might be unnecessary. The bottom line of Fig. 2 shows plots for Everest simulations with and without transition regions. This difference will be investigated in depth in the future and benchmarked against recent new measurements performed with long crystals.

GEANT4 AND FLUKA

The integration of Geant4 into Xsuite was initiated at an early stage, capitalising on the existing Collimasim and BDSIM software tools that establish the connection between Geant4 and various tracking codes [43, 44]. Recently, progress has been made towards incorporating this framework into the Xcoll package. While this remains a work in progress, an initial loss map has been generated, as illustrated in the mid left plot in Fig. 1.

Likewise, efforts have begun to translate the SixTrack-FLUKA coupling into Xcoll, as indicated by the mid right loss map in Fig. 1. However, this process is considerably more intricate, involving multiple layers of code nesting within one another. A similar approach is being employed as in the previous translation of K2 to Everest [3], where the existing FORTRAN code is initially encapsulated and invoked from Python. Subsequently, this encapsulation layer is gradually phased out, culminating in direct calls to the FlukaIO code responsible for the coupling from within the underlying Xobjects API in C. This transition is expected to yield significant improvements in computation time. Furthermore, the development of a user framework capable of generating the requisite FLUKA input files from within Xcoll is essential. This will enable the harnessing of Xsuite's modularity and flexibility for FLUKA coupling simulations.

CONCLUSION

Recent developments in Xcoll have brought critical features for collimation simulations to the Xsuite framework. The user interface of Xcoll continues to expand, while the updated crystal routine in Everest facilitates more precise modelling of crystal interactions. Finally, the incorporation of Geant4 and FLUKA is progressing at a steady pace, with the partial integration already being used for various physics studies like in Refs. [36, 45], yielding promising results.

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