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RELEASE OF CRYSTAL ROUTINE FOR MULTI-TURN PROTON SIMULATIONS WITHIN SIXTRACK V5

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Abstract

Crystal collimation is studied as a possible scheme to further improve the efficiency of ion collimation at the High-Luminosity Large Hadron Collider (HL-LHC), as well as for possible applications in the CERN program of Physics Beyond Colliders. This concept relies on the use of bent crystals that can deflect high-energy halo particles at large angles, of the order of tens of µrad. In order to reproduce key experimental results of crystal collimation tests and predict the performance of this system when applied to present and future machines, a dedicated simulation routine was developed. This routine is capable of modeling both coherent and incoherent interactions of beam particles with crystal collimators, and is fully integrated into the magnetic tracking and collimator modeling provided by the single-particle tracking code SixTrack. This paper describes the implementation of the routine in the latest version of SixTrack and its most recent improvements, in particular regarding the treatment of the crystal miscut angle.

INTRODUCTION

SixTrack [1–3] is a single-particle tracking code widely used at CERN for simulating beam dynamics in circular accelerators. It performs a symplectic and fully chromatic tracking of protons and, as of recently, ions [4, 5] through a magnetic lattice which includes all the different elements of the machine that affect the beam dynamics (such as magnets, RF cavities, etc.).

Collimation studies require a specific version of SixTrack, which implements essential physics to treat the interaction of beam particles with the constituting material of machine elements [6, 7]. The code is routinely used to predict the distribution of losses in the ring [8], which can be compared to the loss distribution measured in operations.

Crystal collimators, however, require a dedicated simulation routine which was originally implemented in SixTrack v4 [9, 10]. This routine models the interaction between proton beams and crystal collimators via a Monte-Carlo simulation based on the theoretical description of coherent interactions between charged particles and bent crystals [11, 12]. Only simulations of proton beams are supported.

A series of major changes implemented in SixTrack over the years were grouped in a new version of the code, named SixTrack v5 [13]. The crystal simulation routine, on the other hand, was never part of the official release. As such, it was never made available to the general public and could not profit from these improvements, remaining instead based on SixTrack v4.

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In 2019, a code development effort was launched in order to make the crystal routine compatible with SixTrack v5 and, as of version 5.4.1, the routine is part of the official SixTrack release [14, 15]. This process offered the chance to develop new features such as an improved treatment of the crystal miscut angle.

MOTIVATION FOR IMPLEMENTATION IN SIXTRACK V5

Since the first implementation of the original crystal simulation routine, many features where added to SixTrack [16–19], such as:

- The *online aperture check*, i.e. the capability to check if particles are lost on the machine aperture while the simulation is running, instead of saving their trajectories for an offline check by a separated program.
- The possibility to run large statistics simulations on BOINC [20], a platform that supports parallel computing on distributed systems.
- The ability to dynamically allocate data arrays.
- The DYNK module, used to change element settings within a simulation on a turn-by-turn basis.
- The coupling with other codes (such as FLUKA [21] and Geant4 [22]) to treat interactions with materials.
- A generally more streamlined structure for the input files to set the parameters of the simulation.
- Various other code optimizations that reduced the time required to run simulations in many scenarios.

The implementation of the crystal routine in SixTrack v5 takes advantage of all of these features. In the porting, all the crystal-related physics calculations were kept in their own separate modules, which are independently called whenever a crystal collimator is encountered in a simulation.

BENCHMARK AGAINST THE ORIGINAL VERSION

The original routine was benchmarked against data gathered during crystal tests at the H8 extraction line in the CERN North Area [11, 23], at the SPS [10, 24] and at the LHC [15, 25, 26]. In order to verify that there were no changes in the crystal physics after the implementation in SixTrack v5, the same setup used for the benchmark against H8 data was chosen to compare the output of the two versions of the routine.

A single passage of a double Gaussian distribution of 400 GeV protons through a silicon crystal placed at the center of the beam line is simulated. The crystal is 2 mm long

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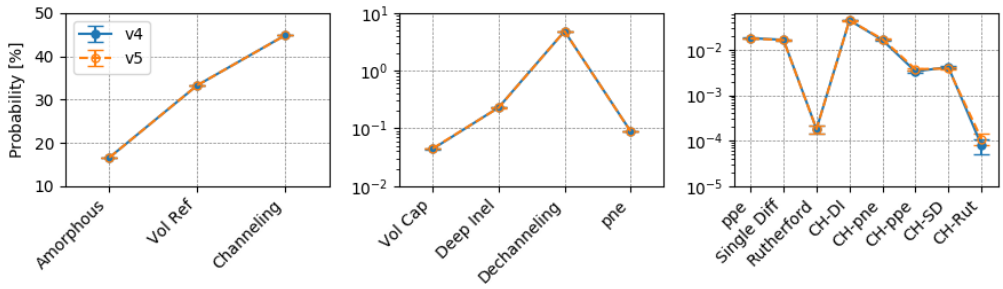

Figure 1: Process probability comparison between SixTrack v4 (blue) and v5 (orange) for 10^7 simulated protons interacting with a silicon crystal. Statistical errors are calculated as $\sqrt{N}$, where N is the number of particles experiencing each process.

and its bending angle is 149 µrad. The outcome of the interaction, in terms of the fraction of particles that experience each specific process, is visually compared in Fig. 1. The comparison shows no significant differences, aside from very small variations in the least likely processes (probability lower than 0.02%) that are within the statistical errors.

In order to further assess the reproducibility of the results between the two routines, the respective output was also processed to reproduce some of the typical plots used to analyze and display data gathered at the H8 extraction line [11]. A typical quantity that can be extracted from measurements and then compared with simulations is the channeling efficiency of the crystal, i.e. the percentage of particles hitting the crystal that actually experience channeling for the entire crystal length. This quantity can be estimated from the distribution of the deflection angle, typically filtered by selecting only particles whose impact angle falls between $\pm\theta_c$ (i.e. 10 µrad for this particular benchmark setup). The channeling efficiency is calculated as the ratio of the 3σ integral of the Gaussian fit to the channeling peak and the statistics of the whole distribution [11, 27]. The results of this analysis are shown in Fig. 2. The deflection angle distributions produced by the two routines perfectly overlap, and the channeling efficiency calculated with the method described above for this setup (10^7 simulated protons) yields compatible values.

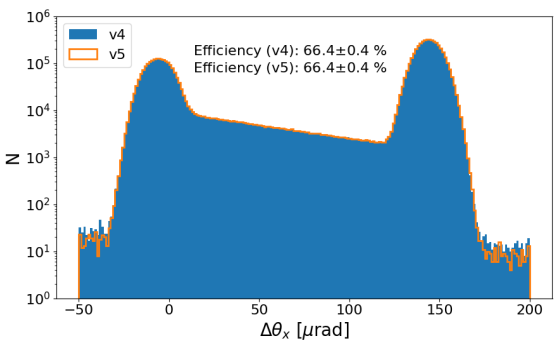

Figure 2: Simulated deflection angle distribution produced by SixTrack v4 (blue) and v5 (orange) for a silicon crystal, after a 10 µrad angular cut has been applied. The resulting channeling efficiency is reported in the plot for both routines.

Additional benchmark studies were dedicated to the complex multi-turn simulation setup at the LHC. Angular scans performed with proton beams at the LHC with the crystal as primary collimator [25] are simulated, in order to compare the results of the two routines at higher energy and taking into account multi-turn effects. The chosen setup is based on the machine settings used during crystal collimation tests at the LHC in 2018, with particular focus on the horizontal crystal installed on Beam 1. This is a 4 mm long silicon crystal with a bending angle of about 65 µrad. Different values of tilt angle with respect to the optimal channeling orientation are applied to the crystal. For each orientation, the percentage of simulated particles that is absorbed at the crystal is calculated in order to reconstruct the profile of local losses as a function of the tilt angle (i.e. the angular scan), which can be experimentally observed at the LHC. The results for a simulated scan at 450 GeV are shown in Fig. 3. The two routines produce consistent results, as the profiles overlap very well aside from fluctuations that are within the acceptable range for this kind of setup.

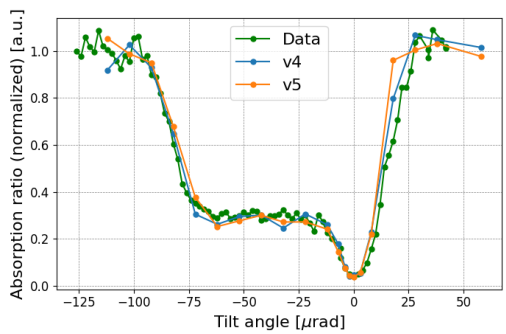

Figure 3: Simulated angular scan for the Beam 1 horizontal crystal at 450 GeV, compared with experimental data.

Running these simulations on the HTCondor batch system [28], widely used at CERN for high statistics simulations, it was possible to compare the mean CPU time needed by the two versions of the routine to simulate each angular orientation. Figure 4 shows the ratio between the original and the new version. A factor higher than 1 indicates that the average CPU time required to run a simulation for that specific orientation is reduced when using the newly implemented routine. A general improvement can be observed at injection and even more noticeably at flat top. The detailed comparison shows the expected results of the migration from SixTrack v4

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to SixTrack v5, i.e. the most significant improvements are observed when the crystal is in amorphous orientation. In this configuration, the crystal acts as a very thin primary collimator, so a large number of turns is needed for a particle to be either absorbed at the crystal or lost elsewhere. To check which particles hit the machine aperture, SixTrack v4 spends a lot of time writing and reading the trajectory of all particles not lost on collimators at the end of the simulation. The *online aperture check* implemented in SixTrack v5, however, takes care of this passage automatically while the simulation is running. As a result, the required CPU time is greatly reduced for simulations which involve the tracking of large particle distributions for a significant amount of turns. A significant, albeit lower, reduction is also observed for orientations closer to channeling, where a smaller amount of simulated turns is required.

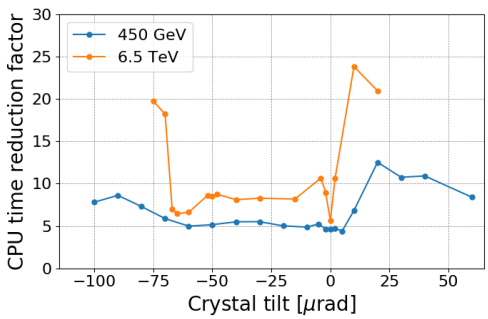

Figure 4: CPU time reduction factors between the original and new routine for the Beam 1 horizontal crystal at 450 GeV and 6.5 TeV. For each orientation, 640 particles per job are simulated. The number of turns increases from a few hundreds to a few thousands when changing the crystal orientation from channeling to amorphous.

Furthermore, the reduced size of the trajectory files produced by SixTrack v5 makes it possible to take advantage of LHC@Home, a volunteer computing project based on BOINC that uses internet-connected computers to carry out complex simulations of accelerator physics [29]. This was one of the key motivations, from a technical standpoint, to implement the crystal routine in SixTrack v5.

UPDATED MISCUT ANGLE TREATMENT

Crystal collimation simulations normally consider perfectly cut crystals with crystalline planes aligned to the lateral surface of the crystal facing the beam. In this case, a channeled particle will always experience a deflection equal to the nominal bending angle irrespective of its impact parameter, defined as the transverse distance between the lateral surface and the particle impact point. However, in reality a non-zero angle between the crystalline planes and the lateral face of the crystal is unavoidable. This is defined as a *miscut angle* and causes a series of edge effects that are especially important for particles that hit the crystal at impact parameters smaller than a certain critical value.

A first treatment of the miscut angle was implemented in the original crystal routine [9]. The migration of the routine to SixTrack v5 offered the opportunity to upgrade the treatment, using geometrical considerations to calculate the effective deflection angle and the distance traveled by channeled particles through the tilted planes of the crystal [15]. Furthermore, the coordinate transformations necessary to move from the machine reference system used for the tracking to the crystal reference system used for the treatment of the interaction are applied consistently in the new version, removing some artifacts introduced by the original version.

Simulation studies were carried out to investigate the effects of the miscut angle on particles with different impact parameters. Figure 5 shows preliminary results of the integrated beam profile obtained for different values of miscut, with impact parameters of the order of a few μm. For a negative miscut angle, channeled halo particles with small impact parameter exit from the side of the crystal rather than from the front face and experience a lower deflection than the crystal bending angle, populating the region between the fully deflected peak and the primary beam. As a result, a slow rise in the integrated beam profile is observed, rather than a saturation after the channeling peak is integrated. This effect is more noticeable for large values of the miscut angle. The new model is planned to be further benchmarked, in view of including it in the official release and using it to study the impact of these effects on crystal collimation.

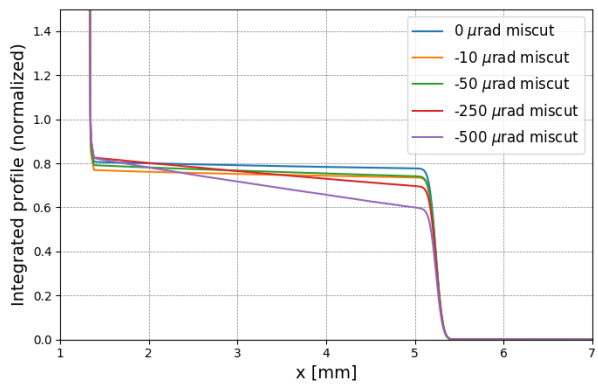

Figure 5: Integrated beam profile obtained in simulations for the LHC at 6.5 TeV with a primary crystal collimator with different values of miscut, as a function of the distance from the beam axis.

CONCLUSIONS

The simulation routine for the interaction of protons with bent crystals is now part of SixTrack v5 and available to the general public. This makes it possible to profit from the latest improvements of the tracking code, in particular recent developments of parallel computing on distributed systems. An updated treatment of the crystal miscut angle was developed and is currently being tested before the inclusion in the officially released routine.

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REFERENCES

[1] SixTrack – 6D Tracking Code, http://sixtrack.web.cern.ch/SixTrack/.

[2] F. Schmidt *et al.*, "SixTrack user's reference manual, Version 5.4.3", CERN, Geneva, Switzerland, Rep. CERN-SL-94-56, Dec. 2019.

[3] G. Ripken and F. Schmidt, "A symplectic six-dimensional thin lens formalism for tracking", CERN, Geneva, Switzerland, Rep. CERN-SL-95-12-AP, 1995.

[4] P. D. Hermes, "Heavy-ion collimation at the Large Hadron Collider: Simulations and measurements", Ph.D. thesis, Westfälischen Wilhelms-Universität Münster, Münster, Germany, 2016.

[5] N. Fuster-Martínez *et al.*, "Simulations of heavy-ion halo collimation at the CERN Large Hadron Collider: Benchmark with measurements and cleaning performance evaluation", *Phys. Rev. Accel. Beams.*, vol. 23, no. 11, p. 111002, Nov. 2020. doi:10.1103/PhysRevAccelBeams.23.111002

[6] G. Robert-Demolaize, R. W. Assmann, S. Redaelli, and F. Schmidt, "A New Version of SixTrack with Collimation and Aperture Interface", in *Proc. 21st Particle Accelerator Conf. (PAC'05)*, Knoxville, TN, USA, May 2005, paper FPAT081, pp. 4084-4086.

[7] R. Bruce *et al.*, "Status of SixTrack with collimation", in *Proc. ICFA Mini-Workshop on Tracking for Collimation in Particle Accelerators*, Geneva, Switzerland, Oct. 2015, pp. 1–10. doi:10.23732/CYRCP-2018-002.1

[8] S. Redaelli, *CERN Yellow Reports: Conference Proceedings*, Geneva, Switzerland: CERN, 2018.

[9] V. Previtali, "Performance evaluation of a crystal-enhanced collimation system for the LHC", Ph.D. thesis, EPFL, Lausanne, Switzerland, 2010.

[10] D. Mirarchi, "Crystal collimation for LHC", Ph.D. thesis, Imperial College, London, UK, 2015.

[11] D. Mirarchi, G. Hall, S. Redaelli, and W. Scandale, "A crystal routine for collimation studies in circular proton accelerators", *Nucl. Instrum. Methods Phys. Res. Sect. B*, vol. 355, pp. 378–382, Jul. 2015. doi:10.1016/j.nimb.2015.03.026

[12] D. Mirarchi, S. Redaelli, and W. Scandale, "Crystal implementation in SixTrack for proton beams", in *Proc. ICFA Mini-Workshop on Tracking for Collimation in Particle Accelerators*, Geneva, Switzerland, Oct. 2015, pp. 91–108. doi:10.23732/CYRCP-2018-002.91

[13] R. De Maria *et al.*, "SixTrack Version 5: Status and new developments", *J. Phys. Conf. Ser.*, vol. 1350, p. 012129, Nov. 2019. doi:10.1088/1742-6596/1350/1/012129

[14] SixTrack release version 5.4.1, https://github.com/SixTrack/SixTrack/releases/tag/v5.4.1/.

[15] M. D'Andrea, "Applications of crystal collimation to the CERN Large Hadron Collider (LHC) and its High-Luminosity upgrade project (HL-LHC)", Ph.D. thesis, Università degli Studi di Padova, Padova, Italy, 2021.

[16] R. De Maria, A. Mereghetti, J. Molson, and K. Sjobak, "SixTrack status", in *Proc. ICFA Mini-Workshop on Tracking for Collimation in Particle Accelerators*, Geneva, Switzerland, Oct. 2015, pp. 11–15. doi:10.23732/CYRCP-2018-002.11

[17] E. Skordis *et al.*, "FLUKA coupling to SixTrack", in *Proc. ICFA Mini-Workshop on Tracking for Collimation in Particle Accelerators*, Geneva, Switzerland, Oct. 2015, pp. 17–26. doi:10.23732/CYRCP-2018-002.17

[18] R. De Maria *et al.*, "SixTrack Project: Status, Runtime Environment, and New Developments", in *Proc. 13th International Computational Accelerator Physics Conference (ICAP'18)*, Key West, Florida, USA, Oct. 2018, pp. 172-178. doi:10.18429/JACoW-ICAP2018-TUPAF02

[19] K. Sjobak *et al.*, "Dynamic simulations in SixTrack", in *Proc. ICFA Mini-Workshop on Tracking for Collimation in Particle Accelerators*, Geneva, Switzerland, Oct. 2015, pp. 123–133. doi:10.23732/CYRCP-2018-002.123

[20] BOINC, https://boinc.berkeley.edu

[21] FLUKA, http://www.fluka.org/fluka.php/.

[22] Geant4, https://geant4.web.cern.ch

[23] W. Scandale *et al.*, "Study of inelastic nuclear interactions of 400 GeV/c protons in bent silicon crystals for beam steering purposes", *Eur. Phys. J. C*, vol. 78, no. 6, p. 505, 2018. doi:10.1140/epjc/s10052-018-5985-8

[24] W. Scandale *et al.*, "Observation of strong leakage reduction in crystal assisted collimation of the SPS beam", *Phys. Lett. B*, vol. 748, pp. 451–454, 2015. doi:10.1016/j.physletb.2015.07.040

[25] R. Rossi, "Experimental assessment of crystal collimation at the Large Hadron Collider", Ph.D. thesis, Università La Sapienza di Roma, Roma, Italy, 2017.

[26] D. Mirarchi *et al.*, "Reducing Beam-Related Background on Forward Physics Detectors Using Crystal Collimation at the Large Hadron Collider", *Phys. Rev. Applied*, vol. 14, no. 6, p. 064066, Dec. 2020. doi:10.1103/PhysRevApplied.14.064066

[27] R. Rossi, G. Cavoto, D. Mirarchi, S. Redaelli, and W. Scandale, "Measurements of coherent interactions of 400 GeV protons in silicon bent crystals", *Nucl. Instrum. Methods Phys. Res., Sect. B*, vol. 355, pp. 369–373, Jul. 2015. doi:10.1016/j.nimb.2015.03.001

[28] HTCondor, https://research.cs.wisc.edu/htcondor/.

[29] J. Barranco *et al.*, "LHC@Home: a BOINC-based volunteer computing infrastructure for physics studies at CERN", *Open Eng.*, vol. 7, no. 1, pp. 378–392, Feb. 2017. doi:10.1515/eng-2017-0042