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ANALYSIS TOOLS FOR NUMERICAL SIMULATIONS OF DYNAMIC APERTURE WITH Xsuite

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Abstract

Recently, several efforts have been made at CERN to develop a new tracking tool, `Xsuite`, which is intended to be the successor to `SixTrack`. In this framework, analysis tools have also been prepared with the goal of providing advanced post-processing techniques for the interpretation of dynamic aperture simulations. The proposed software suite, named `Xdyna`, is meant to be a successor to the existing `SixDesk` environment. It incorporates all recent approaches developed to determine the dynamic aperture for a fixed number of turns. It also enables studying the time evolution of the dynamic aperture and the fitting of rigorous models based on the stability-time estimate provided by the Nekhoroshev theorem. These models make it possible to link the dynamic aperture to beam lifetime, and thus provide very relevant information for the actual performance of particle colliders. These tools have been applied to studies related to the luminosity upgrade of the CERN Large Hadron Collider (HL-LHC), the results of which are presented here.

INTRODUCTION

The dynamic aperture (DA), i.e., the extent of the connected region in phase space where the bounded motion occurs for a finite number of turns N_{max}, is a key quantity characterising the nonlinear beam dynamics and in particular the performance of high-energy storage rings and colliders. In fact, with the advent of superconducting magnets, which feature unavoidable magnetic field errors, the dynamics of charged particles in a circular accelerator turned intrinsically nonlinear. DA poses a challenge to accelerator physicists in terms of theoretical understanding of its features and computational evaluation. In the first domain, several studies were devoted to determine the appropriate models to describe how DA evolves as a function of N_{max}. Several solutions to this problem have been found [1–3] using the stability time estimate provided by the Nekhoroshev theorem [4–6]. The interest of this approach consists in the fact that once the DA evolution over time has been determined with a set of numerical simulations, the analytical model describing such an evolution can be fitted to the numerical data, and the resulting function can be used to extrapolate or predict the DA value for a number of turns beyond that used in actual numerical simulations. The advantage of this approach with respect to a plain brute-force computation is clear, in particular for the large high-energy colliders and even more so for the future ones, such as the Future hadron Circular Collider under study at CERN [7–10]. These new developments in the field require a sophisticated post-processing of the tracking data, which was initially partially implemented for the `SixTrack` code [11, 12].

The new Python modular simulation package `Xsuite` [13–16] has the ambition to combine previous single-particle simulation tools developed at CERN during the past decade, such as `SixTrack`, as well as collective effects codes, such as `PyHEADTAIL` [17, 18]. Therefore, new efforts have been devoted to the implementation of DA techniques developed in the recent past using the new computational paradigm, and all this has been incorporated in the new `Xdyna` module.

BRIEF DESCRIPTION OF XDYNA

`Xdyna` [19] has been developed with the idea of providing a user-friendly environment for beam stability simulations and all the necessary tools for dynamic aperture (DA) analysis. The tools developed are capable of performing analyses similar to those implemented in `SixDesk`, also providing new tools such as the evaluation of DA versus turn and machine learning techniques to optimise the selection of initial conditions for DA computation. The development of `Xdyna` is also an opportunity to review the definition of DA and to provide new reflection paths on this topic. A brief description of the functionalities of this package is outlined in the following:

1. **Creation of a study:**

   For each study, a configuration file is created, which contains all the information about the working units such as: the study name, the normalised emittances, the turn number used, the number of realisations of the magnetic field errors (also called seeds), as well as information about the `MAD-X` [20] scripts that need to be used.

2. **Generate a distribution of particles:**

   `Xdyna` can generate different types of initial distribution of particles: a Cartesian grid, a polar grid, or a random grid. By default, and for the sake of backward compatibility, the radial distribution is the same as that generated by `SixTrack`. Note that `Xdyna` also manages pairs of particles, similar to `SixTrack`. Furthermore, the user can also specify a custom distribution of initial conditions. The post-processing will be performed similarly to that for a random distribution of particles.

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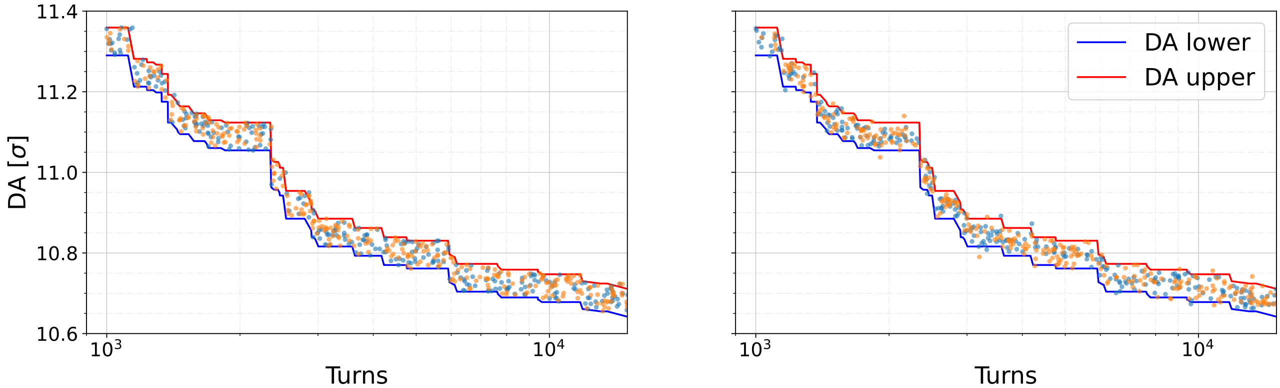

Figure 1: Illustration of the randomly-generated set of points used for the fit of the DA vs. turn. Continuous curves represent DA_l (blue) and DA_u (red), and uniform and Gaussian random generators are shown in the left and right plots, respectively.

3. **Tracking and post-processing:**

   Once the initial conditions are generated, the tracking can be performed. For each session, a number of particles can be specified, and Xdyna automatically selects which particles to track. Note that future development is planned to make Xdyna capable of running simulations on a new version of the volunteer-based computing system BOINC [21–23].

   After tracking ends, post-processing can be performed. The tools implemented in Xdyna allow detection of the stability border in the (x, y) space. They allow calculating the minimum, maximum and average DA, all computed over the angle, as well as the computation of the statistic over the seeds. As usual, the determination of the stability border is implemented so as to discard stable islands of stability disconnected from the origin.

   Xdyna generates two DA estimates: a lower bound corresponding to the border of the connected part of the stability domain, corresponding to what is calculated by SixDesk, and an upper bound corresponding to the lower border of the unstable region.

4. **DA vs turn:**

   A new feature added to Xdyna is the possibility of computing the evolution of DA over time and fitting it with specific models developed for the stability time estimate provided by the Nekhoroshev theorem [3]. A user-defined model can also be applied. The detail of the fitting process is discussed in the following sections.

Note also that Xdyna is capable of using SixDesk outputs to analyse SixTrack tracking data with the new tools.

TOOLS FOR DA STUDIES IN XDYNA

The models developed to describe the evolution of DA over time in [3], are used in the fit procedure, and are implemented in Xdyna. Their free parameters are computed using a least-square minimisation. The built-in models, selected from all those derived in [3], are (using the same numbering used in [3]):

- Model 2 type:

$$DA_2(N) = \rho \left(\frac{\kappa}{2e \ln(N/N_0)} \right)^{\kappa} \quad (1)$$

- Model 4 type:

$$DA_4(N) = \frac{\rho}{\left(-e\, \mathscr{W}_{-1} \left(\frac{-1}{e} \left(\frac{\rho}{6}\right)^{1/\kappa} \left(\frac{8N}{7}\right)^{-2/\kappa} \right) \right)^{\kappa}} \quad (2)$$

where $\mathscr{W}_{-1}$ stands for the negative branch of the Lambert function [24]. ρ and N_0 are scaling parameters for the DA and turns, respectively, and κ is related to the curve shape [3].

Because of the strongly non-linear behaviour of these models and in particular of the parameter interdependence, some bounds, such that $\rho > 0$, $\kappa \in [0.01, 2]$, and $N_0 \in]0, N_{max}]$, have to be provided to the fit routine. Model 2 can be used with two parameters, namely ρ, κ with $N_0 = 1$, or with three parameters, where also N_0 is a parameter.

In principle, the time evolution of the lower and upper DA estimates, DA_l and DA_u, can be determined by post-processing the tracking data and fitting their evolution over time. This provides a region (e.g., that delimited by the blue and red curves in Fig. 1) within which the fitted DA vs. turn should pass. A set of randomly generated points is used in the fit procedure, and two options have been implemented, depending on the type of random generator used, namely a uniform or a Gaussian one. In the first case, the range of the uniform generator along the DA axis is set equal to the interval between the lower and upper DA estimates. In the latter case, the rms of the Gaussian generator is chosen so that $\sigma = (DA_u - DA_l)/4$, which enables some points to be outside of the region delimited by the time evolution of DA_l and DA_u. An example is given in Fig. 1, where the uniform generator (left) and the Gaussian generator (right) are compared. The Gaussian distribution gives a higher weight to the centre of the region between DA_l and DA_u.

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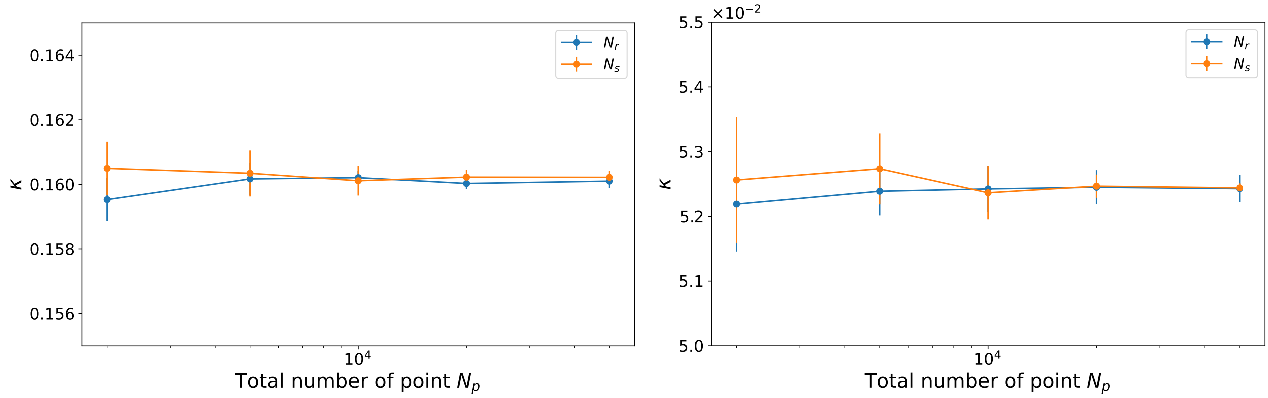

Figure 2: Dependence of κ on N_p when two (left) or three (right) parameters are used for fitting the model of Eq. (1). A Gaussian random generator has been used. The two curves represent separate scans of N_s or N_r.

EXAMPLES OF XDYNA APPLICATIONS

The fit procedure is implemented as follows: N_s samples of N_r randomly generated points are used to fit the DA through these points and the average and rms of each fit parameter are returned and used in our analyses. The total number of points ($N_p = N_r \times N_s$) is a useful quantity to study the accuracy of the fit and the CPU time.

Figure 2 shows how κ depends on N_p for a two- (left) or three-parameter (right) fit. The curves represent independent scans of N_s or N_r, using a Gaussian generator, although similar results are obtained with a uniform generator. $N_p \approx 10^3$ is already enough to ensure that κ has settled to the correct value and that the associated error is at the percent level. Note the large difference in the value of κ depending on the number of free parameters used in the model. This feature is well known for this type of fit function and suggests that two free parameters should be used to avoid interplay between the fit parameters.

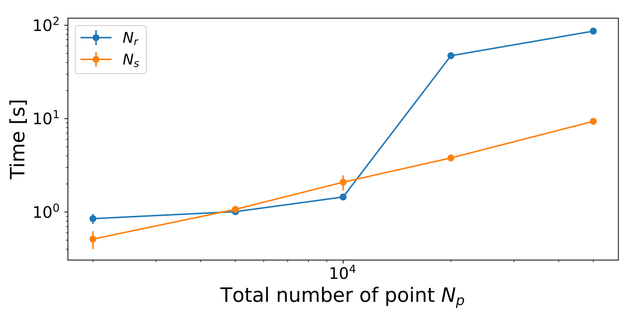

Figure 3: CPU time of the fit procedure as a function of N_p. The two curves represent separate scans of N_s or N_r.

Figure 3 shows the dependence of the CPU time on N_p. The dependence is represented by a power law, but a sudden jump is observed when N_r is varied: this could be related to the behaviour of the routine as a function of the number of points used for the optimisation process.

Finally, Fig. 4 shows the results of the actual fitting of the DA vs. turns. The region delimited by DA_l and DA_u is clearly visible, with the DA curves for the two- or three-parameter fit of Model 2 obtained by the fitting procedure well adjusted within the acceptable region.

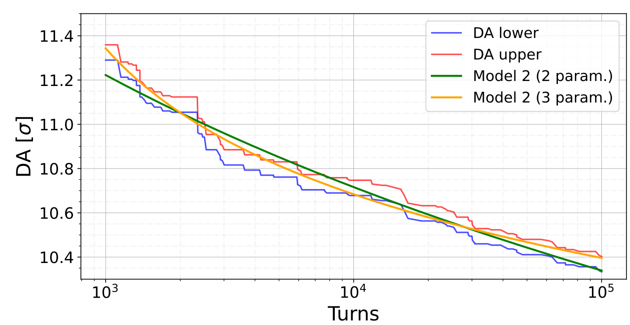

Figure 4: DA versus turn and fit results for Model 2 using 2 and 3 parameters, respectively. A Gaussian random generator has been used.

CONCLUSIONS

Thanks to recent developments in the new tracking code Xsuite, the new module Xdyna has been developed to incorporate sophisticated tools to perform post-processing of the tracking data to estimate the DA of the system under consideration. Several features have already been implemented and tested, such as the determination of the stability boundary for fixed N_{max}, the calculation of the DA vs. turns, and the fit of several models to the DA vs. turns data.

The next steps consist of consolidating the structure of the Xdyna module to make it fully operational for Xsuite users, and then the new features will be applied to the analysis of the large data set of DA simulations collected over the years in the framework of LHC and HL-LHC studies.

It should be clear that although the tools described above have been developed and tested using numerical simulations of the beam dynamics in the LHC, such tools are of general validity and can be applied to any circular hadron accelerator.

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