

CODE BENCH-MARKING FOR LONG-TERM TRACKING AND ADAPTIVE ALGORITHMS

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Abstract

At CERN we have ramped up a program to investigate space charge effects in the LHC pre-injectors with high brightness beams and long storage times. This is in view of the LIU upgrade project [1] for these accelerators.

These studies require massive simulation over large number of turns. To this end we have been looking at all available codes and started collaborations on code development with several laboratories: MAD-X frozen & adaptive mode [2] and integration into the main branch of the MAD-X in-house development [3] code, PyORBIT [4] from SNS, SYNERGIA [5] from Fermilab, MICROMAP [6] from GSI .

We have agreed with our collaborators to bench-mark all these codes in the framework of the GSI bench-marking suite [7], in particular the main types of frozen space charge and PIC codes are being tested.

We also include a study on the subclass of purely frozen and the adaptive frozen modes both part of MAD-X in comparison with the purely frozen MICROMAP code.

Last, we will report on CERN's code development effort to understand and eventually overcome the noise issue in PIC codes.

INTRODUCTION

The aim of this study is threefold. On the one hand we would like to present the completion or near-completion of the GSI Bench-Marking Suite [7] of 2 PIC codes and the comparison with the results from 3 participating frozen SC codes. The second task is to report about the on-going study to understand how SC experiments compare with the various SC codes. To this end we are studying both the PS [8] and the SPS [9] at the integer resonance. This study of SC at the integer resonance in view of evaluating which tools are most suited to understand the dynamics is part of the mandate of a PhD [10] at CERN. Here we can just present a snapshot of what could be achieved up to this conference. Lastly, we would like to remind the community about the effect of grid noise on individual particles in the distribution. Techniques to overcoming this issue or at least minimizing its fake impact on the emittance evolution and particle loss will be crucial to see if PIC codes can be taken to use for long-term SC simulations or not. In fact, at this conference new concepts will be discussed that might do the trick. At CERN Malte Titze's [10] second part of his thesis is dedicated to such techniques.

GSI BENCH-MARKING SUITE

With the upcoming Fair [11] and LIU [1] projects at GSI and CERN respectively, a new sequence of SC workshop has been started to review how our codes can be used to predict long-term SC effects on the dynamics of storage rings in the regime of high intensity. During this first joint GSI-CERN Space Charge Workshop [12] held at CERN in 2013, with a follow-up collaboration meeting in 2014 [13] it had been decided to start a collective effort to bench-mark several PIC codes with the GSI bench-marking suite that has been used for code bench-marking of a number of frozen SC codes in previous years. In particular, the teams of PyORBIT [4] from SNS, the latest incarnation of ORBIT, and the SYNERGIA [5] team of FERMILAB have made the effort to go through all the nine steps of this GSI bench-marking suite.

Figure 1 shows the 9th step of a long-term simulation over 100'000 turns of the SIS18 GSI ring. It is quite interesting to note that for some 10⁶ macro-particles the SYNERGIA (2.5D solver) reproduces the results of the frozen SC codes. What is remarkable about this finding is the fact that also SYNERGIA as a PIC code is suffering from grid noise as shown below.

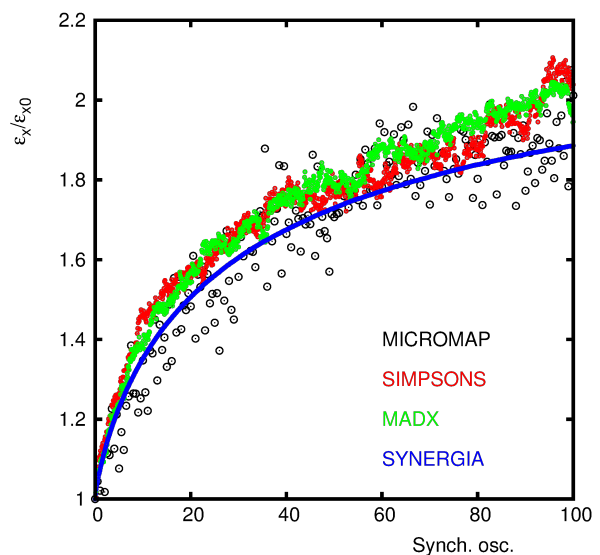


Figure 1: Emittance Evolution of the GSI SIS18 ring simulated with the 3 frozen SC Codes: MICROMAP, SIMPSONS, MAD-X and the PIC code SYNERGIA (1M macro-particles).

The complete results for both codes will now be introduced into the GSI bench-marking web site [7].

CODES IN COMPARISON WITH MACHINE EXPERIMENTS

Adaptive Mode

At first sight it seems astounding that a purely frozen code should be sufficient to describe the long-term evolution of the particle dynamics under the influence of SC and an ever changing particle distribution. On the other hand, a self consistent treatment is very slow in comparison and also burdened by grid noise. It seems therefore like an ideal approach to search for an intermediate solution that remains fast but also adapts the frozen distribution turn by turn closer to the actual distribution. To this end a very fast iterative algorithm [14] has been developed and implemented [15] into MAD-X that fits a Gaussian to whatever the actual distribution might be and thereby ignoring tails that might not be significant for the dynamics anyway. On top of this emittance recalculation, MAD-X allows to also recalculate the optics, so that even the beam sigmas are re-normalized occasionally. It goes without saying that this is indeed quite time consuming and therefore done only every 1000 turns in the case of the PS simulations.

However this approach is not really cost-free:

Pros: If a bench-marking as attempted in this study is successful one might have a unique manner to capture at least partially the self-consistent nature of the SC force. Moreover, the algorithm does degrade the speed only slightly. In fact, there has been a considerable effort with our collaborators at BNL [16] to optimize the speed of MAD-X with the help of OPENMP techniques.

Cons: On the other hand, for a true assessment of the speed one has to consider that in the case of the purely frozen mode one can completely serialize runs, since no cross talk between particles is required, and thereby gain a tremendous speed-up. The intermittent TWISS is quite a burden because it complicates the re-entry into the MAD-X tracking routines which has been an implementation nightmare, quite feared in the community of code developers. Besides these more technical problems, there is a more general and more serious issue which concerns the possibility that the continuous upgrade of the emittances may introduce some kind of statistical noise because it changes quasi random from turn to turn. This will have to be studied carefully.

Machine Parameters

Table 1 holds the most basic parameters of all machines that have been studied here. It is important to point out that there is a particular problem with the PS which consists of combined function magnets. These cannot easily be split into drift and kicks while keeping the full Hamiltonian intact, but rather this transformation leads to the expanded Hamiltonian. As a result the chromaticity is modified by some 16% for the

Table 1: Machine Parameters

Parameter	SIS18	PS	SPS
Length [m]	216.71	628.32	6911.5
Kin. E. [GeV]	0.0114	2	25.079
Tuneshift	-0.1/-0.1	-0.05/-0.07	-0.1/-0.19
Special Features	Sextupole	Sextupole	Optimal adjusted
	Uncorr. Chromaticity		

PS after creating a thin-lens lattice. Therefore, our student Malte Titze has re-derived, from first principles, a thin model of the combined function model [17] that agrees with the full Hamiltonian in the limit of large number of kicks in the splitting of the thick combined function magnet.

PS Experiment

In 2012 we have done SC studies at the PS [8] with special sextupoles excited to allow for a code bench-marking with experiments. In Fig. 2 a measured loss scan is shown as a

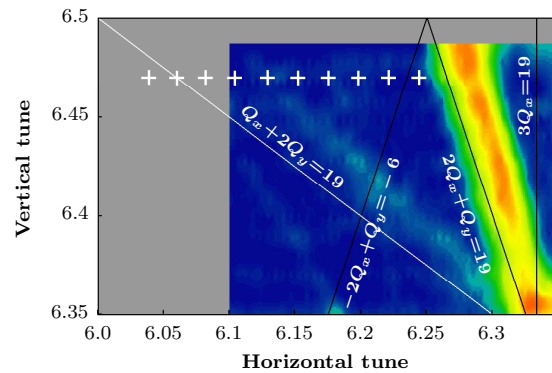


Figure 2: PS SC study with sextupoles excited. The sextupolar resonance $Q_x + 2Q_y = 19$ is shown with a white solid line and the working points used for the systematic study are indicated with the white crosses.

function of tunes together with 10 tune WPs (white crosses) being used to sample the $Q_x + 2Q_y = 19$ normal sextupole resonance and testing the SC tune-shift of $-0.05/-0.07$. Figure 3 shows the comparison of the measured emittance growth ratio (dashed lines) with those from MAD-X in adaptive mode (solid lines). While the overall agreement is excellent at medium and large horizontal tunes the MAD-X simulations predict a distinct increase of the horizontal emittance when approaching the integer tune that is not found in the experiment. When re-doing the simulations (see Fig.4) either with MICROMAP [6] which only has the frozen mode or with MAD-X in frozen mode there is no such increase to be found. Nevertheless, the understanding is less than evident at this point: on the one hand in discussions [18] – the author of the adaptive mode in MAD-X – we tend to believe that the procedure seems to drive particles onto the integer resonance. This may explain why we could not perform TWISS calculations during the run at $Q_x = 6.039$. On the other hand we are puzzled why we cannot find the

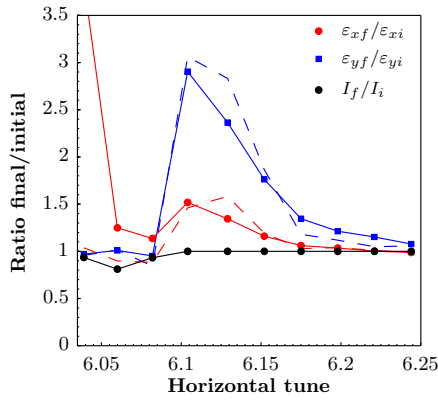


Figure 3: PS Emittance Evolution (adaptive).

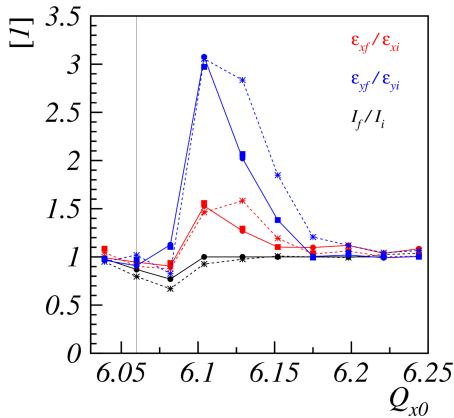


Figure 4: PS Emittance Evolution (frozen).

usual large horizontal emittance blow-up close to the integer resonance as for instance at the SPS (see below). In fact, we have planned simulations with PyORBIT for the PS at these smaller horizontal tunes to determine if this behavior in the adaptive mode is a code feature or if we do not understand something in our experimental set-up. Unfortunately, these studies are not yet ready to be presented here. For a

Table 2: Emittance Ratio in the PS Experiment: Adaptive versus Frozen Mode

Q_x	Mode	Experiment
6.039	Frozen	0.97/1.077
	$1.07 \pm 0.06/0.99$	
6.104	Adaptive	1.553/2.974
	$1.73 \pm 0.03/0.97 \pm 0.02$	

better understanding of the adaptive and frozen mode we have done extensive simulations just at $Q_x = 6.039$ and $Q_x = 6.104$. To this end we have made a systematic check of how the simulations are done: standard MAD-X versus a

better model of the combined function magnets and several options to enact the adaptive mode, leading us to present the average and RMS. We used a polar Gaussian distribution in NormalForm space and transferred it to the laboratory system via the full 6D linear transformation. This makes sure that the beam distribution is matched in 6D. We do not make additional adjustments since in the PS experiment we have a similar set-up. The table shows that apparently the adaptive mode is indeed overstating the presence of the integer for the case $Q_x = 6.039$ while the frozen mode is reproducing what is found in the experiment quite well. For $Q_x = 6.104$ the results are mixed in the sense that the frozen mode better agrees for horizontal emittance growth while for the vertical plane the results are better for the adaptive mode. In conclusion we are not completely sure what the optimal approach is in understanding the results from our machines. In fact, this will be covered by the thesis work of Malte Titze [10].

SPS Experiment

Very detailed studies have been launched for the SPS but the full analysis will come in a few weeks only. In Fig. 5 the horizontal emittance blow-up has been recorded when approaching the integer resonance. It shows both the initial

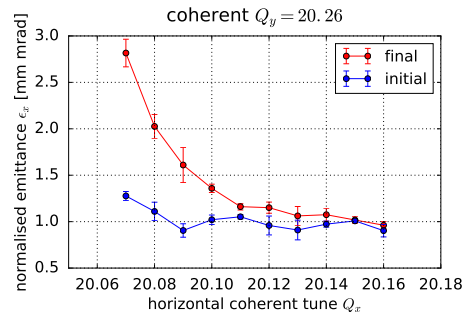


Figure 5: SPS Emittance Evolution Close to the Integer Resonance.

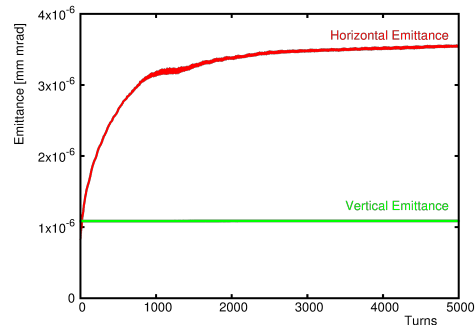


Figure 6: Preliminary Results with PyORBIT for SPS Emittance Evolution at $Q_x = 20.07$.

emittance and the final one after 3 sec of storage time. Note that the blow-up close to the integer resonance is quite fast and therefore increasing values are measured already for the

initial emittance. Therefore, we should estimate the “real” horizontal emittance to be slightly below $\epsilon_x < 1\mu\text{m}$.

Preliminary studies with PyORBIT (2.5D solver, 500k macromacro-particles) confirm that the horizontal emittance blow-up indeed amounts to about a factor of 3 (Fig. 6). Moreover, we are also investigating with MAD-X both frozen & adaptive to see how well the horizontal emittance blow-up can be predicted by either code variant. We must wait until our findings are conclusive and Malte’s PhD thesis [10] should provide those results.

THE NOISE ISSUE OF PIC CODES

The grid noise is the standard nuisance of PIC codes and at CERN we are following closely the new developments to overcome this problem by introducing symplectic PIC codes. In fact, we have started our own effort to understand the symplectic violation of PIC codes as presented at this conference [19] and we are actively investigating to create our own symplectic SC module in the future. In the mean-

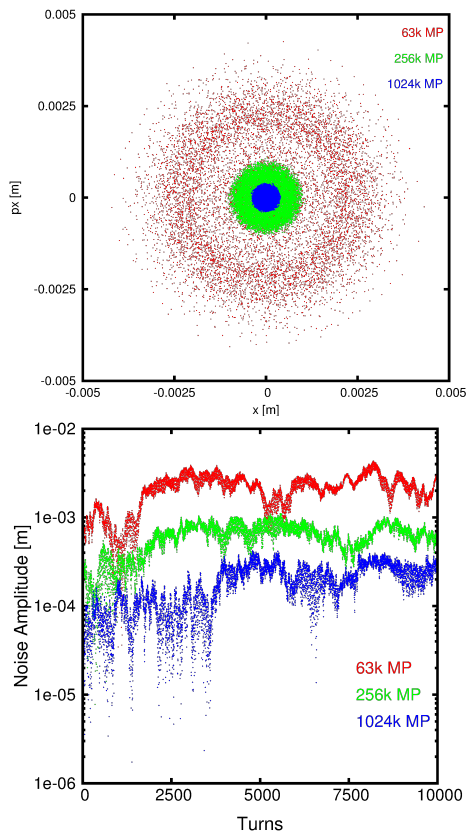


Figure 7: Small Amplitude Jitter study and growth in the horizontal Phase Space with SYNERIA; shown is the artificial phase space of a particle starting with zero amplitude: RED, GREEN & BLUE for 63k, 256k and 1025k Macro-Particles respectively.

time we are looking at the effect of the noise present in today’s PIC codes. To this end we have started a zero amplitude particle together with a distribution of particles for 63k, 256k and 1025k Macro-Particles respectively. In ab-

sence of noise, e. g. in the case of the frozen mode, this zero amplitude particle should rest at zero indefinitely. In Fig. 7

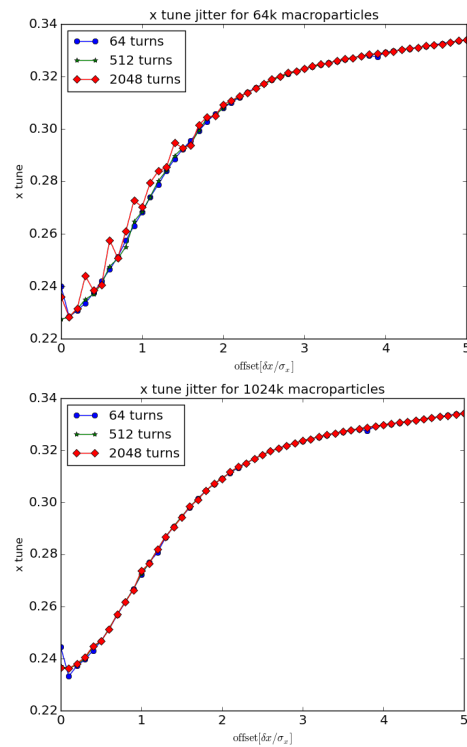


Figure 8: Tune Jitter with SYNERGIA for 64k and 1024K MP respectively.

we find that the noise creates artificial deviations from this expected symplectic behavior that does decrease with the number of macro-particles but nevertheless remains quite large. This is also visible in view of tune jitter (Fig. 8) that unexpectedly becomes larger when the time sequence for the FFT is enlarged. This effect even prevails for the very high number of macro-particle numbers of up to 10^6 .

CONCLUSION

The frozen, adaptive symplectic codes are being compared with the intrinsically noisy PIC codes. Surprisingly the PIC codes are doing quite well to predict general parameters like emittance blow-up. Despite best efforts it is still too early to call the shots of which code variants are best suited to understand our experimental data. However, we have made tremendous progress and in a year or two we should have a definite answer to this question. We are also fully involved in understanding the non-symplectic nature of PIC codes and creating CERN’s next symplectic PIC tracker. Moreover, the experimental procedures and data quality are rigorously improved for all CERN LHC pre-injectors.

The international collaborations have proven incredibly fruitful in this effort! We are determined to continue with this collective effort until we have a better understanding of SC effects in the presence of non-linear lattices and the codes to deal with them.

REFERENCES

- [1] J. Coupard *et al.*, “LHC Injectors Upgrade, Technical Design Report, Vol. I: Protons”, LIU Technical Design Report (TDR), CERN-ACC-2014-0337.
- [2] V. Kapin, Fermilab, F. Schmidt, CERN, “MADX-SC Flag Description”, CERN-ACC-NOTE-2013-0036, <http://cern.ch/Frank.Schmidt/report/MADX-SC.pdf>.
- [3] L. Deniau, G. Roy, and F. Schmidt, “Integration of MADX-SC into the general MAD-X version”, (2013), <http://mad.web.cern.ch/mad/>.
- [4] Andrei Shishlo *et al.*, “The Particle Accelerator Simulation Code PyORBIT”, *Procedia Computer Science*, Volume 51, 2015, pp.1272–1281.
- [5] E. Stern *et al.*, “SYNERGIA”, <https://cdcvs.fnal.gov/redmine/projects/synergia2/wiki>; J. Amundson *et al.*, “High Performance Computing Modeling Advances Accelerator Science for High Energy Physics”, *IEEE Comput.Sci.Eng.* 16 (2014) no.6, pp.32-41.
- [6] G. Franchetti *et al.*, “MICROMAP LIBRARY”, http://web-docs.gsi.de/~giuliano/micromap_manual/micromap_reference_manual.html.
- [7] G. Franchetti, “The GSI Bench-Marking Suite”, http://web-docs.gsi.de/~giuliano/research_activity/trapping_benchmarking/main.html.
- [8] G. Franchetti *et al.*, “Space charge effects on the third order coupled resonance”, to be published in *Phys. Rev. ST Accel. Beams* and presented at HB’16, Malmö, Sweden, paper TUAM6X01, this conference.
- [9] H. Bartosik *et al.*, “Space Charge Studies with high Intensity single Bunch Beams in the CERN SPS”, in *Proc. of IPAC’16*, Busan, Korea, paper MOPOR021, pp. 644-647, doi: 10.18429/JACoW-IPAC2016-MOPOR021
- [10] M. Titze, “On the Impact of Non-Symplecticity of Space Charge Solver”, PhD Thesis (see [19]).
- [11] P. Spiller and G. Franchetti, *Nucl. Instrum. Methods Phys. Res.*, Sect. A **561**, 305 (2006).
- [12] Joint GSI-CERN Space Charge Workshop, held at CERN, April 2013, <https://indico.cern.ch/event/221441/>.
- [13] Space Charge Collaboration Meeting, held at CERN, May 2014, <http://indico.cern.ch/event/292362/>.
- [14] Y. Alexahin, “Computation of Eigen-Emittances (and Optics Functions!) from Tracking Data”, presentation given at the Space Charge Joint GSI/CERN workshop held at CERN (2013).
- [15] V. Kapin, Y. Alexahin, “Space Charge Simulation Using MADX with Account of Synchrotron Oscillations”, in *Proc. of RuPAC’10*, Protvino, Moscow region, Oct 27, 2010, pp. 204-206.
- [16] N D’Imperio *et al.*, “Experience with OpenMP for MADX-SC”, CERN-ACC-2014-0075, BNL C-A/AP/515 (2014).
- [17] M. Titze, “Approach to combined-function magnets via symplectic slicing”, *Phys. Rev. ST Accel. Beams* 19.054002 (2016).
- [18] Y. Alexahin, private communication.
- [19] M. Titze, “On the Impact of Non-Symplecticity of Space Charge Solvers.”, presented at HB’16, Malmö, Sweden, paper MOPR029, this conference.