CODE REQUIREMENTS FOR LONG-TERM TRACKING WITH SPACE CHARGE

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Abstract

In view of the LHC Injectors Upgrade (LIU) program of the LHC pre-accelerators LEIR [1], PSB [2], PS [3] and SPS [4] we have started a new working group at CERN to deal with space charge issues of these machines. The goal is to operate with basically twice the number of particles per bunch which will further increase the space charge tune shifts which presently are already large. Besides obvious remedies like increasing the injection energy we are obliged to better understand the space charge force to optimize our machines. To this end it has become clear that we need computer models that faithfully represent the linear but also the non-linear features of our machines. We have started close collaborations with several laboratories around the world to upgrade existing self-consistent space charge Particle-In-Cell (PIC) codes for our CERN needs. In parallel we have created a frozen space charge facility in CERN's MAD-X code. Both types of codes are being used to study long-term stability and to compare it with machine experiments.

INTRODUCTION

It has been realized in 2011 that at CERN a concerted effort was needed to study the space charge (SC) effects in the pre-accelerators of the LHC in view of achieving a two-fold increase of beam intensity needed to fulfill the goals of the LIU project. To this end a SC working group has been established to build a new team of competence in the field of space charge effects at CERN. Students and staff members have been won to study the 4 circular machines LEIR, PSB, PS and SPS both with experiments and simulations. In the meantime there is also a team to study SC effects in more general terms.

In regular meetings [5] the machine related SC issues are being discussed but also an educational series of talks has been started given by experts from inside CERN and other laboratories.

From the beginning it has been clear that one need to know well the non-linear dynamics in conjunction with SC forces to allow for a full understanding of emittance growth and losses in any of the machines. Expertise is required in both regimes and also a close collaboration with magnet experts is mandatory to get a good modeling and measurements of critical magnets in the rings.

* Speaking as the representative of the CERN Space Charge working group

The codes would need to be adapted towards an adequate treatment of both the non-linear machine models and SC. A decision has been made to invest into existing codes and adapt them to CERN needs, unless we could modify CERN codes with moderate effort. Essential is that any code would have to pass a rigorous benchmarking test before the code results could actually be trusted. Ease of use, flexible structure and computing performance are further critical issues for the LIU studies. Last and not least a code benchmarking with machine experiments is the ultimate way to give us confidence that the whole chain from magnet modeling, the codes and the experimental data taking are all sufficiently well prepared and mastered so that the machines can be understood well enough to minimize the combined effect of machine non-linearities and SC.

Intense collaborations have been initiated around the world and we have started series of workshops [6] [1] and collaboration meetings [7] [2] to make progress on the open issues in the theoretical understanding and program development.

This report is based on the outcome of those two meetings and an outlook is given for the next steps. We concentrate here on CERN machines where presently there is a high demand for SC studies. Many of these discussed issues should be of wider interest to the SC community as a whole.

We have added an Appendix about CERN's new method to create perfectly matched 6D distribution that hasn't been discussed anywhere before.

CODES

In the SC field there are basically two classes of codes: on the one hand there are the self-consistent PIC codes with 2D, 2.5D and 3D SC treatment. These codes are most relevant over a short period at the beginning of injection when the coherent SC are largest, the fields may be time dependent and the dynamics are most complex. Despite these advantages the codes tend to be slow and the results suffer from PIC noise. On the other hand frozen SC codes are being used over longer time ranges and when non-linear resonances play a decisive role in conjunction with SC. These second type of codes perform much better due to a much simpler 2D treatment of SC and they do not suffer from PIC noise. It remains to be fully understood when either approach is truly required and how one might combine them. To this

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end the CERN SC working group is planning a dedicated effort to resolve these issues.

The collaboration on PIC codes concerns 3 codes: pyORBIT [8], SYNERGIA [9] and IMPACT [10]. MADX-SC [11] has been used with a frozen SC implementation. More recently a frozen SC implementation has been added to pyORBIT [12] and is in a testing phase.

All codes are in preparation to cover the needs for the CERN accelerators of which the most relevant are:

- Time varying field
- Double RF system
- Acceleration

In particular pyORBIT, an update of the PTC-ORBIT code with a PYTHON front-end, is now ready for the CERN machines, this naturally implies that PTC is also part of pyORBIT. SYNERGIA is still in a benchmarking phase of the single particle code CHEF compared to MAD-X/PTC. IMPACT is in the process of building up the single particle part. Both pyORBIT and SYNERGIA have done most of the GSI benchmarking suite [13] and the results will be introduced into that benchmarking suite by the end of 2014.

In fact SYNERGIA has done all steps and in particular step 9 which is a long-term check over 100’000 turns of the emittance growth. To this end the standard convergence test of the emittance growth had to be carried out over the full 100’000 turns instead of just a few 1’000 turns, 71 SC kicks were needed with a grid of $64 \times 64 \times 64$. It turns out that 4 million macro-particles were needed for a successful convergence of the emittance growth. The SYNERGIA team has shown, for the first time, that a self-consistent PIC code can carry the tracking over 100’000 turns and find perfect agreement with several frozen SC codes that have also been tested in the GSI benchmarking suite. The upper graph of Fig. 1 shows the emittance growth as predicted by several frozen SC codes and in the lower graph (notice that the scales are identical) one finds basically the same curve except that the fluctuations are very small due the large number of macro particles being used.

It has been agreed that all three PIC codes should publish releases after a full benchmarking of their codes including all features required by CERN machines by the end of the year.

There has been development on the MADX frozen SC code, which has already been benchmarked in the GSI suite. In particular, the re-normalization of the sigma values (the emittance is re-calculated every turn whilst the TWISS parameters are recalculated typically every 1’000 turns) has proven essential in correctly reproducing experimental studies at the CERN PS (see below). Further work on the code is being planned in collaboration with Fermilab.

One obvious question concerning codes is their performance on various platforms. By the nature of simulating a large ensemble of macro particles all codes either operate under MPI or OPENMP to speed up the performance by

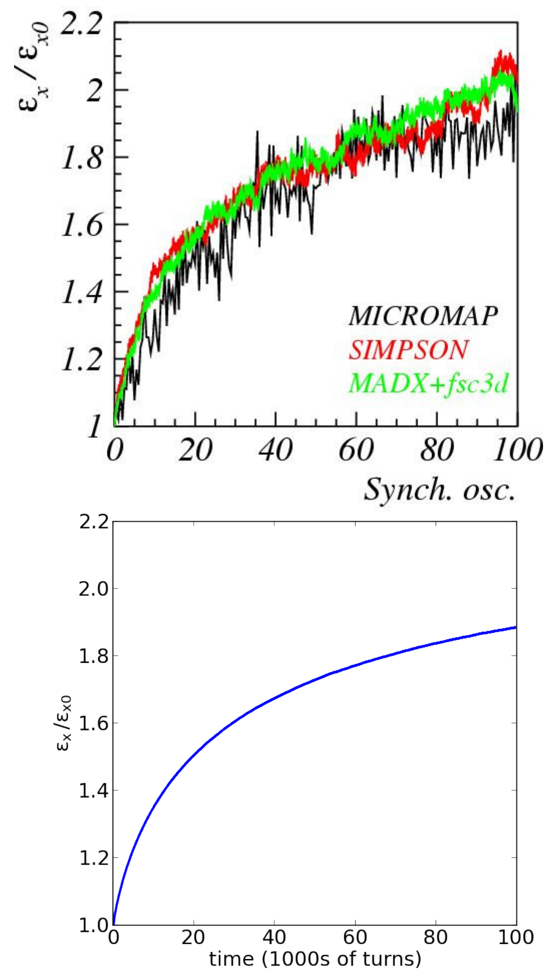

Figure 1: Emittance evolution for SIS18 over 100’000 turns performed by 3 frozen SC codes (top) and (bottom) by the PIC code SYNERGIA [9]. One complete synchrotron oscillation takes 1’000 turns.

parallelization. Nevertheless, optimization of speed must have priority throughout of the development phase of any type of code. In particular, two speed issues are important:

- Is the scalar speed optimized?
- How well does the code scale on platforms with very large number of cores?

The next step is to figure out the optimal computing system: some clusters of multicore machines, super computers with core numbers as large as 100’000 or even GPU systems.

NOISE ISSUES

In the SC workshop in 2013 the issue of noise in PIC codes has been addressed [14] by following the motion of a few test particles in a large distribution with a PIC code. Apparently, all such test particles exhibit chaotic motion. This chaotic behavior may be weak for large amplitudes but gets stronger for smaller amplitudes. The conjecture is that since the SC force is strongest at zero amplitude, it apparently shakes

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single particles erratically and proportional to its strength. The SYNERGIA team [15] has followed single particles over 100'000 turns and recorded the tunes evolution over time (see Fig.2). The analysis as described above seems valid in this long-term simulations: at the smaller amplitude the tune is changing a lot but small tune variations can even be found at larger amplitudes.

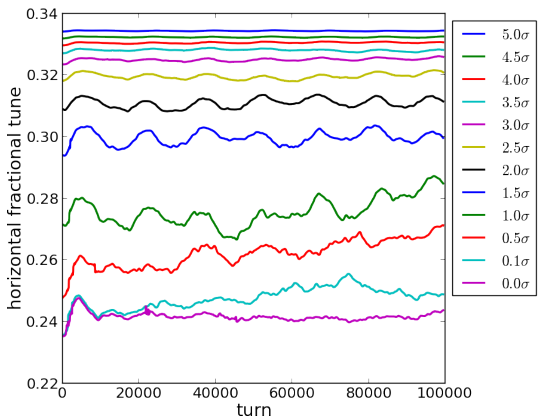

Figure 2: Evolution of the hor. tune for SIS18 calculated in a sliding 1024 turn window over 100'000 turns performed by SYNERGIA [9]. The results are shown for 12 different hor. beam sigmas ranging from 0 to 5 σ.

These findings have caused the SC community to revisit their theory of noise in PIC codes that has been studied decades ago. Struckmeier [16] reminded us that space charge effects include Intra Beam Scattering. His involved theoretical analysis leads to the conclusion that some kind of temperatures can be defined for each motion plane and that the entropy may increase when those individual temperatures are not balanced. Apparently, this holds also in PIC simulations. A team from GSI [17] has picked up from this anisotropic phenomenon and has found that in FODO structures there is an additional component of grid noise that is there even for zero anisotropy.

At SNS [18] there has been an attempt to use the FMM (Fast Multipole Method) that should in principle overcome the discretization problem that causes the grid noise. However, it turns out that anomalous pair-wise forces slip into the calculation such that effectively the noise is not reduced compared to the standard PIC codes. It was also shown that in PIC simulations for very long constant focusing channels eventually even zero amplitude particles grow in amplitude. This is an independent confirmation of the chaotic behavior of single particles in PIC simulations.

Noise in PIC simulations has also been studied at Fermilab [15]. As discussed in the section on Codes above they find good agreement for global properties like emittance growth with the frozen SC codes although all particles them selves are chaotic. The conclusion is that the individual particles mix in the distribution without actually destroying its global properties.

Lastly, there has been a more systematic numerical approach to study PIC noise [19]. A scaling law has been found for the growth of PIC noise in 2D simulations. Tracking of noisy beams may conveniently be explained by a random walk, which shows a tendency of larger steps to the outside resulting in emittance blow-up. It has also been very instructive to see that the grid structure becomes graphically visible in the plots of the standard deviation of the electric fields.

SC EXPERIMENTS

Various studies have been done at the PSB [20] and the PS [21] and the simulation results are starting to be convincing. At the PSB booster it could be demonstrated that good agreement between simulations (PTC-ORBIT) and experiments could be achieved for particle motion close to the $^1/_2$ integer resonance where large losses do occur. Precondition

Figure 3: Intensity evolution for PSB in the vicinity of the $^1/_2$ integer resonance without the usual operational corrections turned on (in which case no beam loss is observed). [20]

for these nice results has been to include in the model both the measured quadrupole and misalignment errors. This is a confirmation of the strategy to complete our model evaluation before we study SC effects. An interesting theoretical side issue is the fact that the tune footprints should not use the phase advance per turn but rather the tune values (phase advance averaged over many turns) for every particle, which implies to average over full synchrotron periods.

In 2012 PS experiments have been performed in the vicinity of the coupled third order resonance $Q_x + 2 \cdot Q_y$ and in presence of SC [21]. MADX-SC simulations with frozen SC and a beam sigma re-normalization every 1'000 turns seem to be in remarkable agreement with the experiments in terms of reproducing different final beam distributions for various working points close to the normal sextupole resonance $Q_x + 2 \cdot Q_y$. Figure 4 shows the experimental results (hor. & ver. variance and particle loss) in the upper graph (errors are determined by repeated measurements) whilst the simulation results are shown in the lower graph, notice that the measurement results are shown as dashed lines to demonstrate excellent agreement except for the fact that the

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horizontal integer line is not correctly reproduced in the simulations (red curve at small tunes). Additional studies are currently being carried out to investigate this effect. On

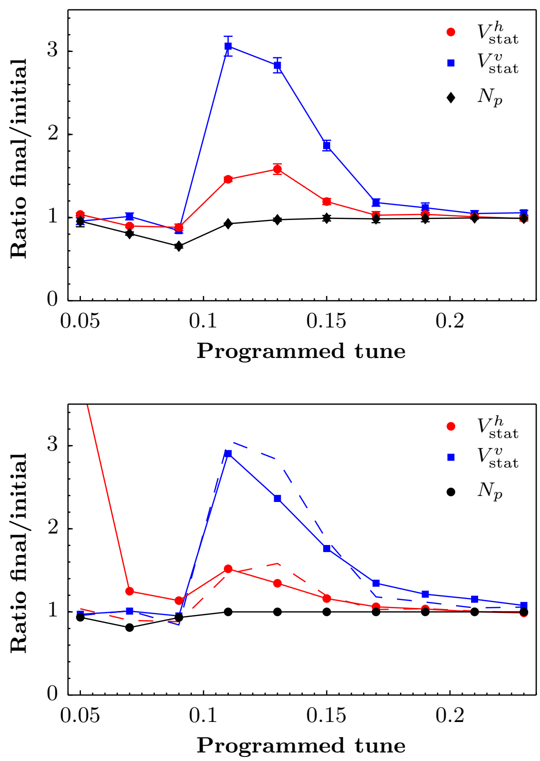

Figure 4: Horizontal & vertical variance and loss as a function of programmed tune for the 2012 PS experiment [21]. The top graph shows the experimental results whilst the lower plot shows the results of the simulations (sold lines) in comparison with the experimental data (dashed lines).

the other hand, the studies at GSI show similar results [22]. There are first indications that the beam distributions, which may be different in the 2 transverse planes, are due to the crossing of 4D fix-line structures caused by the coupled sextupole resonance [23]. Of course, the strong detuning from SC plays an important role.

A measurement campaign at the PS has shown that the resonance $4 \cdot Qy = 25$ is excited and driven by space charge [24]. Besides the integer resonance it is this 4^{th} order resonance that is limiting the PS performances for the production of the future high brightness beams. The symmetry of the lattice (h=50) apparently excites the structure resonance $8 \cdot Qy = 50$ which is driven by space charge. Presently a PS measurement study is under way to change the vertical integer tune such as to mitigate this structure resonance [25]. First simulations using PTC-ORBIT, IMPACT and Simpsons [25–27] have confirmed the potential of this idea.

At RHIC the MADX-SC code is being used with completely frozen SC, i.e. without re-normalization of the beam sigmas, for sub-injection energies at RHIC [28]. These simulations also included the BB effect induced by the two counter-rotating and colliding beams. Comparison with the real machine data are soon to be expected.

CONCLUSION

The international collaboration on all relevant fronts: codes, noise and experiments is in full swing. In particular the benchmarking effort has progressed well and one of the PIC codes (SYNERGIA) has finished the GSI benchmarking suite completely. For the first time it has been demonstrated that a PIC code can be used for long-term tracking over 100’000 turns and simulating 4 million macro-particles on a 144 core machine taking 2 weeks of CPU time, thereby agreeing with the results from frozen SC codes.

Despite the fact that non-negligible PIC noise renders every macro particle in the distribution chaotic, a PIC code can nevertheless reproduce the long-term evolution of global parameters. This makes us hopeful that PIC codes will indeed be useful for storage rings over many turns which up to now has never been demonstrated.

In parallel, the theoretical analysis of PIC noise has been reviewed and extended but no remedies have yet been found to overcome the problem. In fact, even for 4 million macro-particles the noise effect can easily be seen for each individual particle.

On the other hand we are still working on getting all tools ready for the work on CERN machines and presently only PTC-ORBIT or the newest pyORBIT incarnation of the ORBIT code fulfill this requirement. The other PIC codes are still in a state of development. The plan is to have up to 3 PIC code releases ready by the end of 2014: pyORBIT, SYNERGIA and IMPACT.

The frozen SC extension MADX-SC has shown to reproduce well the beam dynamics of the PS close to the sextupole coupling resonance $Q_x + 2 \cdot Q_y$. A prerequisite is a constant re-normalization of the beam sigmas, but it remains to be seen how the unavoidable jitters of the beam sigma from turn to turn is causing some kind of noise phenomenon, albeit of a different nature than PIC noise.

APPENDIX

Traditionally, the SC community has been using standard techniques using TWISS parameters to set-up reasonable well matched distributions. However, with the NormalForm method becoming mainstream there are now ways to achieve this in a more systematic way that will work for systems that are fully coupled in 6D. At CERN [29] we have now established the following procedure:

- Create independent 2D polar Gaussian distributions via the Box-Muller transform [30].
- Multiplied by the square root of the emittance of the horizontal, vertical and longitudinal phase space respectively.

  Eq.1 relates the emittance ϵ_z to the beam-size σ_z and the β_z in the longitudinal plane. The latter can be obtained by the generalized 6D TWISS parameters [31].

$$\sqrt{\epsilon_z} = \sigma_z / \sqrt{\beta_z} \qquad (1)$$

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- Transform coordinates to real space via the linear NormalForm of the 6D one-turn map including BB or SC kicks [31].
- Method can be extended to higher order NormalForm and the initial distributions could be different from Gaussian.

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