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BENCHMARKING AND APPLICATION OF SPACE CHARGE CODES FOR RINGS

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Abstract

This presentation should present an overview of efforts for benchmarking and application of space charge codes for rings. After briefly recalling the historical background of the simulation efforts of space charge effects in rings, we will overview the present benchmarking efforts against experimental results.

INTRODUCTION

Benchmarking of a code in the accelerator community is usually referred to as an effort to confirm validity of a code by comparing the prediction of a code 1) with measured data, 2) with theory based on the same physics and 3) with other similar codes. In this paper, we will discuss why the benchmarking of space charge codes is important and still a challenge now.

Space charge codes using macro particles[#] consisting of two parts. The first part is to update macro particle coordinates as a result of space charge effects integrated in each small time step. The second part is to advance macro particle coordinates in the same time period, which is entirely determined by the external lattice elements. Separation of the two parts and alternative evaluation of them are thought to be essential in order to take into account local details of the beam envelope and the *s*-dependent space charge potential, where *s* is the direction of the beam travel. If the beam emittance in transverse and longitudinal directions evolves, the space charge potential is updated so that the calculation is self-consistent. Although the second part, which is free from space charge, can be easily symplectic, that is the essential feature for long term tracking, evaluating space charge effects is susceptible to any kinds of modelling details. It is possible that the symplectic condition is violated if we employ the Particle in Cell (PIC) method (see below) to obtain a non-smooth space charge potential. Ref. [1] further discusses the conditions of symplectic time evolution when using PIC.

The idea of evaluating the space charge potential using macro particles came from plasma physics [2]. A brute force way of calculating the space charge potential is to sum up the binary interaction among the whole macro particle ensemble (Particle Particle or PP method), but it is not efficient from the computational point. A more practical approach is to divide the configuration space using a grid and then allocate macro particles to and calculate the Coulomb potential at each grid point. This is called the Particle Mesh method or the Particle in Cell (PIC) method [3].

Whether the PP or the PIC method is employed, the number of macro particles is much less than reality, several orders of magnitude less, e.g. 10^6 macro particles to represent 10^{12} real particles, and that may introduce non-physical effects. One of them is the numerical intrabeam scattering, which causes continuous emittance blow up [4].

A different approach is to fix the space charge potential at the beginning and keep it unchanged during the tracking. This is not a self-consistent calculation. However, when the space charge effects are a small perturbation, the change of charge distribution and therefore the change of the space charge potential are negligible and the dynamics is mainly determined by the external lattice elements. In fact, space charge effects in rings are relatively small because the periodic structure excites resonances and tune is allowed only a small shift, e.g., a few per cent change in terms of tune shift, so that the approximation is well justified. The advantage is that it is free from the numerical noise which the PIC method cannot avoid and can make the whole tracking exactly symplectic. On the other hand, some kind of instabilities, such as envelope instabilities due to space charge cannot be modelled [5].

One day in the not too distance future, the same number of macro particles as real particles in rings may be tracked in simulation with space charge effects once computational power has progressed significantly. Space charge codes at present, however, have to use some approximation, often drastic one as we mention later, and the validation of codes are essential.

In this paper, we will briefly review the benchmarking efforts of space charge codes in the past. We will then overview the present activities in detail. It is interesting to see that each period places different emphasis on the benchmarking because of the accelerator projects at that time, available computational resource and theoretical understanding. We would like to note that there was a similar review paper 10 years ago [6].

BACKGROUND

In the accelerator community, the first time when a space charge simulation code for rings was used was probably in the 80s. Although space charge codes for linacs had existed earlier, codes for rings were not easy to write because the number of calculation steps was much larger so it demanded heavy computational power.

There was the demand to preserve transverse rms emittance in high energy hadron colliders and avoid luminosity deterioration. There was also the need to minimise beam loss in high intensity hadron accelerators and so allow hand-on maintenance. It was the time when Superconducting Super Collider (SSC) in the US and KAON Factory in Canada were proposed. People knew

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[#]Numerical Vlasov solver is another way for space charge codes without macro particles, but we do not discuss it here.

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how to calculate the tune spread due to the space charge repulsive force including image charges and image currents arising from the boundary of vacuum chamber and magnets. A theory existed to predict how the beam reacted when coherent resonances were excited with lattice magnet errors. But they were not enough to predict how much emittance growth and beam loss occurred, which was crucial information to design and operate facilities. Although experimental attempts to measure emittance existed [7], the results were not conclusive or inconsistent with theory.

One way to reduce the time of computation was to fix the space charge potential at the beginning and kept the same potential throughout the tracking [8]. It was called the weak-strong model as an analogy with the model of beam-beam interaction. Interestingly, this is nowadays called the frozen space charge model and again is used extensively. The other way was to use a few macro particles (could be as few as 16) which represented a rough shape of the beam. The space charge potential was updated based on those particles with some assumption of the charge distribution function [9].

Space charge codes using a massive number of macro particles and tracking for the many number of turns in rings later became feasible [10,11] and were applied for the integer resonance crossing of high intensity beams [12] and for the half integer resonance crossing with the Alternating Gradient (AG) focusing lattice [13]. The results were consistent with the theory based on the smoothed approximation which was established many years ago [14]. Interestingly, the simulation efforts helped people to be aware of the old theories and the importance of coherent beam oscillations, not only dipole coherent oscillation, but also all higher order oscillations [15].

In the 90s, proposals for high intensity accelerator facilities: ESS, SNS and JHF (later becomes J-Parc) pushed the simulation efforts further and a few new codes were written. Orbit [16] is one of them which started development at ORNL for SNS and became one of the standard codes for space charge study now. Simpsons [17] and Track2D [18] were other examples although both were written for different purpose initially.

Although there were some attempts to benchmark the codes with experiments, more efforts were made to compare with the theories [19]. The biggest issue at that time was the accuracy of experimental data. On one hand, simulation could give all kinds of information including single particle trajectory and incoherent tune. Those were not necessarily available from the experiments. The experiment only gave information of the beam, not a particle, such as beam size and beam intensity. Another big issue was the reliability of the accelerator model. Details of the lattice such as multipole errors in individual magnet were not available. Benchmarking of codes was possible, but seemed difficult to make a quantitative comparison.

Also the benchmarking with theories carried more weight because it was the time the coherent resonance theory was revisited after a couple of decades since Smith [20] and Sacherer [14] formulated the resonance condition. The space charge limit imposed by the coherent resonance condition was discussed intensively and many simulations were carried out to study it precisely [21].

Nevertheless, the need for systematic measurements specifically for the code benchmarking purpose was realised in the community and it became a proposal of the space charge experiment using CERN PS in 2002 [22]. The aim was to set up the accelerator under control as much as possible and spend dedicated time for taking data good enough for the comparison with simulation. The large aperture of CERN PS with the relatively small proton beam helped improve the experiment. This was the first effort world wide of benchmarking against measurements and the results were fairly successful, although there was still some difference of a few ten per cents, which was attributed to unknowns in the lattice.

The CERN PS experiment was indeed one of the milestones in the community. It made people realise there were two different regimes of space charge effects. One is the beam loss regime and the other is the emittance growth regime. Space charge made tune spread always below the bare tune. The small amplitude particles in the beam had the largest tune shift and the large amplitude particles had less. When the small amplitude particles interacted with resonance, it caused the growth of particle amplitude around the core so that emittance increased. On the other hand, when the large amplitude particles interacted with resonances, the particles whose amplitude was already large gained even more amplitude. This often resulted in loss. Although agreement between experiment and simulation was not great quantitatively, it was enough to deduce a new understanding.

The model of beam loss was further extended including synchrotron oscillations. Very slow beam loss was explained by either trapping or scattering of particles with moving resonance islands created by either magnet imperfections or space charge itself [23]. A systematic study for different codes to model this very slow beam loss mechanism was established using GSI SIS18 lattice. It is still referred as a standard benchmarking suite among space charge codes [24].

WHAT IS BENCHMARKING?

As we mentioned at the beginning, benchmarking of simulation codes in the accelerator community means the comparison of simulation results against experiment, theory or other codes. Here we elaborate on the concept and explain more details.

Ideally the best benchmarking should be done by the comparison between codes and experimental results. This has to be done with the wide range of parameters so that we are confident of the results. Agreement at some particular tune for example may not be enough to claim that a code is benchmarked. It is true that hadron accelerators have difficulties of precise measurements of beam quantities. However, beam intensity by a current

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monitor, beam size with a profile monitor or a collimator, bunch shape by a bunch monitor are usually available. Frequency analysed signals of the beam position monitor give coherent tune, which is also a useful measurement.

For a simplified case, it is possible to calculate expected signals by theoretical prediction. This is useful to check whether the code is running as expected, especially in the initial stage of the development. The meaning of benchmarking is, however, different from the above because it is based on the same implementation of the physical mechanism. The main aim is rather check of coding or whether an approximation introduced in the code is qualitatively valid or vice versa. There is no chance that the missing physical mechanism in the code could be found in this comparison. Another practice is the benchmarking among the codes. Sometime this is the only way because no experimental observation or theory is available. As with theory, it is useful to check whether approximations and algorithm implemented by codes is valid.

If benchmarking with measurement is successful, we have strong confidence of what is happening in the real accelerators. At least we could conclude that the physics implemented in the codes was sufficient to reflect the reality. Furthermore, once we have the complete model in hand, it would be possible to observe things, which cannot be seen in the real accelerators. This gives a great opportunity to develop a deeper understanding of the beam dymanics.

If benchmarking with measurement is unsuccessful or partially unsuccessful depending on the input parameters, this indicates there must be unknowns in the experiment that the simulation failed to include. Although it may take some time to fix, we should consider this a great opportunity to find a new mechanism in the real accelerators, which we have not thought about before. We will show a few good examples later.

As we have seen, almost all the benchmarking efforts until about 10 years ago was among codes or with theoretical prediction, not against measurement at least in the sense of a quantitative comparison. In the last few years, however, benchmarking of space charge codes has made huge progress. There are several factors that made this happen. One is the increase of computational power. Parallel computing was introduced in the space charge calculation. It was thought to be difficult to implement a parallel algorithm because the potential has to be calculated at every time step using all the macro particles, which is unavoidable because of the long range nature of Coulomb potential. Individual macro particle is not a good variable to be distributed over the CPUs. However, it was managed in some way owing to a development of algorithm.

Another factor is to the way new facilities are constructed in the last few years. New accelerators under systematic management of design and operation efforts make all the relevant information available such as systematic and random multipoles in individual lattice elements. It is a totally different situation from the modelling of accelerators constructed more than a decade ago where we had to guess lattice imperfections. From the benchmarking point of view, this is the essential improvement. Measured magnetic field profile is available.

The progress of the instrumentation cannot be forgotten. Diagnostics device, e.g. for beam size measurement, may not have made a big step forward, but the environment of control and data taking software has been much improved to make it possible to handle the vast amount of experimental data under control. It is also true that book keeping of the huge amount of data associated with each individual lattice element become possible and they are directly connected to simulation codes, avoiding human error in interfacing.

BENCHMARKING TOWARD QUANTITATIVE AGREEMENT

Present benchmarking efforts become more systematic than ever. Modelling of the lattice and the beam is extended to include more details. Physics included in the codes are very modular so that the different assumptions and their impact on the results are easily compared. Operational details are included to make the simulation realistic. Diagnostics in the codes emulate the reality.

Although the importance of the details depends on each benchmarking case and each one is not always required, it is worth listing the key ingredients in the codes when the benchmarking against experiments is carried out.

Lattice

- Beam loss occurs when particles hit the vacuum chamber transversely. A proper model of the vacuum chamber aperture and sometimes its detailed shape is an important factor to compare the beam loss quantitatively.
- Alignment error of the lattice elements is a source of Closed Orbit Distortion (COD), which breaks the symmetry of the lattice and excites all harmonics, not only a multiple of superperiod, of resonances. If available, measured data instead of randomly generated one is preferred.
- Similarly, non-systematic errors of the bend and quadrupole strength either by measurements or by a random number generator should be included. This is also true for higher order multipoles.
- Thanks to a rapid computational development, it becomes easy to include time dependent error sources like a power supply ripple and tracking errors of the bend and quadrupole synchronisation.
- Footprint of the lattices are often arranged to minimise the building space. As a consequence, neighbouring beamlines including injection and extraction could make interference with the main lattice magnets. It should not be overlooked.

Beam

- Ideally we should have a realistic charge distribution with tails to start simulation. This could be obtained

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either by measurement or simulation of the preceding accelerator.

Operational Condition

- The way of injection has a strong impact on the space charge effects at the beginning of a cycle. Whether the injection employs painting, if so, whether correlated or anti-correlated painting should be properly modelled.
- How accurately the beam orbit and optics are matched to the lattice is an important factor for the development of coherent oscillation later on.
- Whether the beam is injected into the lattice which has already started acceleration or has the so-called flat bottom changes the time dependence of space charge effects. Tune spread shrinks and space charge effects diminish with quick acceleration.
- Some accelerators are now equipped with dual harmonic rf to increase the bunching factor. Another common technique is to ramp the transverse tune during acceleration so that the core of the beam does not move in tune space even if the tune spread shrinks.

Diagnostics

- As in the measurement, multi-particle quantities such as the beam intensity and the beam size should be measured in the same way as experiment. Frequency analysis of the centre of charges gives the coherent dipole tune.
- Single particle quantities such as the trajectory in phase space and the incoherent tune is only available in simulation. On the other hand, we have to be careful to use this information. Because of non-symplectic nature of the PIC method when the potential is not a smooth function, single particle trajectory, especially with the small betatron oscillation, often shows stochastic behaviour which is unphysical [25]. Empirically speaking, single particle trajectory with the large amplitude seems more reliable and gives useful information e.g. trapping in a resonance [26].

BENCHMARKING AGAINST MEASUREMENTS

There are several benchmarking efforts against experimental observation. We will describe a few cases.

J-Parc RCS

This is one of the successful benchmarking of a code against experiment. The accelerator is brand new, just finished commissioning a few years ago and the lattice information on multipoles and all kinds of errors is available on individual lattice element basis. Magnetic interference between the ring lattice and the beam transport is included, and it turns out to be non-negligible. Time dependent errors are also included, for example, ripples of the injection bump magnets.

Simpsons is used to model J-Parc and continuous improvements were incorporated by users during the commissioning period. In particular, the input of time dependent errors was extended for a variety of parameters. Evaluation of scattering at the foil is another recent major improvement. Single particle tracking module is parallelised with Open-MP. Operation process is simulated to reflect the reality, e.g., multi-turn injection with H^- stripping.

It is remarkable to see the agreement of the beam loss in the experiment and simulation within error bars [27].

ISIS

ISIS do not have as much detail information as J-Parc and it is unavoidable to keep some free parameters in a simulation model. However, Orbit simulation shows that discrepancy of the total beam loss is within a factor of two and small adjustment, that is the collimator position, gives a good agreement of the time structure as well as the total loss [28]. Fast cycling operation of ISIS (50 Hz) probably makes details of the lattice, e.g. higher multipoles, less important.

SNS Accumulator Ring

The code Orbit was written initially for the SNS project and extensive benchmarking with measurements at the SNS accumulator ring continues for many years. For the same reason as J-Parc RCS, a recently constructed and commissioned accelerator has a big advantage of the whole detailed information on the lattice elements.

Since the SNS ring is to accumulate the linac beam for 1000 turns and extract it by a single turn, modelling of multi-turn injection is the major part of efforts of benchmarking. Beam profile is compared for different intensities with and without a painting process. The agreement is generally good especially with detailed information of the hardware included (discussed below). There is, however, some discrepancy at a particular tune, e.g., at the Montague resonance. In other words, benchmarking has such an accuracy that it can tell the subtle difference and finding the source of the discrepancy is a good challenge.

Orbit code is evolving continuously. Recently it was combined with PTC code [29] that improves the accuracy of single particle tracking. Introduction of a Python interface makes the whole code user friendly whereas the computationally intensive parts remain C++ to keep performance in speed.

CERN LHC Injectors

The preservation of emittance in the LHC injector chain is the strong demand to realize high luminosity LHC in the near future. Space charge effects as a source of emittance growth and beam loss for a high brightness operation of the injectors are studied intensively along with the development of codes.

PSB, PS and SPS have its own space charge problem, but all has to deal with relatively long term behaviour, that is different from J-Parc RCS and SNS accumulator

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ring. It is also a platform to test even more stringent requirements in synchrotron of the FAIR project.

The "master" experiments have been defined for each synchrotron to investigate several aspects of space charge effects and carry out the benchmarking with codes. In PSB, beam loss and profile change around the half-integer resonance is studied and benchmarked with PTC-Orbit. With measured quadrupole field and alignment errors, the simulation replicated beam loss lasting for more than 100 ms [30]. In PS, a coupling resonance by sextupole with influence of space charge effects are studied. The beam profile was measured in 2012 and it was compared with the frozen space charge model, MADX-SC. We will explain a bit more details later. In SPS, the emittance growth around integer tune was measured and simulation efforts are going on. Because of very long time scale in SPS of the order of 10 s, a novel technique is being developed [31].

APPLICATIONS

Since benchmarking has now an ability to tell whether simulation and experiment agree or not, its obvious application is to help troubleshoot hardware defects or deepen our knowledge of the accelerator by looking at the beam dynamics in detail in simulation which is not seen in measurement.

In J-Parc RCS, the main part of the beam loss came from the foil scattering during injection. There was, however, another loss right after injection in the experiment. This beam loss had tune dependence as well. Later they found that the beam loss was due to a 100 kHz ripple induced in the ceramic vacuum vessel screening strip by the injection bump field. This excited additional betatron resonance at the fractional tune of 0.2. When they included the ripple in the simulation, they could reproduce the time structure of the beam loss with another peak. Eventually, they replaced the screening strip to avoid the ripple and the beam loss disappeared [32].

Also in J-Parc RCS, both experiment and simulation predicted that the beam loss was dominated by the scattering at the foil up to a certain beam power around 500 kW, but there was an additional loss suddenly above that power. The mismatch of the beam optics at injection was suspected. The simulation was carried out and it showed the better matching suppressed the additional loss. Based on the encouraging results from the simulation, the optics of the injection beam line into RCS was redesigned for a better matching. Later it was verified that the better matching at injection indeed suppressed the beam loss in the experiment [33].

In SNS accumulator ring, the beam profile was measured as a function of intensity. When the beam was injected without painting, flattening of the beam profile with beam intensity agreed with simulation very well. With painting, however, a discrepancy appeared. The broadening occurred at a different level of intensity. They suspected the painting kicker waveform did not function as expected. Later the waveform was measured and they found that the painting was in fact started a bit later than design and the waveform itself slightly differed from the model. When they included the measured waveform in simulation, agreement in terms of the profile broadening was much better than before.

In CERN PS, the resonance crossing study was performed for a sextupole coupling resonance, Qx+2Qy=19. Observed beam profile was very different in horizontal and vertical directions. In particular, a development of tail in vertical direction was significant whereas overall enlargement of the profile in horizontal direction maintained a Gaussian-like shape. Simulation with the frozen space charge model reproduced the profiles and further study by simulation led to the development of a theory of "fix lines" in 2D coupling resonances similar to fix points in 1D resonances [34].

Also in CERN PS, the beam loss around Qy=6.25 was identified only for high brightness beam. It was not visible in the tune survey with low brightness beam. Simulation indicated that the beam loss was excited by the space charge induced resonance of 8^{th} order which turned out to be the structure resonance if we considered the almost identical 50 FDDF structure of the CERN PS lattice. One way of mitigation of the resonance was to set an operating tune away from the resonance and simulation results with either around Qy=5.25 or 7.25 looked promising. The experiment verified the significant improvement in terms of the beam loss [35].

On ISIS, detailed studies of beam profile evolution near half integer resonance have shown good agreement between experiment and corresponding simulations with Orbit. Variation of intensity, driving term and tune demonstrated the predictive power of simulation over parameter space [36]. These results should provide the basis for predictive theoretical models that describe the observations. Beam motion suggests that understanding of particle growth mechanisms has to start with single particle, incoherent descriptions, but with suitable modifications to motion that derive from coherent beam response.

Those examples tell us that the proper use of space charge codes in rings helps us troubleshoot hardware problems, understand the beam dynamics in the accelerator much better, and sometime give us an opportunity to develop a new theory which we would not come up with otherwise. The power of space charge codes has much progressed for the last few years.

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