Summary of the SC Collaboration Meeting May 2014

F. Schmidt

The SC Collaboration Meeting took place at CERN from May 20th to 21st 2014. It was co-sponsored by EuCARD-2 XBEAM, The program, the presentations and session summaries are available at the indico page:

https://indico.cern.ch/event/292362/

There have been 28 registrants distributed over the following countries and laboratories:

Switzerland (CERN) 14
Germany (GSI, Frankfurt University, Helmholtz-Zentrum Berlin) 8
UK (STFC) 1
USA (Fermilab, Oakridge, BNL, LBNL) 5

The workshop lasted two days and the program has been grouped in the following sessions (in brackets the chairpersons):

20th of May

Welcome
Projects (F. Schmidt)
Codes (E. Benedetto)
Experiments I (H. Bartosik)
Discussion I (S. Gilardoni)

21st of May

Noise I (J. Holmes)
Noise II (G. Franchetti)
Experiments II (I. Hofmann)
Discussion II (F. Schmidt)

Meeting secretary: Delphine Rivoiron

Goal of the meeting

In April last year we have convened the CERN-GSI joint SC-2013 workshop. This has started a new series of workshops to take place every second year. The next one will be at the Oxford College, Trinity in March 2015. The next event is HB which will in fact only be in November of this year, so rather late as well. We therefore thought that we would need an earlier meeting (not in competition with the major workshops!) with all our collaborators in May 2014 to discuss the immediate needs of our SC studies in view of the LIU upgrade. In particular, since we are now restarting the LHC pre-accelerators and will re-start beam experiments at those machines.

Reviewing the lessons of the SC-13 workshop

1. **What are the requirements for SC codes (PIC/Frozen SC/Alternatives)**:
    - Fully operational and benchmarked lattice design tool, e.g. PTC, CHEF
    - SC Benchmarking with the GSI benchmarking suite
    - Special features: time varying fields, double RF, acceleration
    - Code benchmarking with experiments
    - Code availability including support for external modules
    - Speed and platform

   ➔ Full release
2. **Do we now 'fully' understand the noise and can we live with it, i.e. can we go to large number of turns with PIC codes?**
3. **How well can we reproduce the experiments with codes, in particular for the PSB & PS?**

Next Steps

1. **When will we have a code release ready of at least 2 PIC codes?**
2. **We need validity tests of PIC versus Frozen SC codes.**
3. **What hardware and support is required for realistic simulations of our machines?**
4. **Do we have the proper non-linear lattice models of our machines? Is our effort sufficient? Can we measure it?**
5. **Which experiments should be envisaged for a full code versus experiment benchmarking?**
6. **Is our theoretical understanding sufficient?**

Highlights of the Meeting

I will collect the highlights separately in view of Codes, Experiments and PIC Noise.

Codes

During this session progress reports have been given concerning pyORBIT (Jeff Holmes), SYNERGIA (James Amundson), IMPACT (Ji Qiang) and the MADX- with a frozen SC implementation (Valery Kapin). All codes are in preparation to cover the needs for the CERN accelerators. In particular pyORBIT, an update of the PTC-ORBIT code with a PYTHON front-end, is now ready for the CERN machines. 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 (Giuliano Franchetti) and the results will be introduced into that benchmarking suite by fall of this year. For the IMPACT code help was proposed for the details of the benchmarking effort by the SYNERGIA team. 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 the frozen SC codes that have been tested in the GSI benchmarking suite. 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 of the MADX frozen SC code, which has already been benchmarked with the GSI suite. In particular, the re-normalization of the sigma values, ever so often, has proven essential in correctly reproducing experimental studies at the CERN PS. Further developments are being planned in collaboration with Fermilab. At GSI work has been started with pyORBIT and various codes are being compared (Sabrina Appel).

Experiments

Various studies at the PSB and the PS have been presented and the simulation results are starting to be convincing.
At the PSB booster (Vincenzo Forte) it could be demonstrated that good agreement between simulations (PTC-ORBIT) and experiments could be achieved for particle motion close to the ½ integer resonance where large losses do occur. Precondition for these nice results has been to include in the model both the measured quadrupole and misalignment errors. This is a confirmation of our 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 may imply to average over full synchrotron periods.
The collaboration concerning the 2012 PS experiment has presented first results in 2 talks (Raymond Wasef, Giuliano Franchetti). On the one hand, MADX-SC with frozen SC and a sigma re-normalization every 1'000 turns seems 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 Qx + 2 Qy. On the other hand, the studies at GSI show similar results and 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. Of course, the strong detuning from SC plays an important role.
The 4th order resonance at the PS (Raymond Wasef, Shinji Machida) has been studied in an independent collaboration with STFC Rutherford. It has been found that h=50 (i.e. one finds 8 islands instead of the naively expected 4) is most damaging for the PS due to the fact that this machine has a symmetry of 50. It has been shown in simulations with Simpson that a change of the integer part of the tunes could mitigate this problem.
There has also been a study about indirect SC inducing injection oscillations in the PS (Alex Huschauer). For the PSB a study has been presented how to potentially mitigate SC using hollow beams (Adrian Oeftger). Another study on high intensity beams also in the PSB (Magdalena Anna Kowalska) discusses the mitigation of losses at higher injection energy either by a collimation system or transverse beam painting.
Lastly, there has been a report about using MADX-SC with completely frozen SC,

i.e. without re-normalization of the beam sigmas, for sub-injection energies at RHIC (Christoph Montag). These simulations also included the BB effect induced by the two counter-rotating and colliding beams.

PIC Noise

During the SC workshop in 2013 the issue of noise in PIC codes has been re-discussed in view of the fact that all particles in the distribution 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 single particles erratically and proportional to its strength. These findings have caused the SC community to revisit the theory of noise in PIC codes that has been studied decades ago by Jürgen Struckmeier at GSI.
Jürgen reminded us that space charge effects include Intra Beam Scattering. His involved theoretical analysis ends up with 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 (Oliver Boine-Frankenheim, Ingo Hofmann) has picked up from this anisotopic phenomenon and has found that in FODO structures there is an additional component of grid noise that is there even for zero anisotropy. Oliver referred to techniques from the plasma field that try to limit the study to just the part of the distribution that does not belong to the matched part, i.e. the so-called δF-PIC scheme. However, the overall response of the SC community has been rather skeptical. It remains to be seen if that technique would really be applicable for the beam PIC codes.
At SNS (Jeff Holmes) 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 (James Amundson). It was found that in the case of the SIS18 used in the GSI benchmarking the simulation became unstable for certain even numbers of SC kicks while this effect could be dramatically reduced for a prime number of SC kicks. They find that the PIC tracking for this SIS18 structure converges over 100’000 turns when 4 million macro particles are used for a 64x64x64 grid. It is interesting to note that they find good agreement for distribution properties like emittance growth with the frozen SC codes although single particles are chaotic also in their studies. The conclusion is that in the case of convergence 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 (Frederik Kesting). 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.

Summary of the discussion

It is important to mention that the following scientific secretaries have contributed substantially to this workshop by taking note of all responses to the questions and comments during the discussions:

H. Bartosik, E. Benedetto, V. Forte, E. Granemann Souza, A. Huschauer, F. Kesting, M.A. Kowalska, A. Oeftiger, M. Titze, R. Wasef.

Discussion I&II (Chairperson: Simone Gilardoni, Frank Schmidt)

1) Simone made sure that the community is aware about CERN's requirements for the SC codes:
    a. Complete set of magnetic elements, in particular the combined function magnet
    b. Misalignment
    c. Linear and non-linear chromaticity
    d. Multipolar components
    e. Double RF
    f. Time varying magnet strength, RF voltage and phase
    g. Acceleration

    It was confirmed by all code teams that this is well understood.

2) Progress of the code benchmarking with the SIS18 of the GSI benchmarking suite:
    a. For pyORBIT the last (7^{th}) step (100'000 turn tracking and recording emittance growth) is missing.
    b. SYNERGIA is done.
    c. IMPACT still has problem with parameters (James Amundson offers help).
    d. MADX-SC has been fully benchmarked by Valery Kapin several years ago.
    e. The goal is to have full releases of the 3 PIC codes by the end of the year including all CERN requirements and documentation.
    f. It has been proposed to add performance parameters (how fast, how accurate…) in this benchmarking.

3) What hardware and support is required for realistic simulations of our machines?
    a. The CERN SC team presently lacks state of the art computer resources. Neither do we receive sufficient software development support.

b. Besides super computers as used by SYNERGIA and IMPACT the GPU approach might be an alternative. James Amundson is eager to look into this. However, several participants raised doubt concerning this approach since one cannot just compile one's code on those systems but instead for each GPU type special effort is required to get the same code running. Therefore portability is not ensured on GPUs. Instead constant and substantial development work is required to use GPUs in the long run.

4) Proposed code benchmarking with experiments at the CERN machines
   a. Prepare explicitly specified "master" experiment for a given machine with a clearly defined goal and parameters of interest such that both experiments and the simulations can be performed in an unambiguous way. Both incoherent and coherent effects should be tested. Moreover, it should be determined when a self-consistent treatment (slow by definition) is required and when a frozen and fast SC approach is sufficient.
   b. The experimental description should specify the resonance order and also its type. Since progress has been achieved with the 4D analysis either 2D or 4D resonances are okay, except that 2D resonances maybe easier to understand and the effects on the beam distribution could be potentially faster.
   c. Linear and non-linear models of the machines will be made available in MAD-X files at publicly available AFS space of the CERN SC working group.
   d. The experimental data will be made available there, too.
   e. The general advantage of the CERN machines is their availability and the possibility to study many different cases.
   f. For the PS: continue the 2012 experiment in the vicinity of the Qx + 2 Qy resonance. The 4^{th} order resonance study is another candidate.
   g. Equally relevant are experiments at PSB and SPS. With PIC codes we should look for fast phenomena. For the PSB one can create a measurement plateau at a given energy and there are new multipoles with power supplies. Studies at the SPS are interesting since this machine allows the control of the chromaticities and it also has octupoles available.
   h. The question has been raised if one should exclude acceleration for the beginning since some codes do not have acceleration with the notable exception of pyORBIT.
   i. The issue was raised about moderate particle loss in the experiment, which apparently is the most difficult quantity to be determined by simulations but at the same time is one of the most relevant for optimizing the machine performance.
   j. As a deadline it was agreed to have the proposals for the experiments, including the MAD-X input files, ready for discussions at the next SC workshop in March 2015.

In the discussion it was stressed that the complexity of the lattice, needed to fully describe the machines, can also be the limiting factor on speed. In general, there has been across the board agreement to proceed with this plan of benchmarking experiments.

5) Raymond Wasef has raised the issue of scalability of PTC-ORBIT runs that apparently saturate around some 20 cores on a 48 core machine. At Oakridge, ORBIT is typically run on machines with a low number of cores and hasn't been optimized for large number of core machines. SYNERGIA runs are done on 100'000 processors but works effectively only for well prepared cases. However, the code in general seems to scale well with the number of cores. Doubts have been raised about the value of scalability laws. It definitely seems necessary to test the scalability of all PIC codes with real world examples.
   The MADX-SC code is under OPENMP control and scaling has been demonstrated up to 16 core machines if at least 4000 particles are being simulated.

6) An Excel template file has been prepared to hold the available capabilities of the various SC codes. We hope that the code developers will be willing to fill in the details of their codes. This file should be updated whenever a code has been updated substantially.

7) A discussion has been started by Shinji Maschida about the significance of the SIS18 benchmark agreement between the frozen SC codes and the PIC code SYNERGIA for a run over 100'000 turns. Does this imply that the physics is the same? Apparently, the PIC noise did not harm the bulk results but it would be good to check whether the beam distribution deviates from a Gaussian profile during these long-term runs.

8) Considerable effort has been spent by several teams to improve our understanding about PIC noise:

   a. Due to PIC noise the motion of all particles in the distribution becomes chaotic.
   b. Theoretical models of PIC noise, developed long time ago, have been reviewed and extended.
   c. Despite this fine grain noise, long-term PIC simulations over 100'000 turns agree on bulk quantities as emittance growth in the SIS18 benchmarking with frozen SC codes. A precondition is that the convergence tests are done over the full time scale of the simulations.
   d. Ingo Hofmann has proposed a simulation experiment with trapping phenomena in which a code-generated noise level is introduced to check how much noise can be tolerated and if the codes can handle it. The goal of this experiment is to determine the sources which have the potential to break down Hamiltonian mechanics and artificial noise is one of those sources.

There has been a lively discussion on how this noise should be generated. In particular, PIC noise may not be approximated by white noise. Ingo suggested that a group of colleagues should look into defining such an experiment: which model to use, which code to take for tracking, choice of 2D or 4D resonances, which strength of SC force to apply, define adequate type of noise etc.

9) The next SC workshop is planned for March 2015 at the Oxford College, Trinity.