WORKING GROUP C SUMMARY: COMPUTATIONAL CHALLENGES, NEW CONCEPTS, AND NEW PROJECTS

Steven M Lund*, Facility for Rare Isotope Beams, Michigan State University, USA
Giuliano Franchetti, GSI, Germany
Hiromi Okamoto, Hiroshima University, Japan

Abstract

We summarize workshop discussions held in Working Group C at the 54th ICFA Advanced Beam Dynamics Workshop on High-Intensity, High-Brightness, and High Power Hadron Beams (HB2014; East Lansing, Michigan) taking place 10–14, November, 2014. The charge of Working Group C was to formulate a workshop-oriented agenda on *Computational Challenges, New Concepts, and New Projects*. In this summary, we list topics selected and linked presentations that were delivered, and summarize discussions held. Only limited attempts are given to summarize details of individual presentations. Focus is primarily on recommendations based on material presented both in the topically grouped talks and in linked workshop discussion sections immediately following each group of talks.

INTRODUCTION

The charge of Working Group C (WGC) to address *Computational Challenges, New Concepts, and New Projects* is very broad to cover adequately in 14 invited presentations of 25 minutes duration (20 minutes + 5 minutes discussion) each and approximately 100 minutes of workshop discussion time. Moreover, the potential for the WGC charge to overlap and conflict with Working Groups A (*Beam Dynamics in Rings*; WGA) and B (*Beam Dynamics in LINACS*; WGB) was significant. In an attempt to focus to a reasonably limited agenda to be productive, the conveners tried to pick workshop-oriented topics to group into four sessions with 25 minute joint discussion periods held after the topically grouped talks. Care was taken to minimally overlap with topics taken up in WGA and WGB. Topics likely of interest in WGA and WGB were organized in the overall workshop agenda (two parallel sessions) to allow joint sessions. Topical groupings in WGC were as follows:

- First Session, Tuesday morning, Nov. 11th.
  Computational: Simulation Infrastructure
  New Concepts: Scaled Experiments
- Second Session, Tuesday afternoon, Nov. 11th. (Combined with WGA,WGB)
  New Concepts: Nonlinear Integrable Optics
- Third Session, Wednesday morning, Nov. 12th.
  Computational Challenges: Long Path Length Simulations / Benchmarking
- Fourth Session, Thursday afternoon, Nov. 13th. (Combined with WGA,WGB)
  New Projects: New Projects: ISIS Upgrade, FFAG, Beam-Beam, Electron Lenses

In the four WGC topical summary sections that follow, we give titles and speakers of invited presentations delivered and primarily summarize highlights of 25 minute discussions held (following each session listed). Discussions were largely, but not exclusively, stimulated by the talks within the immediately preceding sessions. Individual talks can be obtained (provided speakers did not opt out) on the HB2014 web site [1]. Recommendations given reflect perceptions of the conveners based on discussions held. Efforts were made to be balanced in summary, but limitations on the conveners backgrounds may result in some of these being of limited value.

SIMULATION INFRASTRUCTURE AND SCALED EXPERIMENTS

Framing invited presentations delivered under simulation infrastructure were [1]:

- Jean-Luc Vay (LBNL), *Needs and considerations for a consortium of accelerator modeling*;
- Ji Qiang (LBNL), *Development of integrated workflow for end-to-end modeling of accelerators*;

and a single presentation for scaled experiments was [1]:

- Hiromi Okamoto (Hiroshima University), *Recent results from the S-POD trap systems on the stability of intense Hadron beams*.

The talks by J.-L. Vay and J. Qiang were invited to cover code collaborations and infrastructure issues which could benefit from community discussion in the workshop. The talk by H. Okamoto was grouped since it overviews an experimental alternative to simulation to efficiently model aspects of beam physics with a trap experiment.

Consensus appeared strong that the code consortium initiative (Consortium for Advanced Modeling for Particle Accelerators; CAMPA) reported by J.-L. Vay is a good cause for community support. If successful, many will benefit in the long term and duplicative efforts will be minimized, allowing resources to be more productively employed to extend and improve the simulation tools. The goal is to provide reliable tools for accelerator modeling

* lund@frib.msu.edu

ISBN 978-3-95450-173-1

from components to full systems. A well motivated strategy of integrating new models without disturbing existing users/developers is being employed. Increased reliability, leveraged effort/funding, and benefits for more unified input/output should result from broad acceptance of the model of integration offered by CAMPA. Preliminary DOE funding is limited. Initial (through 2015) members include LBNL, FNAL, and SLAC. Recommendations suggested by discussion points include:

- Efforts should be expanded beyond the three initial CAMPA partners as soon as funding allows.
- National laboratories may be the natural host for CAMPA since it will need consistent long-term support, but a framework should be adopted to allow participation by universities, companies, and international partners to further leverage effort.
- Previous impressive successes with the Los Alamos Code Group (LACG) in distributing legacy codes (POISSON, TRACE, PARMELA, PARMTEQ etc) should not be neglected. Support of such legacy codes as well as possibly more advanced tool kit components could bring many more users and justify more DOE support. LANL reports that updates of widely used LACG codes such as PARMELA (rewritten in C++) are being carried out and will be made available. Incorporating and leveraging these efforts seems logical.
- Codes for design of optical elements (magnetic and electric) and RF cavities should also be included in the effort since they are also central to design activities.
- Issues of ownership, credit, and distribution of funding will need to be addressed for broad participation.

End-to-end modeling efforts such as those outlined by J. Qiang with the IMPACT code can help support performance claims made for proposed facilities to help justify funding and put concepts on a firmer foundation. Efforts like this fit in well with the CAMPA consortium reported on by J.-L. Vay which also includes the IMPACT code and LBNL. Benefits can be obtained by self-consistently simulating systems fully within an integrated suite of simulation tools since many issues can be more efficiently and reliably evaluated. Questions/comments brought up in discussion include:

- Rings may prove especially difficult for self-consistent (including space-charge effects) modeling and injection of beams into rings via multi-turn stacking and painting. Such processes open questions as to whether it is possible, or even necessary, to carry out detailed upstream modeling in an end-to-end context.
- Even in linear accelerators beam sources and the initial transport near the source can be extremely challenging to simulate self-consistently and seamlessly integrating results may be difficult.
- Initiatives like CAMPA proposed above may provide long-range hope for achieving this vision.

Some of these issues are also brought up in the section on Long Path Length Simulations / Benchmarking.

It appears well established with results reported by H. Okamoto that small Paul-trap based experiments can be applied to effectively model various scalable processes in Hadron beams using an analogy between ions confined in the trap and beam-frame processes in an accelerator. Experiments can be small in scale and inexpensive. Low particle energies and apparatus field strengths have no potential for machine damage. These features make such systems ideal for dedicated physics experiments and student training. Processes amenable to scaling such as lattice focusing properties, halo, and space-charge transport limits induced by resonances appear possible to address with these systems. Unfortunately, the US program at the Princeton Plasma Physics Laboratory exploiting this beam frame analogy with a trap to investigate space-charge physics recently lost funding — apparently due to ongoing DOE budget stress in plasma physics. The remaining US program at the University of Maryland [2] using low energy electrons in a ring to investigate scalable physics is considerably larger with different technical issues. Consensus appeared strong that these experiments are beneficial to our community. It is noted that even idealized theory and simulations provide useful guidance for machine tuning. Paul trap experiments augment what is learned from these directions with an experimental and student training component and can be much faster (one machine cycle per ms at Hiroshima U. trap) than even idealized numerical simulations. Rutherford-Appleton Lab reported (D. Kelliher, short discussion presentation) ongoing plans in a collaboration with Hiroshima U. to construct a trap experiment similar to the systems reported by H. Okomoto. This is welcome news given the demise of the US program due to funding issues. Recommendations include:

- The broader Hadron accelerator community should be more active in conveying specific ideas of scalable processes that can be probed with trap facilities.
- Diagnostics presently employed (confined charge and density profile as function of time via dumping) are very limited. This restricts possibilities to exploit the traps more fully. If constraints needed for generation (electron impact ionization and potentially others) can be addressed, the experiments should become more useful with more detailed phase-space diagnostics. We recommend that attention be given to this.
- Paul traps might provide a natural step for laboratory tests of Nonlinear Integrable Optics (see also the summary on Nonlinear Integrable Optics) and this should be examined.

NONLINEAR INTEGRABLE OPTICS

Invited presentations delivered in this section to cover ongoing efforts in Nonlinear Integrable Optics (NIO) were [1]:

ISBN 978-3-95450-173-1

- Sergei Nagaitsev (FNAL), *The IOTA ring: present status and plans*;
- Stephen Webb (Radia-Soft), *Chromatic and space charge effects in nonlinear integrable optics*;
- Rami Kishek (U. Maryland/UMER), *UMER 2.0: Adapting the University of Maryland Electron Ring to explore intermediate space-charge and nonlinear optics for Hadron beam facilities*.

The final presentation by R. Kishek on the University of Maryland Electron Ring (UMER) was also technically a scaled experiment topic, but covered plans to adapt the UMER ring to experimentally explore nonlinear integrable optics by modifying their low energy electron beam ring. The NIO topic is a natural fit to the workshop given the high community interest in improved transport promised by this concept. The session was well attended from other workshop working groups.

The workshop discussion/debate following the presentations on NIO was lively and productive. There appears to be both enthusiasm and healthy skepticism on aspects of and promises afforded by NIO. Much work remains to be done before the concept can be considered as a replacement to conventional (quadrupole) linear focusing in practical applications. However, the promise of having significantly diminished beam halo generation (from mismatch and other sources) and better stability properties (from large intrinsic tune spread) relative to linear focusing, and thereby potentially more compact and cheaper machines is highly significant. Support appeared high on seeing efforts to develop NIO progress. Even in the event of a practical failure, exploring NIO to a definitive conclusion should increase understanding of beam transport and provide excellent student training to support our field. It is worthwhile noting that various laser/plasma acceleration and focusing concepts have received much better funding in the face of significantly larger and more difficult confounding technical issues faced. Even with the significant advances made in those fields, practical applications such as colliders or even compact front-ends based on laser/plasma technology are likely much further from fruition and more expensive to address than for the corresponding case with NIO. We should be doing a better job as a community to support efforts to bring NIO to a logical conclusion — while remaining mindful of not over-selling consistent with a field building significant scale facilities that must deliver. Recommendations include:

- The IOTA ring appears well motivated and the FNAL team is appropriate to investigate/leverage the concept. It is unfortunate that this effort appears stalled due to a lack of funding given that needs are relatively modest. We endorse efforts to secure funding to complete the ring so relevant tests can be expeditiously carried out.
- Efforts to adapt the UMER ring to explore aspects of NIO appear well motivated. This also fits the fundamental physics and student training role of the group. We endorse U. Maryland efforts in this reorientation of their program.
- Paul traps (see H. Okamoto presentation in section on Simulation Infrastructure and Scaled Experiments) with adaptable electric focusing might prove amenable to economically explore long path length transport aspects of NIO. We advocate exploring this more fully. Given funding issues with IOTA, trap experiments might provide a more rapid and economical partial step to explore concept viability.

Constructive criticisms of the ongoing efforts on NIO that may be addressable within the context of ongoing efforts include:

- Single particle analysis of the dynamic aperture with applied magnetic fields as likely manufactured and realistic lattice errors should be clearly presented to better contrast the idealized situation with linear focusing. This may be easier to analyze than issues being presented (chromaticity, halo generation, ..) and help clarify system properties.
- A moment (envelope) level of beam description would be useful, even if idealized, to better understand beam matching properties to the nonlinear lattice at finite intensity.
- Halo contrasts of NIO to linear focusing may be hard to make without matching characterizations to the nonlinear lattice (see above) clarify a consistent basis contrast. Halo production results shown may be misleading given the extreme initialization assumptions made in the linear focusing case. However, useful results on halo *extents* (and apertures needed to contain) in phase-space are probably obtainable at present and could be contrasted between NIO and linear focusing in an "equivalent" focusing and intensity sense to help draw useful conclusions.
- An engineering survey should be carried out to explore potential issues with making magnets needed for NIO lattices including limitations on pole-tip field strengths. Scaling relative to "equivalent" linear optics incorporating aperture clearances to confine halo together with magnet technology limits could better characterize what savings might result if the promises of NIO on improved transport are realized. This could better motivate efforts/funding if potential savings are significant.

LONG PATH LENGTH SIMULATIONS / BENCHMARKING

Invited presentations delivered to cover long path length simulations and code benchmarking were [1]:

ISBN 978-3-95450-173-1

- Frank Schmidt (CERN), *Code requirements for long term tracking with space charge*;
- Jeffery Holmes (SNS), *Status of PY-ORBIT and noise control in PIC codes*;
- Kazuhito Ohmi (KEK), *Artificial noise in PIC codes and consequences on long term tracking*;
- Ingo Hofmann (GSI), *Grid Noise and Entropy Growth in PIC Codes*.

Here, at the request of WGB, we have included the presentation by I. Hofmann in WGB within the scope of our summary discussions since the topic relates to computational issues taken up in WGC. These individual topics were selected to continue previous productive workshop discussions on this long-running and difficult topic [3]. The emphasis was primarily on rings and the issue of self-consistent space-charge modeling. However, aspects are also relevant to linacs and near-source transport.

Presentations on this topic made clear it will likely be a long struggle to self-consistently incorporate space-charge effects within realistic models and gain confidence in results. Much careful work will be required and new or improved simulation methods may prove necessary. Long path lengths and highly nonlinear models combined with difficult to resolve numerical convergence issues in statistics and gridding in many models open considerable challenges. Even with relatively simple idealized particle-in-cell (PIC) models, for example, may be difficult to achieve due to "expensive" scaling in numerical requirements for clear convergence. As F. Schmidt pointed out, benchmarking both in a code-code (also algorithm-algorithm) and code-experiment sense will be needed to gain confidence in results. Needs include analytic results to check simulations against, other "verified" codes, and reliable experimental data. Recommendations and comments brought out be the presentations include:

- Benchmarking libraries should be accumulated to aid sorting out difficult issues. For example, extensions of efforts like the GSI benchmarking efforts on space-charge induced trapping [4] would be useful.
- Needs may change with questions asked and space-charge intensity: particle orbits become nonlinear when space-charge is included and most reasoning is based on idealized KV (linear space-charge) beam models. What is adequate/optimal may change with the specifics of the problem and understanding extreme limits (even if idealized or not accessible) may help guide efforts.
- Even though plasmas are an extreme limit (essentially full space-charge depression), it is possible that our field can derive benefits from the large body of work on self-consistent modeling in plasma physics (see also comments on orbits above).
- It would be useful to see more tests of methods/algorithms by neutral parties who might compare strengths and weaknesses of various methods on a consistent basis. Results may change with system parameters, model dimension, and questions asked.
- Tests might have better guiding value if kept as simple as possible till effects and simulation needs are better understood. Some test cases appear to have multiple effects with significant impact occurring simultaneously making it difficult to draw clear conclusions on needs and limits.
- Can theory (see I. Hoffman presentation) provide guidance on numerical noise properties and the limits imposed if test cases are simple enough?
- Are "frozen" models with high detail (see K. Ohmi presentation) provide a way to bypass present practical difficulties in numerical convergence to address a variety of questions in real systems?

One sub-topic debate opened in the workshop is illustrative on challenges involved. Brief discussions session presentations by H. Zhang (JLAB) and B. Erdelyi (North Illinois U.) suggested intriguing possibilities with employing a Fast Multipole Method (FMM) to efficiently solve Poisson's equation (including structures and boundary conditions in some manifestations). Such methods open prospects for removing grid effects and simulation noise if fields are applied directly to the particles. Insofar as physical particle numbers are used, it was emphasized that collisional effects would be physical though examples cited appeared to have relatively low particle numbers. Results presented suggest advantages of the FMM relative to PIC methods. But the presentation by J. Holmes appeared contradictory with a FMM applied to a ring problem appearing unfavorable relative to a PIC method due, presumably, to numerical capacity limiting particle number resulting in enhanced collisional effects. Continued exploration of such issues to a clear conclusion might provide long-term benefits even if it must first be done within idealized contexts. Guidance on where various methods might prove optimal by a neutral party might provide significant long-term benefit.

NEW PROJECTS

Invited presentations delivered to cover selected new projects which did not all within the scope of the other working groups were:

- Dean Adams (STFC/RAL), *Ring Simulation and Beam Dynamics Studies for ISIS Upgrades 0.5 to 10 MW*;
- Suzie Sheehy (RAL), *Characterization of a 150 MeV FFAG*;
- Christoph Montag (BNL), *Recent results on beam-beam effects in space charge dominated colliding ion beams at RHIC*;

ISBN 978-3-95450-173-1

- Xiaofeng Gu (BNL), *The physics and use of electron lenses at BNL.*

The S. Sheehy presentation was kindly delivered on short notice to fill in an unexpected opening in the schedule and may not be archived on the workshop web site [1]. Because the New Projects component of WGC involves less focused topics, here we carry out a more conventional summary followed by more limited recommendations.

The ISIS upgrade (see D. Adams presentation) is a major project in RAL. One option is to increase the injection energy from 70 MeV to 180 MeV at 8×10^{13} ppp for 0.5 MW operation. A number of studies supporting the upgrade were carried out using the ORBIT code including transverse injection painting and foils, resonances, and longitudinal dynamics. Resonance issues were studied by analyzing working points and driving terms. Detailed simulation studies suggested that losses can be manageable. Another upgrade scenario to a 2-10 MW RCS ring for a short pulse facility was reported initiated with both 1D injection/acceleration and 3D injection studies carried out.

FFAG accelerators will need to accelerate intense beams to realize their full promise. RAL is evaluating their use as part of an alternative upgrade path for ISIS. In the presentation by S. Sheehy, initial activities using a scaling FFAG associated with measuring and correcting the closed orbit (which has properties different from conventional synchrotrons) were reported. To investigate space-charge effects in the complex magnetic geometry and related enhancement by a machine tune migration with energy gain, plans include use of simulation tools in support of the program.

Beam-beam issues are reported on in two presentations from BNL. Potential detrimental space-charge issues have been a concern in beam-beam and research on the issue is covered by C. Montag. At BNL, Au collision at 2.5–10 GeV/nucleon are of concern in RHIC. Results reported suggest that observed beam decay is not related to space-charge and an associated change of tune. Diffusion studies agreed with experimental results from 2010, and helped set a new working point improving performance in 2014. The computer model used was relatively simple, yet adequate to identify physics, match previous experimental results, and guide improvements. Complex hardware needed to evaluate beam-beam mitigation via electron lenses are being developed and the status of these efforts were reported on by X. Gu. Resonances induced by Coulomb forces are not only induced internally within a beam. In colliders, the Coulomb force of one beam influences the other beam with associated resonance effects. Compensation/mitigation of the beam-beam effect is foreseen via electron lenses to produce a "counter" space-charge effect. Hardware needs are considerable. Solenoids with fields up to 6 Tesla are used. In BNL these lenses are constructed and evaluated for use in head-on beam-beam compensation. The effect of the lenses on orbit and tune were measured and found to be as expected. Future steps will require the use of separate, dedicated hardware.

In this topical of WGC, the common theme is that upgrades of existing facilities are reached through detailed space-charge simulation studies. This requires reliable, benchmarked codes. Comments/recommendations include:

- ISIS upgrade activities illustrate well the need for effective benchmarked code tools to explore loss issues guiding significant facility upgrades.
- Support of FFAG development opens needs for code extensions to deal with the complex applied fields, bunch-bunch interactions, and long path length.
- Frozen simulation models (see Sec. Long Path Length Simulations) may address some facility support issues.
- Beam-Beam space-charge appears not to be playing a significant role at RHIC. Nevertheless, results suggest that the facility may be employable in an R&D sense to develop complex plasma lens technology to address the issue for parameters where the effect may be more severe.
- Beyond substantial technical hardware challenges, the effective use of electron lenses to mitigate space-charge tune shift needs a careful study to verify that the lenses will not produce new detrimental resonances (forces compensated on average) to offset benefits suggested.

ACKNOWLEDGMENTS

The conveners wish to thank all participants of WGC. The invited speakers all devoted considerable effort to formulate their presentations and frame the workshop discussions. Many invited speakers and C. Prior (RAL) in particular assisted editing this summary. These contributions are appreciated. Support for the conveners is as follows: S. Lund, from the U.S. Department of Energy Office of Science under Cooperative Agreement DE-SC0000661 and the National Science Foundation under Grant No. PHY-1102511; G. Franchetti, from the European Commission under the FP7 Research Infrastructures project EuCARD-2, grant agreement No. 312453; H. Okamoto, in part by a Grant-in-Aid for Scientific Research, Japan Society for Promotion of Science.

REFERENCES

[1] Presentations are archived on the HB2014 web site: http://frib.msu.edu/misc/hb2014/index.html

[2] See information presented on: http://www.umer.umd.edu

[3] The topic was discussed at HB2012 (see: http://hb2012.ihep.ac.cn and associated material archived on jacow at http://jacow.elettra.eu) and the 2013 CERN space-charge workshop (see http://indico.cern.ch/event/221441/).

[4] See: http://web-docs.gsi.de/~giuliano/research_activity/trapping_benchmarking/main.html

ISBN 978-3-95450-173-1