WISH-LIST FOR LARGE-SCALE SIMULATIONS FOR FUTURE RADIOACTIVE BEAM FACILITIES

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Abstract

As accelerator facilities become more complex and demanding and computational capabilities become ever more powerful, there is the opportunity to develop and apply very large-scale simulations to dramatically increase the speed and effectiveness of many aspects of the design, commissioning, and finally the operational stages of future projects. Next-generation radioactive beam facilities are particularly demanding and stand to benefit greatly from large-scale, integrated simulations of essentially all aspects or components. These demands stem from things like the increased complexity of the facilities that will involve, for example, multiple-charge-state heavy ion acceleration, stringent limits on beam halos and losses from high power beams, thermal problems due to high power densities in targets and beam dumps, and radiological issues associated with component activation and radiation damage. Currently, many of the simulations that are necessary for design optimization are done by different codes, and even separate physics groups, so that the process proceeds iteratively for the different aspects. There is a strong need, for example, to couple the beam dynamics simulation codes with the radiological and shielding codes so that an integrated picture of their interactions emerges seamlessly and trouble spots in the design are identified easily. This integration is especially important in magnetic devices such as heavy ion fragment separators that are subject to radiation and thermal damage. For complex, high-power accelerators there is also the need to fully integrate the control system and beam diagnostics devices to a real-time beam dynamics simulation to keep the tunes optimized without the need for continuous operator feedback. This will most likely require on-line peta-scale computer simulations. The ultimate goal is to optimize performance while increasing the cost-effectiveness and efficiency of both the design and operational stages of future facilities.

INTRODUCTION

The study of the properties and reactions of short-lived isotopes is a key to our understanding of fundamental questions in nuclear physics, nuclear astrophysics and the study of fundamental interactions at low-energy. This has long been recognized by the international nuclear physics community and is reflected by the investments in that field that have been or are being made in North America, Europe, and Asia. The U.S. nuclear physics community addressed the importance of such studies in its 2002 Long Range Plan [1] where an advanced facility called the Rare Isotope Accelerator (RIA) was identified as its highest priority for new construction. A paper on the computational needs of RIA was given at ICAP 2004 [2].

In this paper the needs and opportunities for peta-scale simulations applied to advanced exotic beam facilities, in general, will be discussed. Examples of such facilities in Europe and Asia will be presented in the following section. All of these examples, RIA or RIA-lite in the U.S., the GSI FAIR facility in Europe, and the RIKEN RIBF project in Asia, are based on high power heavy ion driver accelerators, each using a different accelerator technology.

The following three sections cover the expected availability of peta-scale computing facilities in the near future, the needs for large-scale simulations in the design of next-generation advanced exotic beam facilities, and the opportunities to use peta-scale computing to support the operation of advanced facilities with near real-time simulations for a "model-driven accelerator."

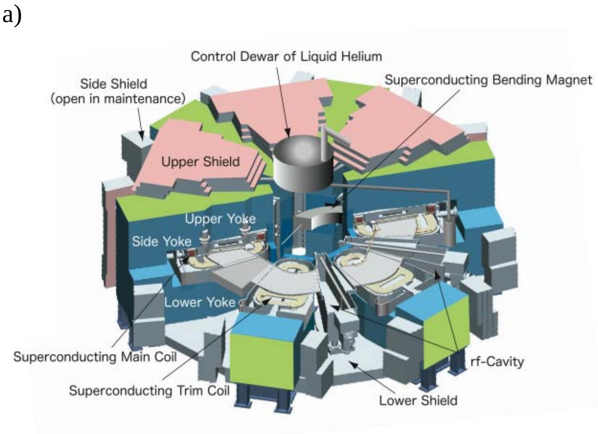
NEXT GENERATION RADIOACTIVE BEAM FACILITIES BASED ON HEAVY-ION DRIVERS

RIKEN/RI Beam Factory in Japan (superconducting cyclotron)

The first of the next-generation exotic beam facilities based on a powerful heavy ion driver accelerator is the one at RIKEN in Japan, the Radioactive Ion Beam Factory (RIBF). This facility is based on a series of isochronous cyclotrons with the final one being the world's largest cyclotron, a K2500, 8000 ton superconducting ring cyclotron (see Fig. 1). This facility is currently in its commissioning stage and an overview and status report was given recently [3].

When fully commissioned, CW heavy ion beams up to uranium with one particle microamp (6E12 ions/s) at 350 MeV/u and lighter ions at the same current or more with energies up to 400 MeV/u will be available for the production of intense secondary beams of rare isotopes. The research program at this new facility is to begin in 2007 and will be based initially on the large fragment separator BigRIPS and a zero degree spectrometer.

The high beam power of this new facility, up to 80 kW, brings with it the need for detailed analysis of thermal and radiological issues. There are challenges associated with heating of cryogenic components especially in the superconducting cyclotron and the superconducting magnets of the fragment separator, high power densities and associated potential for both thermal and radiation damage at the beam dumps, thermal stresses especially in a)



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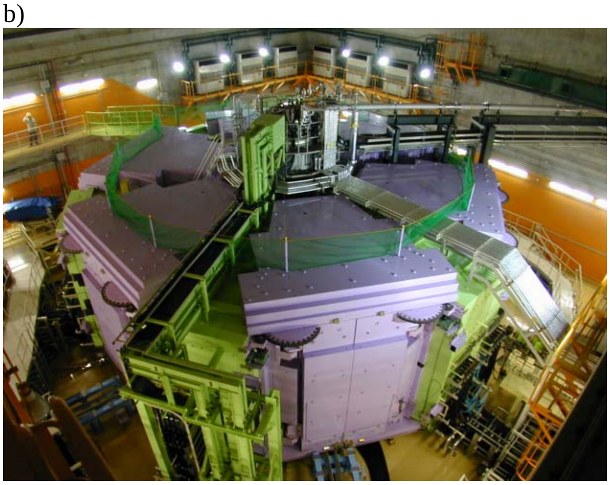

Figure 1. CAD model (a) and photograph (b) of the K2500 superconducting cyclotron at the RIKEN Radioactive Beam Factory which is currently being commissioned.

the production targets and stripper foils, and in detailed simulations and associated tuning of the fragment separator for optimal rare isotope production and secondary beam purification.

GSI/FAIR in Germany (superconducting synchrotron)

The Facility for Anti-proton and Ion Research (FAIR) is planned as a major upgrade of the GSI laboratory in Germany. This facility has several important research thrusts including a program using intense secondary beams of rare isotopes produced via fragmentation and in-flight fission of heavy ions. An overview of the proposed expansion of the existing GSI facility is shown in Fig. 2 and the facility was also described recently [4].

The main accelerators of FAIR are the two large superconducting synchrotrons, the SIS100 and SIS300 rings as shown in Fig. 2. It is proposed to operate FAIR with several simultaneous users by intermingling cycles of the synchrotrons and storage rings. For exotic isotope production via in-flight fission uranium beams up to 1500 MeV/u and ~3E11 ions/s will be available, and they can

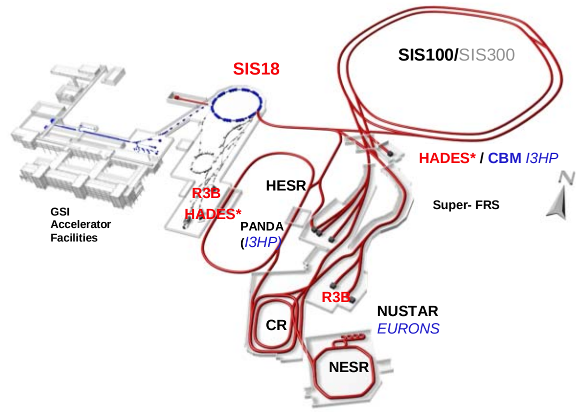

Figure 2. Overview of the proposed layout of the accelerators and experimental instruments at the GSI FAIR facility.

be delivered to the production target of the large superconducting fragment separator, the Super FRS, also indicated in Fig. 2. Both slow extraction with high duty cycle and fast extracted beams, in pulses ~50 nsec long, will be available. The fast extracted primary beams are used to produce short pulses of secondary beams to enable storage of rare isotopes for research in the New Experimental Storage Ring, NESR.

The FAIR project involves a large number of participants from many countries around the world. The construction schedule is coordinated so that research capabilities will come on line in phases, with phase 1 research beginning as early as 2011 with beams delivered to the new Super-FRS and NESR directly from the upgraded SIS18 prior to the completion of the new synchrotron rings.

Large-scale simulations of many aspects of the accelerators and instrumentation are necessary for this complex facility both in the design and construction stages as well as for efficient operation in the future multi-user mode.

RIA-lite in the U.S. (superconducting linac)

Concept development and R&D to support the proposal for RIA, a high-power next-generation radioactive beam facility for the U.S. has been on-going for more than 10 years. An overview of the RIA proposal was presented in [5]. However, with an estimated total project cost of about $1.1B, it has recently been decided to investigate the capabilities of an approximately half-scale version of this facility, sometimes called RIA-lite.

The concept developed for RIA, and retained as much as possible for RIA-lite, comprises a powerful combination of new technologies that enable great advancements in this field of nuclear physics. Some of the factors contributing to the enhanced capabilities are:

- Use of a variety of production techniques for short-lived isotopes including new approaches that remove the main previous limitations of standard ISOL techniques.
- A powerful superconducting driver linac capable of accelerating any stable ion from protons to uranium and designed to allow simultaneous acceleration of multiple charge states of a given ion to attain unprecedented power for the heaviest ions.
- A very efficient post-acceleration scheme based on a superconducting linac injected by low frequency RFQs capable of accelerating singly charged radioactive ions of mass up to 240 amu from ion source energy.
- First rate experimental equipment and multiple user capability to maximize use of the facility.

The charge from the U.S. funding agencies to the Nuclear Science Advisory Committee involves consideration of "a modified RIA that focuses on capabilities which would make it unique in the world and would complement the rare isotope capabilities elsewhere." The present plan is for completion of this study in early 2007 so that the recommendations can be provided as input to the upcoming long-range plan for nuclear physics in the United States which is due to be completed by the end of 2007. Concepts for the reduced-scale facility are being developed by both Argonne [6] and Michigan State University [7].

To achieve the cost savings while retaining as much as possible of the original goals of RIA, as listed above, the proposed superconducting driver linac beam energy is reduced by a factor of two, but the output beam power is retained at 400 kW. The factor of two increased beam current required for beams up to uranium is expected to be feasible due to recent advances in ECR ion source technology [8]. Sample beams and their intensities and energies available from the driver linac proposed for RIA-lite at Argonne (called the Advanced Exotic Beam Laboratory, AEBL) are shown in Table I. Other cost savings come from concentrating on a subset of the experimental capabilities of the original RIA proposal, with an emphasis on those that complement the capabilities of advanced ISOL and fragmentation facilities elsewhere in the world. At Argonne the emphasis is on secondary beams produced by heavy ion fragmentation or in-flight fission combined with helium gas catcher technology [9, 10] followed by post-acceleration of the rare isotopes in the existing ATLAS superconducting linac. A preliminary layout of AEBL at Argonne is shown in Fig. 3.

There are many computational challenges associated with the various simulations required to achieve an optimal, robust design for the RIA-lite facility. This facility involves, for example, multiple-charge-state heavy ion acceleration with stringent limits on beam halos and losses from high power beams [11], thermal problems due to high power densities in targets and beam dumps, and

Table I. Beam list for selected ions from the AEBL Driver Linac. The output currents indicated correspond to 400-kW beam power.

A	q_{source}	I_{source}	q_{out}	I_{out}	Energy
		pμA		pμA	MeV/u
1	1	880	1	692	578
3	2	390	2	312	427
2	1	728	1	582	344
18	6	101	8	73	305
40	8	47	18	34	297
86	14	24	35	18	266
136	18	17	50-52	12	237
238	33+34	6+6	77-81	8	200

radiological issues associated with component activation and radiation damage. Currently, many of the simulations that are necessary for design optimization are done by different codes, and even separate physics groups, so that the process proceeds iteratively for the different aspects. There is a strong need, for example, to couple the beam dynamics simulation codes with the radiological and shielding codes so that an integrated picture of their interactions emerges seamlessly and trouble spots in the design are identified easily. This integration is especially important in magnetic devices such as heavy ion fragment separators that are subject to radiation and thermal damage.

At the commissioning and operational stage of this facility there is also a strong need for large scale simulations as an aid to operators for efficient and robust tuning of the accelerator and beam delivery systems. This is discussed in section 5 below.

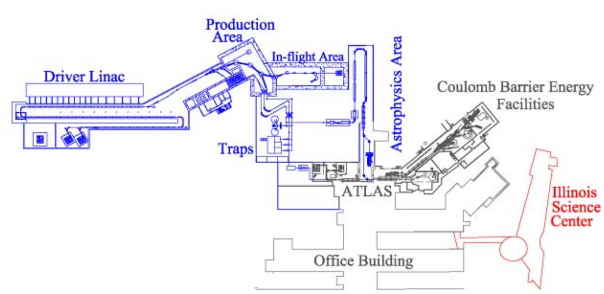

Figure 3: Preliminary simplified schematic layout of AEBL at Argonne.

PETA-FLOP COMPUTING POWER IN THE NEAR FUTURE

There are currently many super-computer projects running and many more in the planning stage. Currently there are several systems on the TOP500 list [12] with ratings of ~100 TF/s, with the #1 being the BlueGene/L 65,536 dual-processor compute-node cluster at LLNL at an achieved performance of 280 TF/s. Smaller clusters with ratings of a few TB/s are generally available for the development of large-scale simulations for accelerator facilities such as the ones discussed in this paper. For example, at Argonne there is currently a single-rack BlueGene/L cluster (1024 nodes/2048 processors) with a peak performance of 5.6 TF/s. Figure 4 is a schematic indicating the components of BlueGene/L clusters. There are plans for significant expansion of the Argonne computing power in the near future [13], with plans to evolve towards petaflop/s computing speeds in a few years. In the U.S. there are several projects for the development of general tools for large-scale accelerator simulations being done under the DOE SciDAC program. This program was summarized at this conference by Spentzouris [14].

With the continued rapid growth in both computing hardware and powerful simulation systems, it seems wise to envision the use of peta-scale computers for future accelerator facility design, commissioning, and operation.

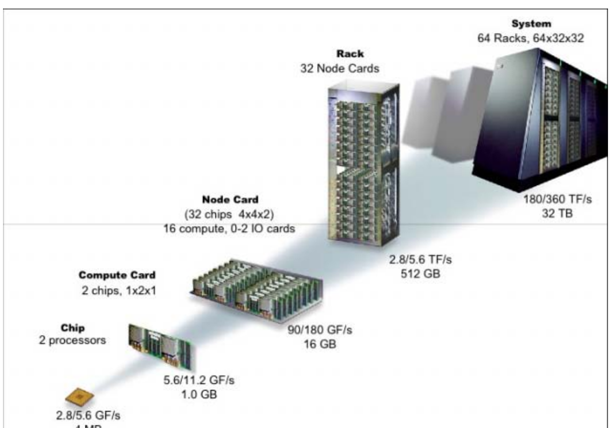

Figure 4. Schematic showing the components of an IBM BlueGene/L computer cluster. Available systems range from single racks (2048 processors) with peak performance of 5.6 TB/s to the “#1” 64-rack cluster at LLNL with an achieved speed of 280 TB/s.

LARGE-SCALE SIMULATION NEEDS FOR DESIGN OPTIMIZATION

The large-scale parallel processing computing power at the design stage of next-generation radioactive beam facilities can greatly decrease the time required and also lead to much better optimization, in turn leading to more robust and cost-effective solutions to technological problems.

Examples of the current categories of simulations that are required during the design optimization process are:

- Complex magnet and RF cavity design
- Detailed 3D electromagnetic models are essential to adequate beam dynamics simulations
- Detailed beam halo and loss sensitivity to alignment and parameter uncertainties are required
- Space-charge tracking, possibly implemented via 3D Vlasov solver – discussed at this conference [15]
- Detailed determination of the necessary diagnostics information to ensure adequate instrumentation
- Shielding and activation models integrated with the beam halo and loss simulations
- Fragment separator resolving power optimization coupled to radiological heating, activation, and damage minimization
- Use of rigorous global optimization – discussed at this conference [16]

An example of a useful interface between large aperture 3D magnet modeling and beam dynamics codes is the work presented at this conference by Manikonda, Berz, and Makino [17].

Future improvements in the design process will come from integration of what is currently done by independent simulations into a more coherent package. A prime example is to integrate the 3D design process for magnets, resonators, and other facility components with the beam dynamics and radiological simulations. Seamless interfaces between the codes are required.

As an example of a possible future improvement in the design optimization, consider the iterative process of the 3D design of a superconducting resonator such as is illustrated in Fig. 5 [18, 19]. Currently this is done via iterations of approximate geometries of the resonator with a 3D electromagnetic code with the goal of optimizing the accelerating voltage of the cavity while minimizing the peak surface electric and magnetic fields. Following this process the resulting 3D electromagnetic fields are processed and used as input to the beam dynamics simulations. In some cases, such as in multi-gap resonators at low velocities or in resonators that have significant 3D steering effects, there are further optimizations to be done based on the results of the beam dynamics. Better integration of this process would speed up the optimization, possibly leading to a higher degree of optimization, and ultimately producing a more cost-effective and/or a more robust design.

Similarly, it would be good to couple an advanced beam dynamics code, such as COSY Infinity or TRACK, to the radiological codes such as MCNPX. Presently beam losses are simulated with high-order beam tracking codes and then the results are taken manually to a radiological transport code to determine shielding and radiological heating and damage effects. Lower order electromagnetic transport models that are currently incorporated in some radiological codes, such as PHITS, do not have the

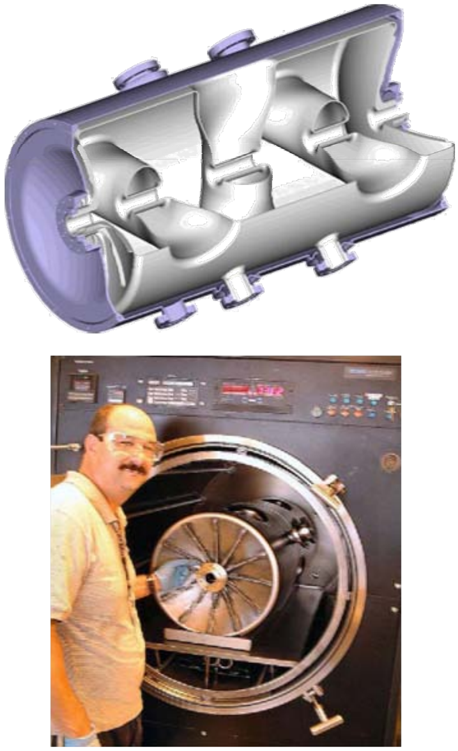

Figure 5. A 3D CAD model and a photograph of a superconducting triple-spoke resonator developed for the RIA driver linac.

accuracy required for complex systems with low beam loss. Improved coupling of the models would lead to better optimization and more cost-effective shielding design. Similar gains are envisioned for improved modeling of the beam dynamics coupled to radiological transport in large aperture fragment separators at high power radioactive beam facilities where superconducting magnets are used in the vicinity of high power beam dumps.

Another example of the need for large scale simulations and close coupling of two design steps is at the front end of high intensity linacs where space charge effects are important in halo generation especially for pulsed beams with low duty cycle. A large-scale parallel computer-based simulation was done with the TRACK code [20] for a pulsed beam in an RFQ at the injector of the FNAL proton driver [21]. The RFQ simulations were done on the ANL BlueGene/L cluster with 1000 processors, and included 100 million particles which is the total number in an RF bunch for this accelerator. Figure 6 shows a 3D view of the bunch of particles at the exit of the RFQ.

LARGE-SCALE COMPUTATIONS APPLIED TO OPERATION: A MODEL-DRIVEN ACCELERATOR

For accelerator facilities that are being designed today and expected to come on line about 10 years from now, it is reasonable to assume that peta-scale computing power will be available in the control room. On-line peta-scale

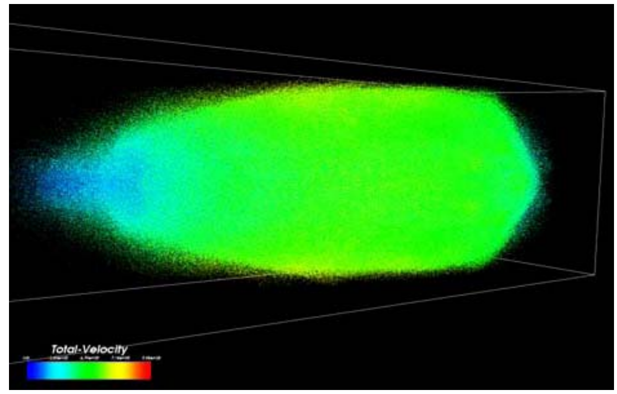

Figure 6. A 3D display of 100 million particles corresponding to the actual number of particles in the 40 mA peak current RF bunch of the FNAL 8-GeV proton driver. [21]

computing could be used for near real-time tune optimization based on diagnostics feedback and detailed facility model.

Such capability would greatly improve operational efficiency and reliability, thereby increasing the cost-effectiveness and the scientific output of the facility.

There are many challenges here, such as determining the requirements and providing an adequate set of diagnostics information, the time response and accuracy of the diagnostics information, the validation of the hardware calibrations with the model parameters, and the integration of the model simulations with the diagnostics information and the control system.

Such capability should be envisioned for the new facility already at the design stage. P.N. Ostroumov has proposed developing this concept of a "model-driven accelerator" for the RIA-lite project. He has pointed out that the concept should be on line and running at the commissioning stage to validate the simulations and ensure proper calibration of the diagnostics devices.

SUMMARY & FUTURE DEVELOPMENTS

Tera-flop-scale simulations of many aspects of accelerator facilities are already currently fairly routine and being used in present day design of advanced accelerator facilities. Further integration of codes to enhance the optimization processes will continue with consideration of scalability to peta-flops/s in the coming years. Full integration of detailed accelerator models, feedback from diagnostics devices, and control systems has the potential to greatly improve operational efficiency and reliability of future facilities.

REFERENCES

[1] Opportunities in Nuclear Science, A Long-Range Plan for the Next Decade, Ed. J. Symons, et al., April 2002. http://www.er.doe.gov/np/nsac/nsac.html

[2] P.N. Ostroumov, J.A. Nolen, and B. Mustapha, “Computational needs for the RIA accelerator systems,” Nucl. Instr. and Meth. in Physics Research **A558** (2006) 25–31.

[3] Y. Yano, “The RIKEN RI Beam Factory Project: A Status Report,” 19th Int. Conf. on the Appl. of Accel. in Res. and Ind., Ft. Worth, TX, August, 2006, to be published in Nucl. Inst. and Meth. B.

[4] I. Augustin, “Status of the FAIR Project,” ibid.

[5] J.A. Nolen, “Overview of the U.S. Rare Isotope Accelerator Proposal,” Nucl. Phys. A734 (2004) 661-668.

[6] J.A. Nolen, “Plans for an Advanced Exotic Beam facility in the U.S.,” IX International Conference on Nucleus-Nucleus Collisions, Rio, Brazil , August 28-September 1, 2006, to be published.

[7] B.M. Sherrill, “RIA: Study of nuclei far from stability,” INTERNATIONAL SCHOOL OF NUCLEAR PHYSICS, 28th COURSE, Radioactive Beams, Nuclear Dynamics and Astrophysics, ERICE-SICILY: 16 - 24 SEPTEMBER 2006, http://www.uni-tuebingen.de/erice/2006/sec/final_program.html

[8] D. Leitner, C. M. Lyneis, T. Loew, D. S. Todd, and S. Virostek, “Status report of the 28 GHz superconducting electron cyclotron resonance ion source VENUS,” Rev. Sci. Instrum. **77** (2006) 03A302, 1-6.

[9] G. Savard, *et al.*, "Development and Operation of Gas Catchers to Thermalize Fusion-evaporation and Fragmentation Products," Nucl. Instr. Meth. in Phys. Res. **B204** (2003) 582-586.

[10] G. Savard, “Ion manipulation with cooled and bunched beams,” Eur. Phys. J. A 25, supplement 1 (2005) 713-718.

[11] P. N. Ostroumov, V. N. Aseev, and B. Mustapha, “Beam loss studies in high-intensity heavy-ion linacs,” Phys. Rev. ST/AB **7**, (2004) 090101.

[12] Top 500 computer sites: http://www.top500.org/lists/2006/11

[13] Argonne Leadership Computing Facility, http://www.alcf.anl.gov/

[14] P. Spentzouris, “Accelerator Modelling under SciDAC: Meeting the Challenges of Next-Generation Accelerator Design, Analysis, and Optimization,” 9th International Computational Accelerator Physics Conference, Chamonix, France, October, 2006.

[15] M. Berz, K. Makino, “A Differential Algebraic High-Order 3-D Vlasov Solver,” ibid.

[16] K. Makino and M. Berz, “Rigorous Global Optimization for Parameter Estimates and Long-Term Stability Bounds,” ibid.

[17] S. L. Manikonda, M. Berz, K. Makino, “A Highly Accurate 3-D Magnetic Field Solver,” ibid.

[18] K.W. Shepard and M. Kelly, PAC2005, Knoxville, TN, TPPT099, TPPT100, May 16-20, 2005.

[19] M. Kelly, “Superconducting Spoke Cavities,” 39th ICFA Advanced Beam Dynamics Workshop on High Intensity Brightness Hadron Beams (HB2006), Tsukuba, Japan, May 29 - June 2, 2006.

[20] V.N. Aseev, P.N. Ostroumov, E.S. Lessner and B. Mustapha, “TRACK: THE NEW BEAM DYNAMICS CODE,” Proc. of the 2005 Part. Accel. Conf., Knoxville, Tennessee, p 2503-2505. http://accelconf.web.cern.ch/AccelConf/p05/PAPERS/TPAT028.PDF

[21] J. Xu, B. Mustapha, V.N. Aseev, P.N. Ostroumov, “Parallelization of a beam dynamics code and first large scale radio frequency quadrupole simulations,” Phys. Rev. ST/AB, to be published (2006).