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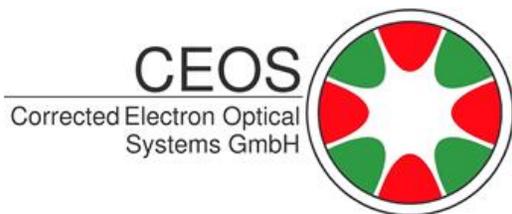
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# CPO-10 ABSTRACTS

## A HIGH BRIGHTNESS FIELD EMITTER BY USE OF NOBLE METAL COATED NANO SCALE PYRAMID FORMED ON TUNGSTEN TIP

Hiroataka Asai, Ryota Kawai, Fumiya Matsubara,  
Hidekazu Murata, and Eiji Rokuta

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**Keywords:** Nano tip; field ion microscopy; field emission microscopy

Nano tips have attracted large attention as the novel electron source with high brightness in high performance electron microscopes. In field emission electron guns, the brightness is improved as the width of electron source is decreased. This is because the electric field converges to the single atom at the tip end, resulting in a dramatic collimated electron beams. Tungsten (W) nanopyramids coated with monolayer films of noble metal (NM) are potential for a material of highly coherent electron sources. Sides of a tungsten (W) needle was coated with collodion containing powder of palladium oxide (PdO) at first. The W needle was subsequently annealed under ultrahigh vacuum to supply palladium (Pd) atoms to an apex of the W needle via surface diffusion and to produce a W nanotip coated with monolayer Pd films. Field ion microscopy (FIM) revealed {111} planes of the W nanotip were contracted by faceting 211 planes surrounding the 111 plane, of which the structural change is analogous to a formation of three sided W nanopyramids. General appearances of the W nanopyramids were the same as those shown by the existing naopyramids. The opening angle corresponding to FWHM of the beam profile of a nanopyramid with a top consisting of fifteen atoms was about 9.4 degree at extractor voltage of 711 V and emission current of 0.6 nA. In order to evaluate the brightness of the single atom tip, we adopted a regular triangle with a side of 0.18 nm was regarded as emission region and source area estimated  $1.4E-14 \text{ cm}^2$ . We evaluated the brightness of  $2.0E4 \text{ A str}^{-1} \text{ cm}^{-2} \text{ V}^{-1}$ . The evaluated value is higher than that of the conventional FE source ( $5.0E3 \text{ A str}^{-1} \text{ cm}^{-2} \text{ V}^{-1}$ ).

## THE ION-OPTICAL DESIGN OF THE HIGH RIGIDITY SPECTROMETER HRS FOR FRIB

G.P.A.Berg

University of Notre dame

### Invited Talk

**Keywords:** Spectrometer, Ion-optical design, Rare Isotopes

With the ongoing construction of the Facility for Rare-Isotope Beams FRIB for the production of high-intensity rare isotopes (RI), several electro-magnetic experimental analysis systems are under construction and design to exploit these beams for a wide experimental science program. A large part of the science program can be executed using the HRS as outlined in the White Paper "HRS A High Rigidity Spectrometer for FRIB" (December

2014, ed. A. Gade and R. Zegers). The HRS will enable gains in luminosity for experiments with rare-isotope beams at FRIB by factors of 2-100, with the highest gains for the most neutron-rich isotopes, including those in the path of the astrophysical r-process. Therefore, the HRS will add tremendously to the discovery potential of FRIB. In this presentation the ion-optical design of a beam line/spectrometer system will be presented that satisfies all essential design requirements. This includes two modes of operation for missing mass experiments with MoNA-LISA and high-resolution spectroscopy. Both modes can operate with the Gamma Ray detector GRETA at the target and allow full dispersion matching of beam line and spectrometer for high resolution without dramatically reducing the beam intensity using momentum slits. The matching conditions also allow the reconstruction of the properties of the reaction products using the detector system. This work is supported by the U.S. Department of Energy Office of Science under Grant DE-SC0014554, ION-OPTICAL AND ASSOCIATED MAGNET FEASIBILITY STUDY OF A HIGH RIGIDITY SPECTROMETER.

## LENS-MIRROR OBJECTIVE FOR TRANSMISSION ELECTRON MICROSCOPE

S.B. Bimurzaev, N.U. Aldiyarov, E.M. Yakushev

Almaty University of Power Engineering and  
Telecommunication

**Keywords:** lens-mirror objective, transmission electron microscope, spherical aberration, axial chromatic aberration

A new electron-optical scheme of the lens-mirror objective for transmission electron microscopes (TEM), based on the special focusing regime (the so-called superimposed image mode) in the center of curvature of the deflecting magnetic field [1-3], is considered. The magnetic field does not cause an additional distortion of the image, and the problem of calculating the objective is reduced to calculating a relatively simple lens-mirror system with a common rotational symmetry axis. The new data on the parameters of specific lens-mirror systems composed of a well-known magnetic lens with a bell-shaped distribution of the axial field and an electrostatic mirror with electrodes in the form of a set of coaxial cylinders of equal diameter have been obtained. A rather wide family of mirror-lens electron-optical systems with a simultaneous compensation of the main types of aberrations (spherical and axial chromatic) with a large linear magnification has been found. The diffraction limit of the linear resolution of the lens-mirror objective has been evaluated under the joint action of the remaining fifth-order spherical aberrations and the diffraction of electrons by the beam-limiting diaphragm. It has been shown that full elimination of the third-order spherical aberrations can significantly increase the resolution of the transmission electron microscopes (TEM) and, even at moderate accelerating voltages about 100 kV, give high resolution values of less than one Angstrom, inaccessible for modern high-voltage TEM / STEM devices. 1. Bimurzaev S.B. and Yaku-

shev E.M. (2013) Electron lens aberration corrector. // WIPO Patent Application WO/2013/077715 A1. 2. Yakushev E.M. "Theory and Computation of Electron Mirrors: The Central Particle Method." In Advances in Imaging and Electron Physics, Ed: Hawkes P.W. Elsevier. 2013. V.178, P.147-247. 3. Bimurzaev S.B. Aldiyarov N.U. and Yakushev E.M. The objective lens of the electron microscope with correction of spherical and axial chromatic aberrations//Microscopy.-2017. – Vol. 66, Issue 5.- P. 356–365.

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## PLANAR MULTIREFLECTIVE TIME-OF-FLIGHT MASS SPECTROMETER OF A SIMPLE DESIGN

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**Keywords:** mass spectrometer, time-of-flight focusing, time-of-flight dispersion, electrostatic mirror

A scheme of an improved version of a planar multi-reflective time-of-flight mass spectrometer [1], based on the use of two-dimensional electrostatic mirrors and an ion source with an ion accelerator forming an inhomogeneous electrostatic field [2], which provide special focusing modes for ionic fluxes, is proposed. Numerical calculations have been used to determine the conditions that allow, along with the formation of a parallel ion flux, the time-of-flight focusing of ions in energy up to fourth order in the four-electrode ion accelerator in which the first electrode has a planar shape and can be combined with the exit window of the ionization region. The data that determine the conditions of time-of-flight focusing of ions in energy up to the third order inclusive in a three-electrode two-dimensional electrostatic mirror in the regime of a plane mirror have been obtained [3]. Mirror electrodes are pairs of parallel plates symmetrically located relative to the symmetry plane of the mirror field. Two variants of plane mirrors are considered: 1) when the forward and reverse branches of the trajectory coincide; 2) when the forward and reverse branches of the trajectory are symmetric with respect to the plane of symmetry. It is shown that the time-of-flight dispersion of the mirror by mass in the second variant is several times higher than in the first variant. The use of an ion source forming a parallel ion flux in combination with highly dispersive mirrors serves as the basis for simultaneous enhancement of resolution and sensitivity of the mass spectrometer. References 1. Nazarenko L.M., Sekunova L.M. and Yakushev E.M. SU Patent 1725289 A1 (1992). 2. Bimurzaev S.B., Yakushev E.M., Nazarenko L.M. Innovative package of the RK. Author's certificate No. 87127 (2015). 3. Kelman V.M., Fedulina L.V., Yakushev E.M. Deviation of parallel beams of charged parts by a plane electrostatic mirror // Zhurnal Tekhnicheskoi Fiziki, 41 (1971). P. 1825-1831.

## LONGITUDINAL BEAM DYNAMICS STUDIES AT THE PIP-II INJECTOR TEST FACILITY

**J.-P. Carneiro, B. Hanna, L. Prost, A. Saini, A. Shemyakin, D. Sun**

Fermi National Accelerator Laboratory

**Keywords:** Fast Faraday Cup, Bunch Length, Longitudinal Emittance

The Proton Improvement Plan, Stage Two (PIP-II) is a program of upgrades proposed for the Fermilab injection complex, which central part is an 800-MeV, 2-mA CW-compatible SRF linac. A prototype of the PIP-II linac front end called PIP-II Injector Test (PIP2IT) is being built at Fermilab. As of now, a 15-mA DC, 30-keV H<sup>-</sup> ion source, a 2 m-long Low Energy Beam Transport (LEBT), a 2.1-MeV CW RFQ, followed by a 10-m Medium Energy Beam Transport (MEBT) have been assembled and tested. A Fast Faraday Cup (FFC) installed in the MEBT measures the length of a beamlet cut out of the bunch by a small-size entrance hole of the FFC. The information about the bunch length measured at various settings allows for reconstruction of the longitudinal beam dynamics and optimization of injection into the first cryomodule. These measurements are compared with simulations by the beam dynamics codes TRACEWIN and TRACK. The paper describes the experimental procedures of the bunch length measurements with the FFC, presents the measurement results, and compares them with simulations. One of important experimental observations, confirmed by simulations, is the dependence of the FFC beamlet length on the radial position across the beam.

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## THE ORDER 4 ALGORITHM FOR CYLINDRICALLY SYMMETRIC ELECTROSTATICS

**David Edwards Jr**

IJL research center

**Keywords:** Finite Difference Method, FDM, order 4 algorithm, nine point algorithm

It has been ~60 years since Emile Durand first reported the fourth order algorithm for cylindrically symmetric electrostatics (1957). It was immediately clear that using this algorithm the potential could be calculated with precisions significantly higher than the standard 5 point or order 2 algorithm. The solution came at a price however and the price was that it was essentially impossible to implement for boundaries not lying on rows and columns of meshpoints. And this situation is basically the same today as it was 60 years ago in spite of the many attempts at incorporating this algorithm into electrostatics. However in 2014 a solution for the curved boundary problem was found for FDM. Unfortunately as the emphasis in that work was on the higher order algorithms and these were entirely too complex to be detailed no explicit formulations could be given. This significantly limited the usefulness of that work. It has become clear however that the fourth order algorithm, which when implemented by the process for curved boundaries as described in the 2014 report would provide significant gains in precision over the order 2 algorithm

and likely compete favorably with the current BEM and FEM formulations. It is thus to provide such a description of that implementation that the present work is directed. In particular it will allow all points within the geometry, independent of their proximity to the boundary, to use the same 4th order algorithm, the one of Durand. Also the construction employed will in fact be more direct than that used in the standard order 2 implementation for curved boundaries at a cost of only a relatively insignificant increase in computational time. In addition the treatment of boundary singularities by a multi-region construction will be described as such singularities can negate any gains that the order 4 algorithm might yield.

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**ADVANCED BEAM OPTIC OPTIONS FOR  
BROOKHAVEN NATIONAL LABORATORY  
ACCELERATOR TEST FACILITY BEAMLINE**

**Mikhail Fedurin**

Brookhaven National Laboratory Accelerator Test Facility

**Keywords:** masked beam, ultrashort bunch, micro-bunching

The Accelerator Test Facility (ATF) at Brookhaven National Laboratory operates as a National User Facility supported by the Accelerator Stewardship Program in the US DOE's Office of High Energy Physics. The facility presently provides high brightness 70 MeV electron beams and terawatt-class CO2 laser capabilities to support wide program in advanced accelerator R&D. Present design of ATF beamline transport with beam manipulation tools and beam diagnostics together with proposed schemes to generate ultrashort and flat electron bunches will be discussed.

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**GENERALIZATION OF PARAXIAL TRAJECTORY  
METHOD FOR THE ANALYSIS OF  
NON-PARAXIAL RAYS: ELECTRON GUN  
DESIGNS IN TERMS OF OPTICAL PARAMETERS**

**Shin Fujita**

Shimadzu Asia Pacific Pte Ltd.

*Invited Talk*

**Keywords:** ray tracing, numerical calculation, cathode lens

The paraxial trajectory method has been generalized for application to the cathode rays inside electron guns. The generalized method can handle rays that initially make a large angle with the optical axis. The key to success of the generalization is the adoption of the trigonometric function sine for the trajectory slope specification, instead of the conventional use of the tangent. An improved assignment of paraxial trajectory to the actual ray becomes possible by the new slope specification. It is possible to relate the ray emittance condition (the combination of position and slope of rays at reference planes) on the cathode to those at the crossover plane using polynomial functions, whose coefficients can be used as the optical parameters in electron source characterization. The most important among the parameters is the Electron Gun Focal Length, which can be used for quantitative estimate of both the crossover size and the angular current

intensity. Electron gun simulation program G-optk has been developed based on the generalized paraxial trajectory theory. The program calculates the principal paraxial trajectories, optical parameters, as well as virtual emittances solely from the axial potentials and fields. It gives a clear physical picture of electron sources and can be used for the gun design optimization.

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**ELUCIDATION OF ION MOTION IN  
QUADRUPOLE MASS FILTER BY BLOCH  
FUNCTION: IMPROVED PRE-ROD DESIGN FOR  
EFFICIENT ION INJECTION**

**Shin Fujita**

Shimadzu Asia Pacific Pte Ltd.

**Keywords:** phase space, periodic potential, Mathieu-Hill equation, eigen-trajectory

In the optimization of the quadrupole mass filter (QP filter), the understanding of ion motion in terms of the phase space (the combined representation of the trajectory coordinate and momentum) is useful. The phase space representation can give an 'ensemble' behavior of ions inside the filter. Even though each ion trajectory does not have the RF periodicity of the applied voltages to electrodes, the phase space evolution does. It is only when appropriate ensemble ions are considered together that a proper QP filter characterization is possible. We here report a new calculation framework for the phase space of the QP filter. The Mathieu-Hill equation is first solved for 'complex number' eigen-trajectory that has pseudo RF periodicity (Bloch Function). It is then shown that the acceptance phase space can be derived from Bloch Function without a need to calculate each ion trajectory. The ensemble behavior of ions can be estimated from one Bloch Function. The application of the Bloch Function method to the pre-rod effects revealed that the ion injection efficiency may significantly be improved by an appropriate choice of pre-rod ( $q$ ,  $a$ ) condition. Proper addition of DC voltage component will result in the phase space transformation in the pre-rod that enables the efficient ion injection.

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**CS AND RB ION COLDBEAMS SUITABILITY FOR  
CIRCUIT EDIT**

**Yuval Greenzweig, Roy M. Hallstein, Minh P. Ly, Yariv Drezner, Rick H. Livengood, Shida Tan, and Amir Raveh**

Intel Corporation

**Keywords:** Circuit Edit, Focused Ion Beam (FIB), Coldbeam, Cold FIB, Magneto-Optical Trap Ion Source (MOTIS), Low Temperature Ion Source (LoTIS)

Semi-conductor applications of Focused Ion Beams (FIB) have long been enabled by Ga Liquid Metal Ion Source technology, but have been challenged by device density doubling every two years for the last 2-3 decades. One such application, Circuit Edit, has been critically losing performance due to density scaling in

the recent past. The emergence of several new FIB source technologies such as gas field ionization and Coldbeam sources having much smaller probe sizes than Ga LMIS, and in some cases higher secondary electron (SE) yields, promise a revival of FIB capability for Circuit Edit. We report herein the results of our testing of Cs and Rb cold ion beams and their suitability for Circuit Edit. Testing of the Cs coldbeam was performed at ZeroK Nanotech, and Rb testing was performed at TU Eindhoven. We characterized Cs image resolution, beam profile, minimum sizes of micro-trenches etched in SiO<sub>2</sub>, and material properties of Cs deposited dielectric and metalization. For both Cs and Rb we measured residual ion contamination levels and SE yields from several common micro-electronic materials. We established the lack of invasiveness of Cs and Rb for Circuit Edit related operations on 14nm Intel transistors. Lastly, using the Cs coldbeam with gas chemistries for etching and deposition, we demonstrated the first ever Cs based real Circuit Edits, which we performed on Intel 10nm chips.

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## ORBITRAP MASS SPECTROMETRY AND NONLINEAR SPACE CHARGE DYNAMICS

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Makarov

Thermo Fisher Scientific, Bremen, Germany

### *Invited Talk*

**Keywords:** mass-spectrometry, space charge

The Orbitrap (TM) mass analyzer belongs to the family of Fourier transform mass spectrometers (FT MS) in which the ions are trapped between two spindle-like electrodes. The quadrupole-logarithmic field [1,2] provides the quadratic effective potential in the axial direction, in which the oscillatory frequency is independent of the orbital parameters (e.g. the amplitude) so that ions with same mass-to-charge ratios ( $m/z$ ) preserve their common phase in the course of  $1e5 \div 1e6$  oscillations. On the other hand, ions with different  $m/z$  ratios oscillate with different frequencies, and Fourier analysis of the induced-current signal produces a mass spectrum with a resolving power of up to one million [3]. If the number of injected charges is large, however, the ion motion is affected by Coulomb forces. Though the space-charge field constitutes only  $\sim 1e-4$  of the trapping field, the interaction between ions with equal or close  $m/z$  is amplified under the resonance conditions and results in sophisticated, sometimes counterintuitive, ion dynamics. For example, the Coulomb interaction between same charge ions, being repulsive by its nature, generates an effective attraction force. Detected FT peaks of ions with different but close  $m/z$  appear shifted towards each other in frequency. Ultimately, it leads to complete frequency synchronization, referred as coalescence, when the ions oscillate as a single bunch. Coalescence makes the involved ionic species undistinguishable in the FT spectrum and thus deteriorates the mass resolving capability. Basing on the perturbation theory, we have developed a multi-body model and an algorithm characterizing ion dynamics in the presence of Coulomb interactions. Systems of multiple ions were simulated near and beyond the coalescence threshold. It was shown that small non-idealities ( $\sim 1e-5$ ) of the trap's field substantially alter the ion dynamics, decreasing or increasing the threshold by a factor of ten. This

observation suggests approaches to improving space charge capacity of the mass analyzers and, therefore, their dynamic range.

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## ELECTRON OPTICS OF A MULTI-BEAM SOURCE (MBS)

Ali Mohammadi-Gheidari, **Xiaoli Guo** and Pieter Kruit

Delft University of Technology, Lorentzweg 1, 2628CJ  
Delft, The Netherlands

**Keywords:** Electron optics, Multi-beam inspection, High throughput, High resolution

In the field of Charged Particle Optics, more than 50 years of research and development have been devoted to improving the resolution of these systems. Present day systems can easily obtain subnanometer resolution in imaging and sub 10nm resolution in patterning. To preserve the high resolution the current in the probe should be low, only tens of pico-Amps to a few nano-Amps. This makes the throughput of these systems too low for applications such as 3D imaging or wafer inspection. Multi-electron beam systems, in which not one but many electron beams are focused onto the sample simultaneously, can enhance the throughput to a great extent. A Multi-Beam Scanning Electron Microscope (MBSEM) that delivers 196 focused beams onto the sample, based on an FEI Nova-Nano 200 SEM electron optical column was designed and built at the CPO group in Delft University of Technology[1]. The multi-beam source (MBS) for this system, presented by Zhang et al.[2], was based on the principle of the "zero-strength" lens, where the deflection and collimation of the off-axis beams take place in a conjugate plane of the source in order to avoid chromatic deflection aberrations, astigmatism and coma. In further theoretical investigations and simulations, however, it was found that even if the net deflection at the aperture array plane is zero, the axial spherical and chromatic aberrations of the field in front of the aperture array plane can lead to unacceptable astigmatism and extra contributions to the field curvature in the image plane of the array. Therefore, in the design of the MBS, it is not the zero deflection at the aperture plane that should be respected but the minimization of its spherical and chromatic aberration coefficients. In general, the aberrations of round electron lenses cannot be made arbitrarily small or negative. However, the unique property of the present lens allows the aberrations to be made close or even equal to zero! A comprehensive and detailed analysis and design of the MBS will be presented here. [1] A. Mohammadi-Gheidari, C.W. Hagen and P. Kruit, JVST B 28(6) 2010. [2] Y. Zhang and P. Kruit, Physics Procedia 1 553, 2008.

## DECELERATION OF HEAVY IONS, HITRAP AND CRYRING@ESR

Frank Herfurth

GSI Helmholtz Centre for heavy ion research

### *Invited Talk*

**Keywords:** deceleration, highly-charged ions, low energy storage ring, penning trap

To perform precision experiments on exotic ions, if highly charged or rare, it is mandatory to provide means to link high-energy production schemes with low energy storage and measurement schemes. Only low energy storage in rings and traps ensures the required extended observation time and well controlled environment. At GSI/FAIR in Darmstadt/Germany, heavy, highly charged stable and rare ions up to bare uranium are produced in large quantities. Medium charged ions at a few 100 MeV/nucleon will be stripped of all electrons when sent through a thin foil or fragmented in nuclear reactions when interacting with enough material in thicker targets. The deceleration down to MeV/nucleon, keV/nucleon and finally sub meV requires several steps involving storage rings and finally a dedicated linear decelerator coupled to ion traps. Two facilities, the linear decelerator facility HITRAP and the low energy storage ring CRYRING@ESR, will be introduced with planned experiments and status of installation.

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## MULTI-ELECTRODE LENS SYSTEM OPTIMIZATION USING GENETIC ALGORITHMS

N. Hesam Mahmoudi Nezhad<sup>1\*</sup>, M. Ghaffarian Niasar<sup>2</sup>, A. Mohammadi-Gheidari<sup>1</sup>, T. Janssen<sup>3</sup>, C.W. Hagen<sup>1</sup>, P. Kruit<sup>1</sup>

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**Keywords:** Electrostatic lens Optimization, Second Order Electrode Method (SOEM), Genetic Algorithms (GAs)

In electron lens design, finding the optimum lens system for the application at hand, is still quite a challenge. The situation becomes especially more complicated when many lens electrodes are involved, because the number of free parameters of the optimization, such as electrode thickness, radii, gaps between electrodes and voltages, increases rapidly. Therefore, fast optimization routines are needed to tackle the problem. In the past, there have been some attempts to develop such optimization programs. Szilagy et al. [1] and Adriaanse et al. [2], have published some results in 1989 on rough optimization of electrostatic lenses. However, using the above-mentioned methods, one could not get

very accurate results. Now that we have more powerful computers and significantly better software, we revisit the problem. First we applied the so called "SOEM" (Second Order Electrode Method) [2] for a fast ( $\sim 0.1$ sec) calculation of the axial potential. However, the results of the optimization were not accurate enough. To improve the accuracy of the SOEM-based optimization, we integrated a finite element based potential calculation method (using COMSOL). This way the potential calculation and the objective function calculation is more accurate, although the optimization becomes much slower. We propose a new approach that improves on the low speed of optimization while keeping the high accuracy results of the finite element method based potential calculation. This is done by first using a rough optimization based on the SOEM approach, resulting in a few approximately optimized systems. Then, using the parameters of the systems found, new sets of systems were defined using a small range of values around these parameters. Then the more accurate, COMSOL-based optimization was applied to this set of limited systems. We have tested our method on multi electrode systems up to 7 electrodes. We succeeded to very accurately optimize these systems within a few hours, with the electrode radii, gaps and voltages as free parameters, and the focus position as a constraint. [1] M.Szilagi, Yakowitz and M. Duff, Appl. Phys. Lett. 44, pp. 7-9, 1984. [2] J.P. Adriaanse, H.W.G Van der Steen and J.E. Barth, J.Vac. Sci. Technol. B7, pp. 651-666, 1989.

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## CORRELATIVE MICROSCOPY BASED ON SECONDARY ION MASS SPECTROMETRY FOR HIGH-RESOLUTION HIGH-SENSITIVITY NANO-ANALYTICS

Hung Quang Hoang, Jean-Nicolas Audinot, Santhana Eswara, Tom Wirtz

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### *Invited Talk*

**Keywords:** Correlative microscopy, secondary ion mass spectrometry, helion ion microscopy, transmission electron microscopy, scanning probe microscopy

Nano-analytical techniques and instruments providing both excellent spatial resolution and high-sensitivity chemical information are of extreme importance in materials science and life sciences for investigations at the nanoscale. New characterisation tools need to anticipate these research trends, but as more and more techniques approach their fundamental limits it is only by combining multiple techniques that disruptive advances may be made. While techniques such as Electron Microscopy, Helium Ion Microscopy and Scanning Probe Microscopy are commonly used for high-resolution imaging, they provide no or only limited analytical information. In particular, both Energy-Dispersive X-Ray Spectroscopy (EDX) and Electron Energy Loss Spectroscopy (EELS) that are routinely used in electron microscopy have limited sensitivity, neither can distinguish isotopes and both have difficulty with light elements. In contrast, Secondary Ion Mass Spectrometry (SIMS) offers extremely high chemical sen-

sitivity, but it typically suffers from poorer lateral resolution. However, by combining SIMS with one of these high resolution microscopy techniques, these intrinsic drawbacks may be overcome [1]. Therefore, in order to get chemical information with a highest sensitivity and highest lateral resolution, we developed integrated instruments combining SIMS with Transmission Electron Microscopy [2], Helium Ion Microscopy [3-5] and Scanning Probe Microscopy [6] and developed associated correlative methodologies and workflows. These workflows allow TEM, SE and SPM images of exactly the same zone analysed with SIMS to be acquired easily and rapidly, followed by a fusion between the SE and SIMS data sets [7]. In this talk, we will present the concepts, describe the instruments and discuss their performance characteristics. We will then present a number of examples taken from various fields of materials science and life science to show the powerful correlative microscopy possibilities enabled by these new in-situ methods. [1] T. Wirtz, P. Philipp, J.-N. Audinot, D. Dowsett, S. Eswara, *Nanotechnology* 26 (2015) 434001 [2] L. Yedra, S. Eswara, D. Dowsett, T. Wirtz, *Sci. Rep.* 6 (2016) 28705 [3] T. Wirtz, D. Dowsett, P. Philipp, *Helium Ion Microscopy*, edited by G. Hlawacek, A. Götzhäuser, Springer, 2017 [4] D. Dowsett, T. Wirtz, *Anal. Chem.* 89 (2017) 8957-8965 [5] P. Gratia et al, *J. Am. Chem. Soc.* 138 (49) 15821-15824, 2016 [6] Y. Fleming et al., *Beilstein J. Nanotechnol.* 6 (2015) 1091 [7] F. Vollnhals, J.-N. Audinot, T. Wirtz, M. Mercier-Bonin, I. Fourquaux, B. Schroepel, U. Kraushaar, V. Lev-Ram, M. H. Ellisman, S. Eswara, *Anal. Chem.* 89 (2017) 10702-10710

## **SPHERICAL ABERRATION CORRECTION WITH IN-LENS N-FOLD SYMMETRIC LINE CURRENTS**

**S. Hoque**<sup>1,2</sup>, R. Nishi<sup>1</sup>, H. Ito<sup>1,3</sup>, A. Takaoka<sup>1</sup>)

1) Osaka University, 2) Hitachi High Technologies America, Inc., 3) Hitachi High-Technologies Corp.

**Keywords:** Spherical aberration, Hexapole corrector, Sextupole corrector, N-SYLC

We have shown that N number of line currents placed symmetrically about the optic axis generate 2N-pole fields [1]. We call this structure N-fold symmetric line currents, or, N-SYLC in short. We have proposed simple aberration corrector models based on N-SYLC for scanning electron microscopes (SEM) [2][3][4]. The most important feature of N-SYLC is that it is free of magnetic material, thus in principle eliminates the problems of hysteresis, non-uniformity, and magnetic saturation suffered by conventional magnetic multipoles. We have shown theoretically that the conventional multipoles of sextupole doublet model of H. Rose [5][6] can be replaced with 3-SYLC to correct spherical aberration [2]. Here, we consider a new structure superimposing N-SYLC on rotationally symmetric lens fields, which is only possible because N-SYLC is free of magnetic materials. This simplifies the corrector structure, and allow for miniaturization and more versatile design. We call this structure in-lens N-SYLC. We show by analytical calculation that by adjusting certain parameters of the system, in-lens 3-SYLC can generate negative spherical aberration with high sensitivity, so that it can be used to correct the spherical aberration of objective lens. We also verify the results by computer simulation [7]. [1] Nishi R.,

Ito H., Hoque S.: Wire corrector for aberration corrected electron optics, (IMC2014), IT-1-P2984, pp.200-201. [2] S. Hoque, H. Ito, R. Nishi, A. Takaoka, E. Munro: Spherical aberration correction with threefold symmetric line currents, *Ultramicroscopy* 161, (2016) 74-82. [3] S. Hoque, H. Ito, A. Takaoka, R. Nishi, Axial geometrical aberration correction up to 5th order with N-SYLC, *Ultramicroscopy* 182, (2017) 68-80. [4] P. W. Hawkes and E. Kasper, *Principle of Electron Optics*, Volume 2: Applied Geometrical Optics, second edition, chapter 41, p. 986-988, Academic Press, 2017. [5] H. Rose, Correction of aperture aberrations in magnetic systems with threefold symmetry, *Nuclear Instruments and Methods in Physics Research* 187, 187-199 (1981). [6] M. Haider, H. Rose, S. Uhlemann, B. Kabius, and K. Urban, Towards 0.1 nm resolution with the first spherically corrected transmission electron microscope, *Journal of Electron Microscopy* 47, 395 (1998). [7] Spherical aberration correction with an in-lens N-fold symmetric line currents model, *Ultramicroscopy* 187, (2018) 135-143.

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## **HIGH-PRECISION MASS MEASUREMENTS WITH MR-TOF-MS**

Timo Dickel, **Christine Hornung**

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### **Invited Talk**

**Keywords:** TOF-MS, RF traps, mass measurements

At the FRS Ion Catcher at GSI, projectile and fission fragments are produced at relativistic energies at the FRS, separated in-flight, range-focused, slowed-down and thermalized in a cryogenic stopping cell and transmitted to a multiple-reflection time-of-flight mass spectrometer (MR-TOF-MS). The MR-TOF-MS can perform direct mass measurements of exotic nuclei, to provide an isobarically and isomerically clean beam for further experiments, and as a versatile diagnostics device to monitor the production, separation and manipulation of exotic nuclei. At the Justus Liebig University, Giessen, Germany similar MR-TOF-MS have been developed for the ISOL facility TRIUMF, Vancouver, Canada and for applications in analytical mass spectrometry. These MR-TOF-MS consist of an injection RF trap to form the ns ion bunches, a coaxial isochronous TOF analyzer, and a TOF detector for mass measurement and a Bradbury-Nielsen-Gate for spatial mass separation. Several novel principles further enhance the performance and versatility of the MR-TOF-MS, including (i) a post-analyzer reflector, (ii) a dynamical time-focus shift technique and (iii) mass-selective re-trapping in the RF trap. Thus extremely versatile MR-TOF-MS with mass resolving powers beyond 600,000 (FWHM), high transmission efficiency, ion capacities of more than a million ions per second and cycle frequencies as high as 1kHz have been developed. The MR-TOF-MS can also be used as their own isobar separator. Mass measurements of uranium projectile and fission fragments produced at the FRS at 1000 MeV/u have been performed using the MR-TOF-MS of the FRS Ion Catcher. More than 30 short-lived ground state masses have been measured with high mass accuracies (down to 6E-8). The excitation energies of isomers and isomeric ratios were determined using mass spectrometry,

and, for the first time, an isomeric beam was prepared using an MR-TOF-MS. The unique combination of performance parameters make the MR-TOF-MS the system of choice for measuring the masses of very exotic nuclei and for the search for new long-lived isomeric states.

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## LATTICE DESIGN OF THE HEPS

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### *Invited Talk*

**Keywords:** High Energy Photon Source, diffraction limited storage ring, linear optics, nonlinear dynamics

The High Energy Photon Source (HEPS) is the first high-energy diffraction-limited storage ring (DLSR) light source to be built in China, with a natural emittance of a few tens of picometers and a circumference of 1360 m. After 10 years' evolution, the accelerator physics design of the HEPS has been determined. The latest HEPS lattice consists of 48 hybrid-7BAs with a few modifications, such as, antibends, superbends, and alternating high- and low-beta sections. These modifications promise a 34 pm design with high brightness. In this report we will introduce the status of the HEPS accelerator physics design and the linear optics and nonlinear dynamics of the latest HEPS lattice.

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## DETECTION SYSTEMS IN SCANNING ELECTRON MICROSCOPE

Jaroslav Jiruse

TESCAN Brno

**Keywords:** SEM, detection system, secondary electrons, backscattered electrons

Controlling surface sensitivity is becoming increasingly important in SEM. We will present results obtained with ultra-high resolution columns developed recently with extended detection systems optimized for low energies. These systems allow angular filtering of secondary electrons and both angular and energy filtering of backscattered electrons. These filtering possibilities lead to enhanced surface sensitivity of the detected signal.

## DESIGN OF A HIGH-PERFORMANCE POST-COLUMN IMAGING ENERGY FILTER FOR (S)TEM INSTRUMENTS

Frank Kahl, Heiko Müller, Martin Linck, Richard Schillinger

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### *Invited Talk*

**Keywords:** post-column energy filter, ESI, EELS, Electron-Spectroscopic-Imaging, Electron-Energy-Loss-Spectroscopy, spectroscopy

CEOS developed a high-performance post-column imaging energy filter for transmission electron microscopy. It can be used for Electron-Spectroscopic-Imaging (ESI) and Electron-Energy-Loss-Spectroscopy (EELS) for beam energies from 30kV to 300kV. It has been designed as a multi-purpose instrument for zero-loss filtering with large field of view, low-loss and core-loss spectroscopy with highest energy resolution, angle-resolved EELS, and fast STEM-EELS mapping applications. Its exceptionally low remanence and drift effects allow for switching from high-resolution EELS to ESI or another EELS dispersion back and forth with only very little shift or defocus. The excellent stability of the filter supply minimizes the need for regular re-tuning. The filter is supported by a python-based image processing platform featuring automated tuning for maximum ease of use. The users can run their own python scripts, having access to all acquired images plus image processing and display functionality via an Application-Programmers-Interface (API). Third party software can be integrated very easily. The detector interfaces are designed for flexibility. In ESI mode an entrance aperture of up to 12 mm can be used. The filter supports post-filter cameras with detector sizes up to 64 mm side length and fits into the mounting space of all modern (S)TEMs. Three ESI magnifications are supported, imaging a quadratic field of views of 8 mm, 10 mm and 12 mm diagonal length in the entrance aperture plane onto the detector. For those three magnifications the non-isochromaticities, maximum distortions and maximum chromatic distortions are (0.13 eV, 0.9 %, 0.22 %), (0.44 eV, 1.0 %, 0.23 %) and (1.7 eV, 1.4 %, 0.26 %), respectively, for an energy window of 50 eV at 200 kV. The regular EELS aperture is 5 mm. The pre-slit alignment is kept almost identical for the different ESI and EELS modes. Additional spectroscopy modes supporting an extremely large spectral range of up to 4 keV at 200 kV and dedicated alignments for omega-q mapping at higher dispersions are possible. For highest energy resolution a dispersion of 2 meV/channel for 4k x 4k detectors with pixel sizes at the order of 15 um is available. In order to minimize the non-isochromaticity of an ESI image and to improve the quality of focus of the Zero-Loss-Peak (ZLP) in EELS mode, the diameter of the ZLP in the slit plane formed by all electrons over the entire entrance aperture must be as small as possible in the dispersive direction. This is equivalent to minimize the geometric aberrations in the slit plane, which is achieved by combining a sector magnet whose geometry has been optimized for minimum intrinsic geometric aberrations with a set of sextupole, octupole, decapole and dodecapole fields allowing for correcting all residual geometric slit aberrations up to third order and certain aberrations of fourth and fifth order. The aberrations are measured by scanning the ZLP over the edge of one selection slit, recording the attenuation pattern and fitting the aberration coefficients from that. The

pre-slit setting shared by all ESI magnifications is optimized for low residual chromatic distortions in the image while the pre-slit setting shared by all regular EELS modes uses an additional pre-slit sextupole to correct for the spectrum inclination. For all ESI magnifications the projective corrects or adjusts the distortion coefficients of first order, the three intrinsic coefficients of second order, one critical intrinsic coefficient of third order and finally the chromatic distortion coefficients of first degree. Its excellent performance is achieved by an optimized design comprising a minimalistic design of only four main quadrupoles, two weak rotated quadrupoles for correcting parasitic aberrations and three sextupoles. The measureable residual distortions for the 12 mm entrance field of view are very predictable and can optionally be removed by online distortion dewarping.

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## ON SIGNIFICANCE OF 50 KV E-BEAM SHOT NOISE IN LITHOGRAPHY APPLICATION

**Victor Katsap**

NuFlare Technology America

**Keywords:** e-beam lithography, shot noise, acid deficit

In e-beam mask writers, 50-keV e-beam having dynamically controlled rectangular shape strikes mask blank surface. Mask blank consists of thin layers of resist and metal atop of massive quartz substrate. Primary and secondary electrons expose resist by colliding inelastically with resist molecules. Beam dwell time depends on beam spot current density and resist sensitivity. Noise is often defined as ratio of  $\text{SQRT}(\text{var})$  to MEAN value. For e-beam shot noise, it's  $1/\text{SQRT}(N_e)$ ,  $N_e$  being number of electrons in process considered. In a simplified way, e-beam resist exposure may be looked at as a sequence of 3 steps:  $N_e$  electrons enter resist > Na acids get de-protected > Np polymer molecules get exposed in Post-Exposure-Baking (PEB) step. In each step, limited number of particles is involved, and so each process may be described with Poisson-type statistics. These 3 statistics can be summed up to evaluate resulting noise in e-beam exposed and developed resist:  $\text{SQRT}(\text{var})/\text{MEAN} = \text{SQRT}(1/N_e + 1/N_a + 1/N_p)$  This means that step with the least number of particles would dominate resulting noise in the exposed feature, thus defining exposure quality. Typically, Na is smallest of 3 values, facilitating so called "acid deficit". Under realistic conditions, e-beam noise is 1/4 of total, while acid noise may reach 70% of total noise. This could explain a difference in exposing resist with low- and high-energy e-beams: - with low-energy beam, acid yield is close or greater than 1 acid per primary electron, hence no acid deficit, and e-beam noise dominates. - with high-energy beam, acid yield is less than 1 acid per primary electron, hence acid deficit, and e-beam noise is minor factor. However, because of using thinner and thinner resist in commercial process, e-beam noise may become major component of the total exposure noise.

## HIGH-ORDER ABERRATIONS OF LARGE APERTURE MAGNETS AND APPLICATIONS TO THE SUPER-FRS PROJECT AT GSI

**Erika Kazantseva, Oliver Boine-Frankenheim, Helmut Weick**

Technische Universitaet Darmstadt

### *Invited Talk*

**Keywords:** Super-FRS, high-order aberrations, realistic Taylor transfer maps

The magnets of the charged particle spectrometers and separators play a decisive role in the beam quality and transmission percentage, especially for the systems with large geometrical and momentum acceptances. In the case of the Superconducting Fragment Separator (Super-FRS), a core part of the FAIR project being built at GSI, the undesired high-orders aberrations are expected due to the large usable apertures of the magnets ( $38 \times 19 \text{ cm}^2$  in the main dipoles and  $19 \times 19 \text{ cm}^2$  in the multipoles) and wide operation rigidity range of 2-20 Tm. In this work we will analyse the aberrations introduced by the normal conducting dipole magnet of the Super-FRS preseparator. The methods of generating the high-order Taylor transfer maps from the 3D magnetic field distributions and taking the magnetic rigidity into account will be discussed.

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## QUANTUM CHARGED-PARTICLE BEAM OPTICS

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Chennai Mathematical Institute and Dhofar University

**Keywords:** Quantum Mechanics, Charged Particle Beam Optics

Though the classical charged-particle beam optics is very successful, in designing and operating numerous charged-particle beam devices from electron microscopes to particle accelerators, it is natural to look for the quantum theory of such systems handling beams of microscopic particles for which quantum mechanics should be relevant. With the curiosity of understanding how the classical charged-particle beam optics is so successful, the quantum charged-particle beam optics (QCPBO) is being developed by Jagannathan et al. QCPBO is seen to reproduce the classical charged-particle beam optics exactly for the paraxial and aberrating systems in the classical limit of dropping the additional quantum correction terms which depend on the Planck constant and are, of course, extremely small compared to the classical terms. In the classical limit the quantum formalism reproduces the well-known Lie algebraic formalism of classical charged-particle beam optics. QCPBO based on the Klein-Gordon equation is applicable to spin-0 and spinless particles. The formalism of QCPBO based on the Dirac equation provides a unified treatment of orbital and spin dynamics of a Dirac particle with anomalous magnetic moment being transported through magnetic optical elements accounting for the orbital phase-space transfer maps, including the Stern-Gerlach effect, and the Thomas-Bargmann-Michel-Telegdi spin motion. QCPBO based on the nonrelativistic Schrödinger equation emerges as the approximation of the relativistic formalisms based on both the Klein-Gordon and the Dirac equations.

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**A LOW-ENERGY SPREAD GRAPHENE COATED  
NICKEL ELECTRON SOURCE FOR  
LOW-VOLTAGE SCANNING ELECTRON  
MICROSCOPY**

Xiuyuan Shao, Wei Kean Ang, and **Anjam Khurshed**

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**Keywords:** Energy distribution, Boersch effect, Graphene

Field emission energy distribution characteristics of graphene coated nickel emitters have been experimentally measured as a function of cathode extraction voltage and tip radius. These emitters have been recently reported to have significant advantages over conventional cold field tungsten emitters for electron microscopy/lithography applications. Full-width at half-maximum values for their energy spectra were experimentally measured to vary between 0.16 to 0.39 eV. By subtracting the calculated total energy distribution (TED) in the thermal field regime from the experimental spectra, the energy spread broadening due to Coulomb interactions (Boersch effect) was obtained, and found to increase with increasing extraction voltages and decreasing the tip sizes. These results are of particular interest for low-voltage scanning electron microscopy applications where chromatic aberration of the objective lens is the main factor limiting spatial resolution.

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**CONSIDERATIONS ON BEAM OPTICS OF  
SUPERCONDUCTING HEAVY ION LINACS FOR A  
RARE ISOTOPE BEAM FACILITY**

**Jongwon Kim, Brahim Mustapha**

Institute for Basic Science, Korea, Argonne National  
Laboratory, USA

**Invited Talk**

**Keywords:** Superconducting linac, Heavy-ion beam, Rare isotope beam

The rare isotope science project (RISP) was started in Korea from Dec. 2011 to establish an accelerator facility based on superconducting linacs for nuclear and applied science studies under the auspices of the Institute for Basic Science (IBS). The current design was frozen in 2013 in terms of the facility layout and the civil construction began in 2016. In fact, some considerations on alternative linac design were made in 2016 together with the linac development group of Argonne National Lab in search of further optimized configuration of the driver linac, which should have sound lattice design against realistic machine errors. Results of beam optics simulations and error analysis for an alternative design will be presented. Also, considerations on optimized design and operation scheme of the superconducting linac which can accelerate both stable and rare isotope beams simultaneously, will be presented.

**PONDEROMOTIVE GENERATION AND  
DETECTION OF ATTOSECOND ELECTRON  
PULSES**

**Martin Kozak**, Timo Eckstein, Norbert Schönenberger,  
Peter Hommelhoff

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Department of Physics, Friedrich-Alexander-Universität  
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**Invited Talk**

**Keywords:** Ultrafast control of electron pulses, attosecond physics

In this contribution we will discuss recently developed technique for generation and detection of attosecond electron pulses via inelastic ponderomotive scattering of electrons at an optical traveling wave formed by two laser pulses at different frequencies. This scheme represents an analogy to the classical Kapitza-Dirac effect [1], in which the roles of the transverse and longitudinal directions (with respect to electron propagation) are reversed. We demonstrate a large modulation of the kinetic energy of subrelativistic electrons with initial kinetic energy of 29 keV, achieving a peak acceleration gradient of  $G=2.2$  GV/m (energy gain/travelled distance) [2]. A time-correlated modulation of electron energy leads to a ballistic compression and formation of attosecond electron pulses. Detection of the sub-cycle temporal structure of the electron pulse train was performed via energy streaking using a second phase-controlled traveling wave [3]. Measured spectrograms (spectrum as a function of relative phase) and their comparison with numerical calculations allow monitoring the evolution of the electrons' longitudinal phase space distribution. [1] P. L. Kapitza, and P. A. M. Dirac, Proc. Cambridge Philos. Soc. 29, 297 (1933). [2] M. Kozák, T. Eckstein, N. Schönenberger, and P. Hommelhoff, Nat. Phys. 14, 121-125 (2018). [3] M. Kozák, N. Schönenberger, and P. Hommelhoff, Phys. Rev. Lett. 120, 103203 (2018).

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**CORRECTION OF ABERRATIONS IN ELECTRON  
MONOCHROMATORS AND SPECTROMETERS**

N. Dellby<sup>1</sup>, A.L. Bleloch<sup>1</sup>, M.V. Hoffman<sup>1</sup>, T.C.  
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**Invited Talk**

**Keywords:** spectrometers, monochromators, aberration correction

Electron energy loss spectroscopy (EELS) in the electron microscope has progressed remarkably in recent years. In our monochromated microscope system, we have reached 4.2 meV

energy resolution at 30 keV, measured as the full-width at half-maximum of the monochromated zero loss peak (FWHM of ZLP), and 5.9 meV at 60 keV - i.e., energy resolution better than 1 part in  $10^7$ . In both the monochromator and the spectrometer, the energy spectrum contains a small image of the electron source, and the attainable energy resolution is given by  $ER = d / D$ , where  $d$  is the diameter of the source image and  $D$  the energy dispersion. Reaching better energy resolution thus requires making  $d$  smaller, or increasing  $D$ . The second path employs sizable energy-dispersing devices with concomitant weight and mechanical stability issues. We have chosen the more practical first path to better energy resolution, and we pay particular attention to three performance aspects: 1) stability of the source image position, 2) demagnifying the source sufficiently (while retaining a useful electron current), and 3) increasing the convergence angle, to minimize the diffraction limit, and to maximize the probe current. The third aspect requires that aberrations be kept under tight control. Our latest spectrometer design corrects all geometric aberrations up to 5th order, plus mixed chromatic-geometric aberrations up to third rank. It also includes autotuning that measures individual aberration coefficients and corrects them. The talk will review the methods we use to optimize performance aspects 1) and 2), and then focus on the correction of aberrations in the monochromator and the spectrometer. It will also describe our recent work on optimizing probe corrector performance.

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## DOUBLE MIRROR ABERRATION CORRECTOR

Pieter Kruit(1) and Hideto Dohi(2)

(1)Delft University of Technology and (2)Hitachi High-Technologies Corporation

**Keywords:** scanning electron microscope; aberration corrector; MEMS electron optical components

The resolution of scanning electron microscopes (SEMs) is limited by aberrations of the objective lens, mainly the chromatic aberration. It is well known that both spherical and chromatic aberrations can be compensated by placing an electron mirror in the beam path before the objective lens. The effectiveness of this has been proven in LEEM systems. Nevertheless, this approach has not led to use of these aberration correctors in SEMs, probably because aberrations of the bending magnet can be a serious problem. We have proposed a mirror corrector with two mirrors placed perpendicularly to the optic axis of an SEM and facing each. As a result, only small-angle magnetic deflection is necessary to guide the electron beam around the top mirror to the bottom mirror and around the bottom mirror to the objective lens. The deflection angle is only in the order of 50 mrad, and thus sufficiently small to avoid deflection aberrations. In addition, lateral dispersion at the sample plane can be avoided by the correct choice of deflection fields. In order to keep such a corrector system simple, the incoming beam should pass the top mirror at a distance in the order of millimeters. It is proposed that condition can be satisfied with micro-scale electron optical elements fabricated using MEMS technology. Extensive optical calculations were performed. Aberrations of the micro-mirrors were analyzed by numerical calculation. Dispersion and aberrations of the deflectors were calculated by using an analytical field model. We concluded that the proposed corrector system could

be a candidate for aberration correction in low-voltage SEMs. We have started the construction of a system to be tested in an existing SEM. Reference: Hideto Dohi and Pieter Kruit, Design for an aberration corrected scanning electron microscope using miniature electron mirrors, *Ultramicroscopy* 189 (2018) 1-23.

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## SOME DESIGNS FOR QUANTUM ELECTRON MICROSCOPY

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**Keywords:** interaction-free measurement, quantum electron microscope, electron mirror, electron phase manipulation

Following a recent suggestion [1] that interaction-free measurements may be possible with electrons, we have analyzed the opportunities to use this concept for imaging of biological specimen with reduced damage in a Transmission Electron Microscope. This requires that part of the electron wave travels multiple times through the same position on the specimen. We expect this to be an interesting challenge in charge particle optics. We have made preliminary designs for an atomic resolution interaction-free electron microscope, or “quantum electron microscope” [2]. The designs require a number of unique components not found in conventional transmission electron microscopes. These components include a coherent electron beam-splitter or two-state-coupler, and a resonator structure to allow each electron to interrogate the specimen multiple times. A two-state-coupler has the function of moving the electron wave slowly between the reference beam and the specimen beam, as in a Rabi-oscillation. We have suggested and are now investigating, both in simulation and in experiment, whether an electron mirror with a diffraction grating on the reflecting surface can accomplish the two state coupling while at the same time forming part of the resonator. The experimental design consists of many MEMS elements. The same mirror unit might be used for a more advanced manipulation of the electron wave front. This research is funded by the Gordon and Betty Moore Foundation. 1] Putnam, W.; Yanik, M. *Phys. Rev. A* 2009, 80, 040902. 2] Kruit, P.; R. G. Hobbs, C-S. Kim, Y. Yang, V. R. Manfrinato, J. Hammer, S. Thomas, P. Weber, B. Klopfer, C. Kohstall, T. Juffmann, M. A. Kasevich, P.Hommelhoff, K. K. Berggren. *Ultramicroscopy* (2016), 31-45 3] Elitzur, A. C.; Vaidman, L. *Found. Phys.* 1993, 23, 987-997.

## NANO APERTURE ION SOURCE

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**Keywords:** Ion source; brightness; mirror charge

Ion production in the Nano Aperture Ion Source (NAIS) is based on electron impact gas ionization inside a sub-micron sized gas chamber [1]. An important part of recent efforts [2] was devoted to understanding how the relevant physical processes determine the ion beam performance. This has led to interesting insights in charged particle optics. The influence of initial velocity and position distributions of the neutral gas particles, their ionization cross sections, the electron current density, ion-neutral scattering, Coulomb interactions and the electric fields around the double membrane structure are studied by analytical models, numerical calculation, and ray tracing. An unexpected effect is that the low energy ions are deflected by their mirror charge when they exit the submicron sized orifice of the gas chamber. An important finding is that the ion current and the brightness tend to keep increasing with increasing particle density, despite increasing ion-neutral scattering. Ion-to-ion Coulomb repulsion is found to pose a final limit to the achievable brightness. In a realistic configuration, the simulations predict a brightness of about  $3 \times 10^6$  A/m<sup>2</sup>srV in combination with an energy spread of 1 eV. In experiments we have now demonstrated a brightness of  $1 \times 10^5$  A/m<sup>2</sup>srV, which we consider a milestone result because it is already a competitive brightness when compared to a Ga LMIS while there is clearly room for improvement. [1] David S. Jun, Development of the Nano-Aperture Ion Source, PhD Thesis TU Delft, 2014. [2] Leon van Kouwen, The Nano-Aperture Ion Source, PhD Thesis TU Delft, 2017

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## LONGITUDINAL PHASE SPACE MANIPULATION OF ELECTRON BEAMS USING MICROWAVE CAVITIES

Wouter Verhoeven, Jasper van Rens, Peter Mutsaers, Jom Luiten

Eindhoven University of Technology

### *Invited Talk*

**Keywords:** dynamic electron optics, ultrafast electron microscopy, microwave cavities, time-of-flight eels

At Eindhoven University of Technology we are developing resonant microwave cavities as dynamic charged particle optics for electron microscopy (EM). We employ miniaturized and power-efficient dielectric 3 GHz pillbox deflection cavities in TM-110 mode both for creating femtosecond electron pulses by chopping a continuous beam and for measuring pulse lengths by streaking electron pulses across a detection screen. Cavities in TM-010 mode are used as longitudinal lenses to both compress electron pulses (positive focal length), to improve the temporal resolution, or stretch them (negative focal length), to reduce the uncorrelated energy spread. If properly used, microwave cavities do not affect the electron beam quality. The microwave phase can

be accurately synchronized to femtosecond lasers, enabling ultrafast pump-probe experiments. Combining a high-quality continuous electron gun with a special configuration of two TM-110 cavities and two TM-010 cavities, time-of-flight EELS can be realized with few-10-meV energy resolution and few-ps time resolution. This new method does not require femtosecond lasers and may constitute an interesting alternative to magnetic electron spectrometry. The use of microwave cavities is therefore not restricted solely to the burgeoning field of ultrafast EM. In fact, it may become increasingly relevant to EM in general.

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## FOR THE PROMOTION OF MICROSCOPY AND MICROANALYSIS IN ALL RELEVANT SCIENTIFIC DISCIPLINES: THE MICROSCOPY SOCIETY OF AMERICA

Charles E. Lyman and Robert L. Price

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**Keywords:** microscopy society, scientific conference, electron and ion optics, peer-reviewed journal, education

The Microscopy Society of America (MSA) is pleased to support student travel to the 10th International Conference on Charged Particle Optics. Such support is a natural fit for MSA given our mission statement, an excerpt of which forms the title above. Founded 76 years ago, our Society has been a forum for discussion of electron optics, from the early days of the TEM to aberration-correction technology; indeed, the original name of the society was the Electron Microscope Society of America. Today our purview also includes ion optics with presentations and publications that include focused ion beam (FIB) and atom probe tomography (APT) instrumentation and techniques. The Society promotes microscopy and microanalysis in several ways. The Microscopy & Microanalysis (M&M) conference in August is the largest annual microscopy meeting and instrument exhibition in the world. M&M 2018 featured 1236 scientific papers and attracted attendees from 40 countries. Among the many students and post-doctoral scholars attending the meeting, 55 received competitive travel awards. Our student council members are learning leadership skills by independently organizing an annual pre-meeting congress. *Microscopy and Microanalysis*, our peer-reviewed research journal covering both the life and physical sciences, ranks high among microscopy journals in terms of Impact Factor and number of pages published per year. Our technical trade magazine, *Microscopy Today*, reaches a large audience and provides news and research summaries that emphasize advances in instrumentation and methods, as well as hints and tips for novice and experienced microscopists. In addition to the above, our educational efforts include short courses and tutorials at the M&M meeting, a technologist certification program, undergraduate research scholarships, and several outreach programs for students in middle school and high school. Finally, membership in MSA is cost-effective since dues cover subscriptions to our publications and registration discounts at the M&M meeting.

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## ELECTRON OPTICS FOR A MULTI-PASS TRANSMISSION ELECTRON MICROSCOPE

**Marian Mankos**<sup>1</sup>, Stewart A. Koppell<sup>2</sup>, Brannon B. Klopfer<sup>2</sup>, Thomas Juffmann<sup>3</sup>, Vladimir Kolarik<sup>4</sup>, Khashayar Shadman<sup>1</sup> & Mark A. Kasevich<sup>2</sup>

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### *Invited Talk*

**Keywords:** electron optics, multi-pass transmission electron microscopy, electron mirror

Recent advances in cryo-electron microscopy (cryo-EM) and direct electron detection have spurred renewed interest in the development of novel electron imaging techniques for applications in structural biology at atomic resolution. The challenge with imaging unstained biological specimens is that they provide a low scattering cross-section to the probing electrons because they are composed primarily of low atomic number elements. Hence, high electron doses are needed to obtain sufficient signal-to-noise ratios (SNR). Such doses, however, severely damage the specimens. Multi-pass transmission electron microscopy [1] is a promising approach that can reduce the required electron dose for a desired SNR by exploiting the change to the phase of the electron wave that is imparted by the specimen. In this approach, the electron beam interacts elastically with the specimen multiple times so that the change in the phase accumulates before reaching the detector. Here we examine the electron-optical design of a practical implementation of a multi-pass transmission electron microscope (MTEM), which is currently under construction. In MTEM, an electron pulse, triggered by an ultrafast laser beam, is focused by the illumination optics and transmitted by the entrance electron mirror, rendered transparent by a voltage pulse synchronized with the laser beam. The transmitted electron pulse enters an electron resonator, bounded by the entrance and exit mirrors. The resonator includes two objective and field lenses that sandwich the specimen. The electron pulse is collimated by the upper field and objective lens onto the specimen, and refocused by the lower objective and field lens onto the exit mirror, which reflects it back symmetrically so that the electron pulse is collimated again at the specimen. This reflection is carried out multiple times until a second voltage pulse renders the exit mirror transparent to allow the electron pulse with the accumulated phase to proceed into the projection optics, which magnifies the image at the exit mirror onto the detector. Past simulations have predicted an improvement in resolution and sensitivity for a range of electron microscopy imaging techniques, and an order-of-magnitude reduction in damage at equivalent resolution[2]. 1 T. Juffmann, B. B. Klopfer, T. L. Frankort, P. Haslinger, and M. A. Kasevich, Nat. Commun. 7, 12858 (2016). 2 T. Juffmann, S. A. Koppell, B. B. Klopfer, C. Ophus, R. M. Glaeser, and M. A. Kasevich, Sci. Rep. 7, 1699 (2017).

## ULTRAFAST ELECTRON DIFFRACTION USING THE CBETA PHOTOINJECTOR

**Jared Maxson**, William Li

Cornell University

### *Invited Talk*

**Keywords:** UED, photoinjector, time resolved diffraction

In this talk, I will describe perspectives and simulations of the photoelectron injector for the CBETA accelerator (Cornell-BNL Energy Recovery Test Accelerator) as a high average brightness source of short-pulse electrons for femtosecond time-resolved electron diffraction. Specifically, I will discuss the ability of the CBETA photoelectron gun to take advantage of novel high coherence photocathode materials, as well as the extreme flexibility of the RF acceleration system. The acceleration system is composed of five superconducting cavities each with independent phase and amplitude control, which I will show is critical for a number of applications, including longitudinal phase space linearization in velocity bunching, as well as ultrafast time of arrival measurements when used in conjunction with a high resolution spectrometer. These capabilities make the CBETA photoinjector an excellent candidate for use in high spatiotemporal resolution electron scattering experiments.

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## COLD ATOM ION SOURCES

**J. J. McClelland**(1), J. R. Gardner(1,2), W. R. McGehee(1), A. Schwarzkopf(3), B. Knuffman(3), and A. V. Steele(3)

(1) CNST, National Institute of Standards and Technology, Gaithersburg, MD, USA; (2) IREAP, University of Maryland College Park, College Park, MD, USA; (3) zeroK NanoTech, Gaithersburg, MD, USA

### *Invited Talk*

**Keywords:** ion sources; laser cooling; high brightness; focused ion beams

Ionization of laser-cooled atoms has emerged as a new approach to constructing high brightness ion sources for applications such as focused ion beam (FIB) microscopy and milling. While conventional sources, such as the Ga liquid metal ion source (LMIS) or the gas field ionization source (GFIS), attain brightness by emitting from a very sharp tip, cold atom sources reach high brightness through reducing the transverse velocity spread. With the ultracold, microkelvin-range temperatures achievable with laser cooling, the corresponding velocity spread can lead to a brightness significantly higher than typical LMIS values. Moreover, the phase-space shape of the emittance of the source - narrow in velocity, wide in space - brings new opportunities for ion optical design. For example, high currents can be obtained without the high current density present in sharp tip sources. This can result in fewer Coulomb effects, such as increased emittance and broadened energy spread (Boersch effect). In addition, the absence of a sharp tip eliminates a sensitivity to source stability. Other advantages of this type of source include insensitivity to contamination, access to new ionic species, inherent isotopic purity, and fine control over emission, down to the single ion level.

To date, sources have been demonstrated with Cr, Li, Rb, and Cs ions. In this talk I will review progress in the field, focusing on our work with a Li FIB microscope for battery studies and a Cs FIB with brightness 24 times higher than the LMIS.

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### A NEW SIMULATION PROGRAM FOR ELECTRON MIRRORS USING THE BOUNDARY ELEMENT METHOD

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**Keywords:** Electron mirrors, boundary element method, aberration computation, direct ray tracing

Electron mirrors have many applications in charged particle optics, e.g. aberration correctors, beam separators, time-of-flight spectrometers. Optimization of electron mirrors requires high accuracy computation of electric fields, trajectories, focal properties, and geometrical and chromatic aberrations, including both spatial and temporal aberrations. The simulations are more difficult than for electron lenses, because the ray slopes become infinite at the reflection plane, so the trajectories and aberrations have to be computed using time, rather than axial position, as independent variable. This paper presents a new electron mirror simulation software using the Boundary Element Method. This method computes the electric charge distribution generated on the electrode surfaces, by dividing the electrodes into rotationally symmetric rings, and generating a matrix equation expressing the potential on each ring as a weighted sum of the surface charges on all the rings. Since the potentials on each ring are the known electrode potentials, a matrix equation is obtained whose solution yields the ring charges. The potential at any point in the mirror can then be computed by numerical evaluation of a sum of elliptic integrals of the ring charges. This method has several beautiful features: (1) Data input is simple, because only the electrode surfaces need to be discretized, not the intervening space; (2) Numerical accuracy can be verified by evaluating the potential at check-points on the electrodes and comparing these with the known values; (3) The axial potential distribution and its derivatives can be obtained with great accuracy; (4) From these axial functions, all the optical properties can be computed, including geometrical and chromatic aberrations, both temporal and spatial, using a differential algebraic method; (5) The potential and fields at any off-axis point can be computed using elliptic integrals which have great accuracy and stability, and the results are an exact solution of Laplace's equation; (6) These off-axis fields can be used to compute aberrations by direct ray-tracing, providing an independent check on the differential algebra results. The program will be described in detail, and illustrated with practical examples, and the results compared with those from our previous electron mirror program, which used finite element method and Hermite series fits.

### ELECTRON RAY TRACING IN A CYLINDRICAL DEFLECTOR ANALYZER FOR FIELD EMISSION SPECTROSCOPY

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**Keywords:** electron ray tracing; three-dimensional boundary charge method; Runge-Kutta-Fehlberg 4th order method; field emission spectroscopy; cylindrical deflection angle

Field-emission spectroscopy (FES) is a technique that acquires an energy spectrum of the electrons emitted from a field emitter. A cylindrical deflector analyzer (CDA) is often used for FES. Assuming that the electric field in the CDA is an ideal cylindrical field, it is known that the optimum deflection angle is  $127^\circ$ . In fact, there is a deviation from an ideal cylindrical field in the CDA. In particular, a fringing field occurring at the vicinity of entrance and exit of slits is not negligible. Therefore, herein, we performed three-dimensional (3D) electric field calculations and electron ray tracing using a 3D boundary charge method (BCM) that we developed previously. Furthermore, for this purpose, we improved the calculation method of the electron ray tracing. So far, we had used Runge-Kutta-Gill method (RKG method) for the electron ray tracing. In the method, the step size is fixed due to the specification of the method. Therefore, to perform an electron ray tracing with high-accuracy, the step size must be finer. However, extremely-long calculation time is required for the electron ray tracing. Hence, to improve this obstacle, we introduced Runge-Kutta-Fehlberg 4th order method (RKF4 method) into the electron ray tracing calculation so that suitable step size can be controlled automatically while keeping high-accuracy. As a result, we have found that the improved method can reduce the calculation time while keeping high-accuracy. In addition, as a result of the electron ray tracing in the CDA, we also have found that when the potential difference between the inner and outer electrodes is 0.353 V ( $= 2 E_0/e \log 1.8$ ) and the initial energy  $E_0$  of the electrons is 0.3 eV, the optimum deflection angle of the CDA is  $\sim 109$  degree.

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### LARGE MOMENTUM ACCEPTANCE BEAM OPTICS OF A SUPERCONDUCTING GANTRY FOR PROTON THERAPY

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**Keywords:** Beam optics design; proton therapy; superconducting gantry

In proton therapy, the last part of the beam transport system is installed on a rotatable gantry, so that the beam can be aimed at the tumor from different angles. Since such a gantry system consists of many dipole and quadrupole magnets, it is typically a 200 ton device of more than 10 m in diameter. The use of superconducting (SC) magnets for proton therapy allows gantries

to be significantly lighter and potentially smaller, which is attractive for this medical application. In addition to that, SC combined function magnets enable beam optics with a very large momentum acceptance. The latter can be advantageous for patient treatment, since the irradiation time can be significantly reduced by avoiding magnet current changes. A new prototype of a SC gantry with a momentum acceptance of +/- 15 % is under development at PSI. To design such an achromatic system, precise high-order calculations have been performed. In order to reach the required accuracy and to check consistency of the obtained results, we have used several simulation tools in our iterative design approach. Here we will describe how we have combined an initial standard first order calculation with more detailed calculations using the higher order code COSY Infinity and particle tracking using OPAL (open source software from PSI) in 3D field maps obtained from detailed magnet calculations performed in OPERA. A comparison of the results from the beam-optics calculations helped to determine the next iteration step in the design of the SC gantry.

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### ADJOINT VARIABLE METHOD FOR RAPID DESIGN OPTIMIZATION OF ELECTROSTATIC LENS SYSTEMS

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Stanford University, Ion Innovations

**Keywords:** optimization, electrostatic lens design, finite element method, inverse design, electrostatic field solver, adjoint variable method, charged particle optics, einzel lens, velocity verlet

We have implemented a generative algorithm for design optimization of electrostatic charged particle optical devices using the discrete adjoint variable method. In this work, we optimize a series of electrostatic lenses to minimize spherical and chromatic aberrations and perform beam steering. To the best of our knowledge, these are the first charged particle optics systems designed by an adjoint variable based algorithm. Physical systems with many designable parameters (e.g. dimension, shape and applied voltages) are computationally burdensome to optimize. To efficiently improve the device design it is crucial to know how its performance changes under all designable perturbations to its shape, dimensions, and operating conditions. This sensitivity of the design to its design parameters can be obtained by simulating each potential perturbed device in turn. This is a computationally costly approach requiring at least one extra full-system calculation per design parameter. In contrast, adjoint design sensitivity analysis is a method to obtain sensitivities to all design parameters at once through an algorithm with nearly-fixed computational cost. Thus, adjoint methods enable rapid optimization of complex systems. This has led to the pervasive use of these methods in aeronautical, structural and photonic design. To obtain such a rapid algorithm for charged particle optics, we derived and implemented a fully discrete adjoint system solver for the non-linear, coupled system comprising the Laplace equation for the electric potential and an equation of motion based on the Lorentz force law and Newton's second law, using a custom-built electrostatic finite-element method and a charged particle dynamics simulator based on Verlet integration. This solver allows for arbitrary selection of initial designs and number of design parameters

and calculates the sensitivity of the design to charged particle trajectories for each of these parameters. The method demonstrated can be applied to miniaturizing complex systems and optimizing multi-beam applications such as lithography.

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### INVESTIGATION OF ELECTROMAGNETIC-SYLC FOR CHROMATIC ABERRATION CORRECTION

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**Keywords:** chromatic aberration, symmetric line currents, SEM, aberration correction

We are studying a simple aberration corrector for scanning electron microscopes (SEM). We have proposed SYLC (SYmmetric Line Currents) corrector in which parallel line currents are symmetrically arranged instead of usual magnetic multipoles to correct spherical aberration [1, 2, 3]. The main feature of SYLC is being free of magnetic material, thus eliminating the problems of hysteresis, nonuniformity and magnetic saturation of the magnetic material. In addition to spherical aberration, correction of chromatic aberration is also necessary for low acceleration voltage SEM. Therefore, SYLC is expanded to incorporate electrostatic multipole field with magnetic multipole field. Applying positive and negative electrostatic potentials alternately to the conducting lines of SYLC yields a superposition of electrostatic and magnetic 2N-poles, which we call an electromagnetic-SYLC. Moreover, since the direction and distribution of 2N-pole electric and magnetic field are the theoretically same, the number of poles can be reduced by half comparing with a conventional electromagnetic multipole. We show that chromatic aberration can be corrected by a model in which the conventional multipoles of the quadrupole 4-stage corrector proposed by H. Rose [4] are replaced by the combination of electro-and magnetic-SYLC. [1] Nishi R., Ito H., Hoque S., (IMC2014), IT-1-P2984, pp.200-201 [2] S. Hoque, H. Ito, R. Nishi, A. Takaoka, E. Munro, Ultramicroscopy 161, (2016) 74-82 [3] P. W. Hawkes and E. Kasper, Principle of Electron Optics, Vol.2 : Applied Geometrical Optics, 2nd ed., chap. 41, pp. 986-988, Academic Press, 2017. [4] H. Rose, Optik 32, (1970) 144

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### EVALUATION OF A MONOCHROMATOR WITH OFFSET CYLINDRICAL LENSES FOR ELECTRON MICROSCOPY

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**Keywords:** Monochromator, Cylindrical lens, Electron microscope

Monochromators (MCs) have been indispensable optical components for advanced electron microscopes [1-3]. MCs can improve image resolutions at low energy conditions and energy resolutions of EELS spectra. Both are achieved by narrowed energy spreads of electron beams. At the CPO9 conference, a new MC

with cylindrical lenses (CLs) was proposed [4]. The MC consists of two CLs in offset layout with the middle plane symmetry. The strongly excited CLs generate large energy dispersions, which enables the MC optics with high performance and simple structure. Based on theoretical studies on the MC [5-7], a prototype of the MC has been constructed at high mechanical accuracy and combined with highly stable electronics. The MC achieved the energy resolution of 73 meV by measuring energy distributions with an additional energy analyzer [8]. Observation in two conditions with or without the MC confirmed fine beam profiles because of the symmetry of the MC. The results assure applicability of the MC to electron microscopes. At the conference, recent evaluation results of the MC will be presented. References: [1] H. Rose, Ultramicroscopy 78 (1999) 13. [2] H.M. Mook, P. Kruit, Ultramicroscopy 81 (2000) 129. [3] O.L. Krivanek, et al., Nature 514 (2014) 209. [4] T. Ogawa, et al., Microsc. Microanal. 21 (S4) (2015) 112, Proceedings of CPO9. [5, 6] T. Ogawa, B. Cho, Nucl. Instrum. Methods. A 772 (2015) 5, 800 (2015) 18. [7] T. Ogawa, et al., J. Vac. Sci. Technol. B 33 (6) (2015) 06FJ01-1-11. [8] T. Ogawa, Y. Takai, J. Vac. Sci. Technol. B 36 (3) (2018) 032902.

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## SIMULATION OF MOTION OF MANY IONS IN A LINEAR PAUL TRAP

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**Keywords:** linear quadrupole Paul trap, Coulomb crystals, optical atomic clock, micromotion, trajectory simulation

The quadrupole linear Paul trap is one of the key instruments in building highly stable atomic clocks. However, a frequency reference based on a single trapped ion is limited in stability due to the time needed for the interrogation cycle which cannot be further shortened. A promising strategy is the utilization of multiple trapped ions. The ions of the same kind then repulse each other with the Coulomb force, which is countered by the ponderomotive force of the time depended field in the trap. A few ions form a chain along the axis of a linear Paul trap. Adding more ions (a few tens or hundreds) gives rise to Coulomb crystals. We created an efficient simulation code which calculates the motion of such collections of ions in quasistatic radiofrequency fields of real linear quadrupole traps (including the micromotion). We attempt to take into account various methods of cooling the ions. The simulation tool can be used to study the formation and the dynamics of Coulomb crystals under conditions corresponding to various experimental set-ups.

## SIMULATION FOR THE DEVELOPMENT OF PRECISE AUTO-FOCUSING OF SEM LENSES

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**Keywords:** SEM, auto-focus, self-inductance, aftereffect

The latest SEMs in industrial product lines should meet the demands of higher resolution and higher throughput. The higher resolution objective lenses have the shorter depth of focus which require the more precise adjustment of their coil current. The duration of auto focusing should be shorter to obtain higher throughput then the precision of auto-focusing is subject to the delay of current response with the self-inductance and the aftereffect of magnetization. We propose a response function based on those two delay mechanisms while the ratio of the aftereffect is estimated comparing experimental delay times with simulated ones. A function to calculate self-inductance has been built onto an in-house electron optics simulator "EMB2D" which shows the saturation of self-inductance over the permeability of 1000. We demonstrate the ratio of the aftereffect 0.06 with time constant of 1.0 sec. is plausible in this case and our proposed response function is useful to improve the precision of auto-focusing.

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## WIDE-ANGLE ANNULAR ELECTRON BEAM FOCUSING COLUMN.

**Balamuniappan Pranesh, Ang Wei Kean, Anjam Khursheed**

National University of Singapore

**Keywords:** annular focused electron/ion beams, aberration correction, electric sectors

There are many applications in electron microscopy, electron spectroscopy, as well as accelerator physics that require the combination of minimizing a focused electron beam's probe size, while maximizing its beam current. This paper describes how it can be done through the use of annular focused electron beam column designs and cold field emission sources, where an electron beam is propagated and focused in the form of a ring beam. For relatively small probe semi-angles, where the central angle lies between  $1^\circ$  to  $2^\circ$ , a 3 stage deflector-corrector in combination with an objective lens will be presented. The objective lens design can be either magnetic or electric. For probe semi-angles above say  $20^\circ$ , a column consisting of 2 identical electric sectors and 2 identical focusing lenses functioning with odd symmetry will be presented. The column is designed to cancel energy dispersion while limiting geometric aberrations to be of 3rd order at the point of final focus. Both designs predict to have over two orders of magnitude higher beam current than their corresponding conventional electron beam focused columns for the same final probe size. For a 1.2 keV annular electron beam with a semi-angular spread of  $45^\circ \pm 0.1146^\circ$  semi-angle, simulation results predict a final spot size of 5.7 nm at a working distance of 3.4 mm, giving approximately three orders of magnitude larger probe current than its corresponding conventional on-axis electron beam column for a similar probe size.

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## COMPARISON OF BEAM OPTICS FOR NORMAL-CONDUCTING AND SUPERCONDUCTING GANTRY BEAMLINE APPLIED TO THE PROTON THERAPY SYSTEM

**Bin Qin**

Huazhong University of Science and Technology

**Keywords:** Proton therapy, beam optics, superconducting gantry beamline, high order effect

Due to the unique ‘Bragg peak’ dose distribution characteristics of the proton beam, the proton therapy is recognized as one of the most precise and effective radiotherapy method for tumors. A gantry is required to project the beam on tumors with various angle for multiple fields radiation, and a superconducting beamline can significantly reduce the size and the weight of the gantry. A proton therapy system is under development in HUST. This paper will introduce the comparison study of the beam optics for normal-conducting and superconducting gantry beamline. Beam simulation study which demonstrates the influence of high order magnetic field effect in the beamline, will also be described.

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## DIFFERENTIAL ALGEBRAIC METHOD IN ELECTRON OPTICAL DESIGN

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*Invited Talk*

**Keywords:** differential algebraic method, correctors, aberrations, parasitic aberrations

The differential algebraic method is standardly used in particle accelerator design. It provides the high order transfer map needed for simulations of the long-term ring stability. On the other hand, the electron optics community prefers methods having a solution in the form of the aberration integral which provides a deeper view of the effect of each element on the electron optical properties of the system but they became too complicated with increasing aberration order, which is not a case of the differential algebraic method. We show the potential of the differential algebraic method on a design of electron optical systems. The first part deals with simulation of the axially symmetrical systems where the effect of the fringing field regions must be handled to obtain correct values of aberration coefficients. The next part shows the application of the method on aberration corrector design, we propose the efficient combination of the trajectory method used for a qualitative description of the primary aberration behavior and the differential algebraic method providing the quantitative description of electron optical properties. Instead of the aberration integrals the shape of the aberration coefficients is used for estimation of the effect of each electron optics element. The approach is used in the analysis of parasitic aberrations and optimization of the system with corrector. The last part shows the application on the systems whose symmetry was perturbed by the general 3D elements of the in-lens detector.

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## RECENT SUCCESSES OF MULTI-REFLECTION DEVICES AT RIKEN’S RIBF FACILITY AND SOME THOUGHTS ABOUT HIGHLY ACCURATE MASS CALIBRATION USING ION TRAPS

**M. Rosenbusch** (1), Y. Ito (2), P. Schury (3), M. Wada (3),  
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Energy Agency (JAEA), (3) KEK - Wako Nuclear Science  
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**Keywords:** Multi-Reflection Devices, Precision Mass  
Spectrometry, Mass Calibration, Nuclear Masses

By the use of coaxial ion mirrors, very long flight paths of ions to a time-of-flight detector were possible since the early 90’s, when multi-reflection time-of-flight mass spectrometry (MRTOF MS) was invented [1]. The development and usage of MRTOF mass spectrographs has been performed intensely at nuclear-physics on-line laboratories at later time and is still being continued. Due to the high precision of ion masses achieved in times  $<10$  ms, and the single-ion sensitivity achievable for TOF MS, this technique became attractive for high-precision mass determinations of rare and short-lived nuclei. Due to minute production rates and insufficient beam emittances provided by the existing facilities, the MRTOF technique has been developed in combination with ion-trapping techniques, i.e. quadrupole ion traps as accumulators, ion coolers, and injectors into the MRTOF device. At the super-heavy element (SHE)-mass facility of RIKEN-KEK [2] the exotic isotopes of  $^{249-253}\text{Md}$  [3], many other rare species like  $^{210-214}\text{Ac/Ra}$  [4] and about 70 other isotopes have successfully been mass determined with precisions down to several hundred ppb [5]. Reaching extremes for mass precisions, new considerations of the effect of ion traps on the mass calibration of an MRTOF mass spectrograph may become important and have been calculated. Here, the success of a MRTOF MS at RIKEN’s RIBF facility will be presented and later-on, some thoughts on mass calibrations for precisions beyond the so far achieved ones will be discussed. [1] H. Wollnik and M. Przewłoka, IJMS Ion Proc. 96, 267 (1990) [2] P. Schury et al., Nucl. Instr. Meth. B 335, 39 (2014) [3] Y. Ito et al., Phys. Rev. Lett. 120, 102501 (2018) [4] M. Rosenbusch et al., Phys. Rev. C 97, 064306 (2018) [5] S. Kimura et al., IJMS 430, 134 (2018)

## AN ALGORITHM FOR CHARACTERIZING THE GEOMETRIC OPTICS OF CHARGED PARTICLE INSTRUMENTS

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**Keywords:** nonlinear ordinary differential equation solver,  
ray-optical simulator

The proper design of charged particle instruments requires accurate simulations of the particle trajectories within the applied electromagnetic fields. Of interest, in particular, are the small deviations in the trajectories from the optical axis of the instrument. These deviations have linear and nonlinear dependencies on the initial conditions of the particles whose coefficients define the optical properties of the instrument. These coefficients can be computed directly, circumventing the need to simulate the individual trajectories. The traditional methods apply perturbation theory to the equation of motion to manually derive integral expressions for the primary nonlinear (aberration) coefficients. However, the manual procedure is difficult to extend for the computation of the higher order aberrations as the algebra becomes intractable. This difficulty has been overcome by the differential algebraic method, which uses a structure from nonstandard analysis to compute the series expansions of the electromagnetic forces about the optical axis in an automated manner. Here, an algorithm is presented that uses a standard mathematical technique, the binomial theorem, to codify this calculation. This algorithm gives the evolution of the coordinates along the optical axis as a series expansion in their initial values. The series coefficients can be derived up to any order in one of two ways, by either accumulating them serially along the optical axis via the solution to a difference equation or in parallel over the entire region of interest via an iterative solution of an integral equation. The algorithm is not limited to the equation of motion. It can be applied to higher order nonlinear, ordinary differential equations for the evolution of the dependent variables in the neighborhood of a principal path.

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## A HIGH RESOLUTION MULTI-TURN TOF MASS ANALYZER

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**Keywords:** Mass analyzer, TOF mass spectrometer, Ion optics,  
Aberrations

Ion optical design of a high resolution Multi-turn TOF Mass Analyzer (MT-TOF MA) is presented. The analyzer has rotational symmetry of the main electrodes, which allows higher density of turns in the azimuthal (drift) direction compared to MT-TOF MA's linearly extended in the drift direction. The analyzer geometry has mid-plane symmetry and comprises a pair of polar-toroidal sectors S1 (lower) and S3 (upper), a toroidal sector S2 located at the mid-plane of the system, a pair of polar (trans-axial) lenses, and a pair of conical lenses for longitudinal and lateral focusing, each pair of the electrodes being mirror symmetric with respect to the mid-plane. Additionally, drift focusing segments embedded into S2 electrodes are used to provide focusing and spatial isochronicity in the drift direction. Due to an open reference trajectory and static electric fields the analyzer retains the full mass range of the injected ions. Geometry and potentials of the analyzer electrodes are optimized for 5-8 keV ions to provide transverse focusing and isochronicity with some higher order corrections of TOF aberrations. Ion optical properties of the analyzer are described in detail. Several operational modes of the analyzer are feasible. At small turn numbers (up to  $\sim 10$ -12 turns) focusing in the drift direction is not required, and the turn number can be varied by simple injection steering. Maximum  $m/dm$  in this mode is  $\sim 50$ -60 k (fwhm). At larger turn numbers the drift focusing must be used. The ions' drift in the azimuthal direction can be reversed by using a pair of dedicated reversing deflectors. This gives possibility of multiple passes in the drift direction. It was demonstrated earlier that  $\sim 200$  k (fwhm) of mass resolving power is feasible after 2 passes in the drift direction (forward and reversed). Further optimization of the analyzer for 4 passes allowed us to increase  $m/dm$  up to  $\sim 400$ -500 k (fwhm). Respective numerical simulations are presented. Apart from TOF operational modes the analyzer can be optimized for the use as an electrostatic trap with Fast Fourier Transform (FFT) mass analysis.

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## FFT AND TOF OPERATIONAL MODES OF A HYBRID MASS ANALYZER

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**Keywords:** FFT mass spectrometry, Mass analyzer, Ion optics,  
Aberrations

It was demonstrated earlier that a rotationally symmetric mass analyzer can achieve mass resolving power of  $\sim 200$  k (fwhm) in a multi-turn TOF operational mode. The analyzer geometry has

mid-plane symmetry and comprises a toroidal sector S2 located at the mid-plane, a pair of polar-toroidal sectors S1 and S3, pairs of trans-axial and conical lenses for lateral and longitudinal focusing, each pair being mirror symmetric with respect to the mid-plane. In the multi-turn TOF operational mode drift focusing segments are used to provide focusing and spatial isochronicity in the drift direction. In this work we present results of simulation studies demonstrating that analyzers with similar geometries can be used as (i) a pure Fast Fourier Transform (FFT) mass analyzer with image charge detection providing  $m/dm$  of at least  $\sim 800$  k (fwhm), (ii) a pure multi-turn TOF mass analyzer with  $m/dm$  of at least  $\sim 200$  k (fwhm), and (iii) a hybrid instrument providing either  $m/dm \sim 100$  k (fwhm) in multi-turn TOF mode or  $m/dm \sim 800$  k (fwhm) in FFT mode. Analyzers of three different sizes (500 mm, 250 mm and 120 mm of external diameter of S2) have been studied numerically for ions at 5-8 keV energy. The largest analyzer is the best for the use in the multi-turn TOF mode. Its simulated  $m/dm$  for 400 Da ions at 5 keV is  $\sim 200$  k (fwhm) at typical flight times of about 1.1 ms. Large size makes the analyzer rather slow for running it in FFT mode. On the contrary, the smallest analyzer is the fastest of the three and the most appropriate for the use in the FFT mode. The 5th harmonic of the FFT signal provides  $m/dm$  of  $\sim 800$  k (fwhm) after 1 sec of measurement time. Its estimated  $m/dm$  in the multi-turn TOF mode is only  $\sim 15$ -20 k. Hybrid analyzer of the intermediate size (250 mm of S2 diameter) demonstrates  $m/dm \sim 100$ k (fwhm) in the multi-turn TOF mode or  $m/dm$  of  $\sim 800$  k (fwhm) at 2.1 s measurement time in the FFT mode. Similar instruments can be run in one of the two complimentary modes - the multi-turn TOF mode with lower  $m/dm$  and faster mass analysis, or the FFT mode with higher  $m/dm$  and slower mass analysis. Corporate software and SIMION program were used in the studies.

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## ROBUSTNESS CALCULATION OF MAGNETIC SECTORS USING DIFFERENTIAL ALGEBRAIC METHOD

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**Keywords:** SEM, magnetic sector, simulation

In electron microscopes, beam separators are important electron optical components used to separate the signal electrons. In particular, magnetic sectors have a long history of being used for low energy electron microscopes, and in recent years have also been considered for use in scanning electron microscopes (SEMs). To be able to use magnetic sectors, the aberrations introduced must be negligible compared to that introduced by other optical components [1]. Furthermore, the magnetic sectors must be robust enough so that they can be fabricated and operated under practical machining and current source precisions, respectively. Aberrations introduced by magnetic sectors can be calculated using the differential algebraic method to solve the electron beam trajectory as a function of its initial conditions, which are position, direction, and energy [2]. However, to assess their robustness the aberrations must be calculated for many cases, each with different pole piece shapes and excitation currents caused by the machining error and the current source noise. This becomes tedious and increasingly difficult as the number of pole pieces becomes

large. To make the assessment of robustness possible, we have developed a simulator that treats the angles of the grooves forming the pole pieces and the excitation currents of the pole pieces as parameters that are part of the initial condition. Therefore, in addition to the initial conditions of the beam, the aberrations can be calculated also as a function of the groove angles and the excitation currents. Using this simulator, we evaluated the robustness of a chicane-type magnetic sector [3], which only deflects the secondary beam, and found that this chicane-type magnetic sector can be useful for electron optical systems with straight optical axes such as SEMs. References: [1] Y. Shirasaki et al., EIPBN 2016 (2016). [2] M. Berz, Modern Map Methods in Particle Beam Physics. Academic Press (1999). [3] V. Kolarik et. al., "Close packed prism arrays for electron microscopy", Optik 87, 1 (1991).

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## PRISMATIC MASS SPECTROGRAPH WITH A CONICAL ACHROMATIC PRISM AND TRANSAXIAL LENSES

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**Keywords:** prismatic mass-spectrometer, transaxial lens

The conical achromatic prism (CAP) has a record angular dispersion equal to about 50 radians per 100% of mass variation [1]. In CAP, electric and magnetic fields are realized whose potentials in a spherical coordinate system depend only on angular variables. The particles of a homogeneous planar parallel ion beam move in the middle plane of the CAP along similar trajectories and maintain parallelism at the exit from the CAP. The CAP also focuses on energy, and the parallelism of the volume beam is maintained due to its telescoping in the vertical direction. CAP can be used in a prismatic mass spectrometer, which in its scheme is similar to a prism light-optical spectrometer equipped with a collimating and focusing lens. The linear dispersion of the prism spectrometer is equal to the angular dispersion of the CAP multiplied by the focal length of the focusing lens. A prismatic device is designed in which three-electrode transaxial lenses are used as a collimating and focusing lens. Due to the large mass dispersion by using a positional detector located in the focal plane of the focusing lens, a mass spectrograph can also be implemented in such a device. 1. Spivak-Lavrov I.F. Analytical Methods for The Calculation and Simulation of New Schemes of Static and Time-of-Flight Mass Spectrometers. - Advances in Imaging and Electron Physics. - Vol. 193, Burlington: Academic Press, 2016. - P. 45-128.

## DRIFT CONTROL IN ISOCHRONOUS MULTI-REFLECTION TOF ANALYZER WITH ELONGATED ION MIRRORS

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Alexander Makarov

Thermo Fisher Scientific

**Keywords:** mass spectrometry, aberration correction, ion mirror

Ion mirrors are employed to establish a many meters-long flight path in a table-size time-of-flight (ToF) mass spectrometer [1-3] to enhance the mass resolving power. This goal also requires isochronicity, i.e., independence of the travel time with respect to the ion's initial coordinates and velocities. The systems under consideration comprise a pair of ion mirrors facing each other in such a manner that the ions isochronously oscillate between them. To achieve spatial separation between the oscillations, the mirrors are elongated in the direction orthogonal to the line of oscillations. The ions are injected at an angle and slowly drift in the direction of elongation describing zigzag paths. An unavoidable spread of the drift velocities results, however, in the expansion of the ion bunch, and adjacent oscillations start overlapping after just a few reflections. To counteract the drift expansion, the ideal' isochronous 2D electrostatic field  $f_0(z,x)$  should be given a relatively small perturbation  $df(z,x,y)$  that varies in the drift coordinate 'y'. Some designs [3] incorporate an array of three-electrode lenses placed after each reflection, while in other solutions [4] the mirrors are sectioned to reverse the drift direction and refocus the ion bunch. It should be noticed, however, that the y-dependent field breaks the reflection isochronism so that the time of flight becomes a function of the ion's injection position  $y(0)$  and the injection angle  $dy/dz$ , which should be avoided. In this presentation, we develop a perturbation theory of drift control and its impact on the oscillation isochronism. It is shown that some classes of field perturbations generated by inter-mirror electrodes and slight non-parallelism of the ion mirrors counteract the drift expansion while the isochronicity is practically retained. As simulations have demonstrated, these results may be used to build ToF mass spectrometers with improved mass resolving power and throughput. [1] Nazarenko L.M., Sekunova L.M., Yaku-shev E.M., USSR Patent SU1725289 (1989) [2] Wollnik H. and Casares A., Int. J. Mass Spectrom. 227 (2) (2003): 217-22 [3] Yavor M., Verentchikov A., et al., Physics Procedia 1 (2008): 391-400 [4] Sudakov M. and Kumashiro S., Nucl. Instr. Meth Phys Res. A645 (2011): 210-5

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## STATISTICAL COULOMB INTERACTIONS IN MULTI-BEAM SEM

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Faculty of Applied Sciences, Delft University of  
Technology

**Keywords:** Multi-beam; Coulomb interactions; Trajectory displacement

Statistical Coulomb interactions in conventional scanning electron microscopy mostly affect the probe size via energy spread

and virtual source broadening in the emitter vicinity. However, in a multi-beam probe forming system such as multi-beam SEM, the trajectory displacement due to interactions in the whole column can give a major contribution to the final probe size. A theoretical description of trajectory displacement is only known for single-beam systems. It can be expressed using approximate analytical formulae for the total trajectory displacement in a beam segment (Jansen's theory) or by integrating contributions of infinitesimally thin beam slices (the slice method). We build on Jansen's theory of statistical Coulomb interactions and develop analytical formulae for the trajectory displacement in a multi-beam system. We also develop a more precise semi-analytical result using the slice method. We compare both approaches with a Monte-Carlo simulation and show a good agreement thereof. Finally, we discuss the implications of our results for the optical design of multi-beam SEM. In a multi-beam with probe size dominated by Coulomb interactions, an increase in the number of beamlets does not necessarily provide an increase of throughput, because the probe size is limited by the total current. Furthermore, we disprove the notion of "the fewer crossovers - the less coulomb interactions" by showing the quadratic dependence of trajectory displacement on segment length.

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## ACCURATE MEASUREMENT AND CORRECTION OF IMAGE DISTORTION IN TEM WITHOUT REFERENCE

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Science & Medical Systems Business Group, Hitachi  
High Technologies Corporation

**Keywords:** Image Distortion, Aberration, Electron Optics

As well known, transmission electron microscope (TEM) has the image distortion due to lens aberration, and it is not easy to remove. Image distortion lowers the accuracy of image scale and increases the error in computational image reconstruction such as Tomography, Single Particle Analysis, and Ptychography. One of the solutions to this problem is a distortion correction with a known information. However it is difficult to get an exact information of the distortion, because there are no suitable measurement references for high magnification in electron microscopes. To solve this problem, we developed a new method to quantitatively measure the image distortion without reference. This method uses multiple images which are taken in the different fields of view with some amount of overlap. Between each image, there are mainly two kinds of changes. One is a linear image shift which corresponds to the field of view movement and the other is a nonlinear image transformation which originates from the image distortion. From the nonlinear image transformations, differential component of distortion can be obtained, which is then used to calculate image distortion. From numerically generated test images, measurement error less than 0.1% was confirmed for radial distortion which is the main cause of barrel or pincushion distortion. Moreover, post-correction of the image distortion from the measured results and the applicability to experimental images were also confirmed to be possible. This method allows many kinds of typical specimen to be used for dis-

tortion measurement, and the result can be used for both optical system evaluation and real-time or post distortion correction.

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## MUON LOSSES FROM BETATRON RESONANCES AT THE MUON G-2 EXPERIMENT AT FERMILAB

David Tarazona, Martin Berz, Kyoko Makino

Michigan State University

**Keywords:** betatron resonance muon losses

The Muon g-2 Experiment (g-2) at Fermilab is directed toward measuring the muon anomalous magnetic moment with statistical and systematic relative errors smaller than 140ppm. This new measurement will serve as strong indication of yet undiscovered particles beyond the Standard Model and validate or disprove other theoretical models beyond the SM. Of special interest is the reduction of muon losses to achieve the precision needed at the g-2 Experiment. For this purpose, we have developed a detailed and precise g-2 Storage Ring using COSY INFINITY that consider inhomogeneities of the magnetic field, up to the electric 20-pole multipole of the Electrostatic Quadrupoles (ESQ), and injection to the ring based on measurements. In specific, we have recreated lost muons rates for several possible configurations of the ESQ system in order to find the best possible scenarios that minimize muon losses. Additionally, comparison with measurements have allowed to identify possible sources of error due to both the beam dynamics and imperfections in the g-2 storage ring.

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## OPTICAL DESIGN OF THE FIXED FIELD PERMANENT MAGNET GANTRY FOR THE PROTON CANCER THERAPY

D. Trbojevic 1, William Lou 2, Stephen Brooks 1, Francois Meot 1, and Nicholaos Tsoupas 1

1. Brookhaven National Laboratory 2. Cornell University

**Keywords:** Fixed Field magnets, large momentum acceptance, hadron cancer therapy, proton gantry

We present an optical design of the proton therapy gantry with a very large momentum acceptance of  $dp/p = \pm 33\%$ . This momentum range corresponds to the kinetic energy of protons within a range of 65-250 MeV - energies required for the patient proton radiation therapy moving the Bragg peak between 3.5-38 cm. The optics uses combined function magnets with a fixed linear magnetic field. The permanent magnets of the Halbach type, are made of Neodymium Iron Boron - NeFeB. Additional important optics properties is that the gantry is made of chromatically matched parts. The first achromatic part bends protons upwards. The central momentum particles travel in a perfect circle while the rest of them radially oscillate with orbit offsets of +14 -10 mm; positive offsets correspond to the higher while the lower energies, accordingly. The same magnets from the half of the first gantry part continue symmetrically upward but with opposite bending direction. The last part of the gantry brings focused proton beams to the patient. The last gantry magnet is

more than 1.2 meters away from the patient. Two radially scanning magnets are placed within this space to allow  $\pm 10$  cm in the horizontal plane at the patient. There are multiple advantages of this optical design: the large momentum acceptance allows fast energy change without magnetic field variation. The only variable magnetic field comes from the scanning magnets at the end of the gantry. The transverse scanning is significantly slower as the longitudinal energy scanning occurs for each radial position. The patient treatment time is shorter and the operation is simplified due to the fixed magnetic field. There is a significant reduction of power consumption as well as with the overall gantry cost; it is one order of magnitude reduced with respect to the other existing gantries. The weight and size of the magnets is significantly reduced allowing lighter rotating structures.

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## THE ERHIC SPIN ROTATOR AND THE BEAM OPTICS OF THE 400 MEV TRANSFER LINE TO RCS

N. Tsoupas\*, M. Blaskiewicz, H. Lovelace III, F. Méot, C. Montag, V. Pitsyn, V. Ranjbar, S. Tepikian, W. Zhang, G.M. Wang, E. Wang, W. Weng, F. Willeke

Brookhaven National Laboratory

**Keywords:** Spin Rotator

The 400 MeV LINAC [1] is the first acceleration stage of the electron accelerator of the proposed eRHIC collider [1]. The second acceleration stage of the electron bunches is the Rapid Cycled Synchrotron (RCS) which can increase the energy of the electron bunches up to 18 GeV. The function of the transfer line between the LINAC and the RCS (LtRCS) is twofold, first to transfer the electron beam from the exit of the 400 MeV LINAC to the injection point of the Rapid-Cycled-Synchrotron (RCS) [1] and second to rotate the electron spin from the longitudinal direction to the vertical. We will describe the beam optics of the transfer line, and the required constraints on the beam line for the proper beam matching of the 400 MeV LINAC and the RCS and the spin rotation. A section will also be devoted to discuss the spin rotator. \* tsoupas@bnl.gov [1] PCDR of eRHIC Brookhaven National Laboratory

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## DEVELOPMENT OF A DIAGNOSTIC SETUP FOR QUANTUM ELECTRON MICROSCOPY

M. Turchetti, N. Abedzadeh, A. Agarwal and K. K. Berggren

Massachusetts Institute of Technology

**Keywords:** quantum electron microscopy, aberration, ptychography, shadow imaging, ronchigrams

Quantum electron microscopy is one of the most promising approaches that could overcome the resolution limit imposed by the radiation damage especially to biological samples. This microscopy scheme requires the design of novel components such as gated electron mirrors, and the development of a platform for diagnostics of ultra-fast electron optics. This testbed would allow

time-resolved characterization of such elements either isolated or integrated into the system, both in transmission and in reflection modes. In this work, we propose a diagnostic setup comprised of a ptychography and shadow-imaging (Ronchigrams) platform to allow the evaluation of wavefront aberrations in transmission, and a procedure for beam characterization in reflection, which employs an electron mirror with tuneable spherical aberration.

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## ANALYTIC ABERRATION FORMULAS AND TRANSFER MAPS OF ELECTROSTATIC DEFLECTORS

Eremey Valetov and Martin Berz

Michigan State University

**Keywords:** electrostatic deflectors, transfer maps, aberrations, differential algebra

Using an iterative perturbation method, we derived first and second order analytic aberration formulas for the electrostatic deflector, specified by the curvature radius, central angle, and inhomogeneity coefficients. We compared the results with those of numerical differential-algebraic (DA) integration of the ODEs of motion using COSY INFINITY. Additionally, we directly calculated the transfer map of the electrostatic spherical and cylindrical deflectors in the laboratory coordinate system using a Runge-Kutta integrator. For the electrostatic spherical deflector, we also calculated the transfer map analytically and in closed form using the properties of the respective elliptical orbits from Kepler theory. We compared the results with the DA transfer map of COSY INFINITY's built-in electrostatic and spherical deflector elements, as well as with the program GIOS.

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## TRANSVERSE PHASE SPACE TOMOGRAPHY IN BEAMLINES

Adam Watts, Carol Johnstone

Fermilab

**Keywords:** optics, tomography, transverse, phase space

Methods of reconstructing beam transverse phase space using computed tomography are compared and optimized in simulation to improve reconstruction accuracy. Errors and artifacts are shown for both Filtered Back Projection (FPB) and Simultaneous Algebraic Reconstruction Technique (SART) methods as a function of their respective free parameters. Finally, a theoretical discussion of common optics configurations and their effect on the feasibility of computed tomography is shared, and advice is given on choosing optimal sections of rings or beamlines to perform such reconstructions.

## A TRANSVERSE ENVELOPE MACROPARTICLE METHOD FOR MODELING HIGH-GAIN FREE ELECTRON LASERS

Stephen D Webb

RadiaSoft, LLC

**Keywords:** free-electron lasers, reduced models

Recirculating schemes for free-electron lasers, such as the regenerative amplifier FEL, require simulating thousands of passes through a high-gain FEL system. Modeling high-gain FELs accurately requires the inclusion of diffractive effects in the radiation field and transverse motion of the electron beam. Consequently, most simulation codes that study high-gain FELs are three-dimensional self-consistent codes. Using these codes in the aforementioned multi-pass system would be too computationally expensive to produce results in a reasonable amount of time. However, because the transverse dynamics for the electron bunch is largely comprised of linear motion through drifts and quadrupoles, it can be represented by carefully constructed reduced models. Here we present the use of macroparticles with a transverse gaussian envelope to map the three-dimensional problem to a quasi-one-dimensional problem, reducing the computational cost of simulating the high gain FEL. We present the derivation of the algorithm and preliminary benchmarking simulations against GENESIS for both accuracy and computational efficiency.

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## COMPUTATION AND CONSEQUENCES OF HIGH-ORDER AMPLITUDE AND MOMENTUM DEPENDENT TUNE SHIFTS IN THE MUON G-2 RING

Adrian Weisskopf, David Tarazona, Martin Berz

Michigan State University

**Keywords:** Betatron tune shifts, muon g-2 ring, normal form, high-order transfer maps

Betatron tune shifts can influence the coherent betatron oscillation (CBO) frequency of a mismatched beam in an accelerator, in particular the muon beam in the storage ring of the Muon g-2 Experiment at Fermilab (E989). In this case, nonlinear electric fields from the electrostatic quadrupole system (EQS) installed within the storage ring to confine muons vertically and other nonlinearities due to slight errors in the uniformity of the magnetic field produce substantial amplitude-dependent tune shifts. In addition to this, the storage ring momentum acceptance of  $\pm 0.5$  allows for momentum-dependent tune shifts. Motivated by these aspects and by the sensitivity of the final measurement precision at E989 to the CBO frequency, we present a normal-form based method for the calculation of high order energy/momentum as well as amplitude dependencies of horizontal and vertical tune in the storage ring of E989 using the differential algebra framework within COSY Infinity. First, the energy/momentum dependent reference orbit is calculated, which corresponds to the parameter dependent fixed point of the map representing the detailed simulations of the g-2 storage ring. Secondly, the fixed-point map is transformed into normal form coordinates to extract the

high-order tune dependencies. Analytical estimations of those calculations are presented to benchmark the simulation results.

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## MASSIVELY PARALLEL CHARGED PARTICLE OPTICS ENABLED BY MEMS FABRICATION TECHNIQUES

**Marco Wieland**

Mapper Lithography

### *Invited Talk*

**Keywords:** maskless lithography, charged particle optics, MEMS, massively parallel

Mapper Lithography has developed a maskless lithography system, based on massively parallel electron-beam writing with high-speed optical data transport for switching the electron beams. The system, containing 65,000 parallel electron beams, has a 1 wph throughput at 300 mm wafers and is capable of patterning any resolution and any different type of structure all the way down to 28 nm node patterns. The large number of beams is realized by fabricating the electron optics using MEMS fabrication techniques such as lithography and deep dry etching. In this presentation we will discuss the various building blocks enabled by the MEMS fabrication techniques such as lens arrays, aperture arrays, deflector arrays, individually controllable deflectors and beam blanker arrays. Also we will describe how these building blocks are combined to make a massively parallel electron-beam lithography tool.

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## TIME-OF-FLIGHT MASS SPECTROGRAPHS AND THE PRECISE DETERMINATION OF MASSES OF IONS

**H. Wollnik**, M. Wada, P. Schury, M. Rosenbusch, Y. Ito, S. Kimura, H. Miyatake, S. Ishizawa

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5 Institut of Physics, University of Tsukuba, Ibaraki 305-8571, Japan

### *Invited Talk*

**Keywords:** Time-of-flight mass spectrographs, very precise mass determinations, masses of short-lived nuclei

The masses of charged atoms and molecules were first investigated by laterally dispersive sector field mass analyzers, which early on already achieved mass resolving powers  $m/\Delta m \approx 100\,000$  and more. Equally high mass resolving powers were achieved by time-of-flight mass analyzers during the last decades. These measurements became possible when fast and precise electronic circuitries became available. Such techniques have been developed and used extensively for the mass analysis

of short-lived nuclei, which mass values reveal insight in processes that describe the formation of elements in star explosions. Precise mass determinations of short-lived ions have been performed for energetic ions in large accelerator storage rings as well as for low energy ions in time-of-flight mass spectrographs with long flight paths. Similarly precise mass measurements can also be performed for molecular ions that help to reveal the structure of molecules. In case of very high mass resolving powers the mass determination of molecular ions can be so high that the measured ion mass directly reveals the molecule's sum formula.

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## OPTIMIZE THE DESIGN OF CHICANES FOR EEHG SCHEME

**Kaishang Zhou**

Shanghai Institute of Applied Physics

**Keywords:** CSR EEHG fully coherent

The echo-enabled harmonic generation (EEHG) scheme in free electron lasers is one of the most promise ways to generate the fully coherent soft x-rays. However, the increased energy spread of the electron beam causing by the coherent synchrotron radiation (CSR) effect may smear the fine structure introduced by the external seeded lasers. Here, we optimize the design of the chicanes to reduce the increased energy spread causing by CSR effect.

# ICAP'2018 ABSTRACTS

## ZGOUBI: RECENT DEVELOPMENTS AND FUTURE PLANS

**Dan T. Abell** (1), Rob Nagler (1), Francois Meot (2), Damian Rouson (3), and Izaak Beekman (4)

1. RadiaSoft, LLC, Boulder, CO; 2. Brookhaven National Lab, Upton, NY; 3. Sourcery Institute, Oakland, CA; 4. ParaTools, Inc., Eugene, OR

**Classification:** F-1, D-1, D-2

The particle tracking code Zgoubi [1,2] has been used for a broad array of accelerator design studies, including FFAGs [3] and EICs [4,5]. Zgoubi is currently being used to evaluate proposed designs for both JLEIC [6,7] and eRHIC [8,9], and to prepare for commissioning the CBETA BNL-Cornell FFAG return loop ERL [10,11,12]. Moreover, Zgoubi is now the subject of a Phase II SBIR aimed at improving its speed, flexibility, and ease-of-use. In this paper, we describe our on-going work\* on several fronts: (i) parallelizing Zgoubi using new features of Fortran 2018, including coarrays [13,14]; (ii) implementing a new particle update algorithm that requires significantly less memory and arithmetic; and (iii) developing symplectic tracking for field maps. In addition, we describe plans for a web-based graphical interface to Zgoubi. References 1. <https://sourceforge.net/projects/zgoubi/> 2. F. Meot, FERMILAB-TM-2010, 1997 3. F. Lemuet et al., NIM-A, 547:638, 2005 4. F. Meot et al., eRHIC/45, 2015 5. F. Lin et al., IPAC17, WEPIK114, 2017 6. J. Martinez-Marin et al., IPAC18, MOPMF004, 2018 7. A. M. Kondratenko et al., IPAC18, MOPML007, 2018 8. F. Meot et al., IPAC18, MOPMF013, 2018 9. V. H. Ranjbar et al., IPAC18, MOPMF016, 2018 10. G. Hoffstaetter et al., IPAC18, TUYGBE2, 2018 11. F. Meot et al., NIM-A 896:60, 2018 12. F. Meot et al., Full Field-Map Modeling of CBETA 4-Pass ERL, these proceedings 13. J. Reid, ISO/IEC JTC1/SC22/WG5 N2145, 2018 14. <http://www.opencoarrays.org/> \*This work was supported in part by the US Department of Energy, Office of Science, Office of Nuclear Physics under Award No. DE-SC0017181.

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## RECENT DEVELOPMENTS OF THE OPEN SOURCE CODE OPAL

**Andreas Adelman** for the OPAL developer team

PSI

**Invited Talk**

**Classification:** F-1

After a general introduction of OPAL, I will introduce a set of new features available with version 2.0 released in July 2018. All new features will be presented together with examples of ongoing research projects. In the OPAL-t flavour, elements can now be placed in 3D, without restriction. Overlapping fringe fields are handled, and off-momentum beams as occurring in tolerance

studies can be tracked. Furthermore, survey plots of placed elements are a valuable diagnostic when dealing with complex designs. A new element, a flexibly configurable collimator, will be presented. In the OPAL-cyc flavour, a robust way of generating matched distributions with linear space charge is introduced. A new method for describing fixed field accelerators (FFAs) in a very general way will be shown. A new element TRIMCOIL can be used to correct for field-errors in cyclotrons and FFAs. The OPAL language (a derivative of the MAD language) was extended to allow the specification of multi objective optimisation problems, which are then solved with a built in NGSA-II genetic algorithm. A new feature SAMPLER allows you to setup and run random or sequential parameter studies and seamless utilisation of a vast number of computing cores. Finally, a set of Python tools (pyOPALTools) was created for post processing. The manual is now available on the OPAL-wiki as well as in pdf format.

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## SNS BEAM TEST FACILITY FOR EXPERIMENTAL BENCHMARKING OF HIGH INTENSITY BEAM DYNAMICS COMPUTER SIMULATION

**A. Aleksandrov**, S. Cousineau, B. Cathey, A. Zhukov, Z. Zhang

ORNL, University of Tennessee

**Classification:** F-1, D-1

The SNS Beam Test Facility (BTF) is a 2.5 MeV hadron accelerator equipped with state-of-the-art transverse and longitudinal beam diagnostics. The BTF can produce pulsed high intensity H- beam with up to 50mA peak current. The expected available beam-on time of a few thousand hours per year provides an opportunity for carrying out advanced high intensity beam dynamics experiments. The first ever direct measurement of 6D phase space distribution of a beam in an accelerator has recently been completed. Preliminary analysis of the data shows a complex phase space structure that is not visible in measurements below 5D, including correlations between degrees of freedom not customarily measured together. This result opens path forward to solving the long-standing problem of initial condition in hadron linac beam dynamics simulation. An extension of the BTF beam line consisting of a FODO line and high dynamic range emittance monitor is being built to provide a test bench for simulation codes benchmarking against measurements in well controlled environment. This paper describes these efforts along with the longer-term plans.

## QUANTUM STATISTICAL PROPERTIES OF FREE ELECTRON LASER WITH A PLANAR WIGGLER AND ION-CHANNEL GUIDING

Masoud Alimohamadi

Farhangian University

*Classification:* B-1

An analysis of the free-electron lasers (FELs) with a planar wiggler and in the presence of ion-channel guiding, has been carried out using a Hamiltonian quantum field theory. The quantum Hamiltonian of single a particle has been derived in the Bambini-Renieri (BR) frame [1-5]. The equations are valid in a reference frame, moving with a relativistic velocity with respect to the laboratory frame, chosen in such a way that the carrier frequency of the pulse equals the pseudoradiation (wiggler) field frequency. In this reference frame, the equations assume a simple non-relativistic form. Time-dependent wave function and three constants of motion are obtained. The Wei-Norman [2] Lie algebraic approach has been employed to solve exactly the spherical Raman-Nath equation (SRNE) [3-5]. A quantum approach has been used to get photon gain, photon statistics and squeezing properties of a FEL. The quantum statistical properties have also been studied numerically. [1] H. Mehdian, M. Alimohamadi and A. Hasanbeigi, Journal of Plasma Physics 78 (5), 537-544(2012). [2] J. Wei, E. Norman, J. Math. Phys. A 4, 575 (1963). [3] M. Alimohamadi, H. Mehdian and A. Hasanbeigi, Journal of fusion energy 31 (5), 463-466(2012). [4] A. Bambini and A. Renieri. Lett. Nuovo Cimento 21, 399 (1978). [5] F. Ciocci, G. Dattoli, A. Renieri and A. Torre, Physics Reports, 141(1), 1-50(1986).

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## OPTIMIZATION OF HEAVY-ION SYNCHROTRONS USING EVOLUTIONARY ALGORITHMS AND MACHINE LEARNING

S. Appel, W. Geithner, S. Reimann, D. Vilsmeier, M. Sapinski, R. Singh

GSI

*Invited Talk*

*Classification:* E-2

The application of machine learning and nature-inspired optimization methods, like for example genetic algorithms (GA) and particle swarm optimization (PSO) can be found in various scientific-technical areas. In accelerator physics these approaches have not yet found a wide application. Still, in the last years those approaches have been applied to a greater extent. In this presentation, nature-inspired optimization as well as the machine learning will be shortly introduced and their application to the accelerator facility at GSI/FAIR presented. For the heavy-ion synchrotron SIS18 at GSI the multi-objective GA/PSO optimization resulted in a significant improvement of multi-turn injection performance and for the subsequent transmission for intense beams. A range of suitable injector brilliances for given initial loss could be defined. This information is crucial for the layout of the injector upgrade for FAIR. The effect of transverse space charge force on MTI has been included in the optimization studies. An automated beam-setting optimization with ge-

netic algorithms at the CRYRING@ESR ion storage ring has been performed. First results and the experience gained will be presented. The application of machine learning for the reconstructing of space-charge distorted beam profiles from ionisation profile monitors (IGMs) will be shown.

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## SELF-CONSISTENT SIMULATIONS OF SHORT- AND LONG-RANGE WAKEFIELD EFFECTS IN STORAGE RINGS

Gabriele Bassi

Brookhaven National Laboratory

*Invited Talk*

*Classification:* F-1

We discuss the parallel tracking code SPACE, which is capable to simulate simultaneously the effect of short- and long range wakefields on the dynamics of multi-bunch configurations in storage rings. As an example of such a simulation, we present a study, performed at the NSLS-II storage ring, of the influence of bunch lengthening and the microwave instability induced by short-range wakefields, on the performance of a passive higher order harmonic cavity for operation with multi-bunch configurations in hybrid modes.

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## SPIN DYNAMICS IN MODERN ELECTRON STORAGE RINGS: COMPUTATIONAL ASPECTS

Oleksii Beznosov, Daniel Appelo, Desmond Barber, James Ellison, Klaus Heinemann

University of New Mexico, University of Colorado Boulder, DESY, University of New Mexico, University of New Mexico

*Classification:* A-2, F-1, F-2, D-2

In this talk we present some numerical results from our work on the spin polarization in high energy electron storage rings. The motivation of our work is to understand spin polarization in very high energy rings like the proposed Future Circular Collider (FCC-ee)[1] and Circular Electron Positron Collider (CEPC) [2]. This talk is a supplement to K. Heinemann's talk and gives further numerical details and results. As discussed in Heinemann's talk our work is based on the initial value problem of the full Bloch equations (FBEs)[3] which in turn determines the polarization vector of the bunch. The FBEs take into account spin diffusion effects and spin-flip effects due to synchrotron radiation. The FBEs are a system of three uncoupled Fokker-Planck equations plus coupling terms. Neglecting the spin flip terms in the FBEs one gets the reduced Bloch equations (RBEs) which poses the main computational challenge. Our numerical approach has three parts. Firstly we approximate the FBEs analytically using the method of averaging, resulting in FBEs which allow us to use large time steps (without the averaging the time dependent coefficients of the FBEs would necessitate small time steps). The minimum length of the time interval of interest is of the order of the orbital damping time. Secondly we discretize the averaged

FBEs in the phase space variables by applying the pseudospectral method, resulting in a system of linear first-order ODEs in time. The phase space variables come in  $d$  pairs of polar coordinates where  $d = 1, 2, 3$  is the number of degrees of freedom allowing for a  $d$ -dimensional Fourier expansion. The pseudospectral method is applied by using a Chebychev grid for each radial variable and a uniform Fourier grid for each angle variable. Thirdly we discretize the ODE system by a time stepping scheme. The presence of parabolic terms in the FBEs necessitates implicit time stepping and thus solutions of linear systems of equations. Dealing with  $2d + 1$  independent variables poses a computational challenge due to the extreme size of the ODE system if the Fourier modes are coupled extensively. However, thanks to having used averaged FBEs, the Fourier modes are uncoupled in the Fokker-Planck terms. Hence the parabolic terms are separated from the mode coupling terms. We take advantage of this separation by using an implicit/explicit time stepping scheme so that we end up with a large system of only locally coupled ODEs. Since the Fourier mode couplings are local, a parallel implementation with only local communication is possible. Numerical experiments demonstrating efficiency and accuracy of the algorithm will be presented. References 1. FCC-ee webpage <http://tlep.web.cern.ch> 2. CEPC webpage <http://cepc.ihep.ac.cn> 3. Ya.S.Derbenev, A.M. Kondratenko, "Relaxation and exilibrum state of electrons in storage rings", Sov. Phys. Dokl. 19, p.438 (1975); K.A. Heinemann, O. Beznosov, J.A. Ellison, D. Appelö, D.P. Barber, "A Pseudospectral Method for Solving the Bloch Equations of the Polarization Density in e- Storage Rings", <http://ipac2018.vrws.de/papers/thpak144.pdf>

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## EXPLORING THE VALIDITY OF THE PARAXIAL APPROXIMATION FOR COHERENT SYNCHROTRON RADIATION WAKE FIELDS

David Bizzozero, Erion Gjonaj, Herbert De Gerssem  
TU Darmstadt

*Classification:* C-2, F-1

Coherent synchrotron radiation (CSR) is an essential consideration in modern accelerators, yet is often computationally difficult to accurately model. A common approach used in simulating CSR effects uses the paraxial, or slowly-varying envelope approximation with a simple constant cross-section approximation of the geometry. While these approximations are often valid for the simulation of many accelerator components, we aim to more closely analyze the errors introduced by such approximations by comparing them with wake field solutions obtained by full-wave electromagnetic field simulations. The simulations are performed with CSR DG (Coherent Synchrotron Radiation with Discontinuous Galerkin), our GPU-enabled MATLAB code. Presented in earlier work [Coherent Synchrotron Radiation and Wake Fields With Discontinuous Galerkin Time Domain Methods, Proceedings of IPAC 2017, Copenhagen, Denmark], CSR DG evolves Maxwell's equations the time domain using a curvilinear coordinate transformation and a Fourier series decomposition in a transverse direction.

## BEAM STABILITY ESTIMATES AND SIMULATION STUDIES FOR THE FUTURE CIRCULAR COLLIDER (FCC-HH)

Oliver Boine-Frankenheim, Daria Astapovych, Uwe Niedermayer, Sergey Arsenyev, Daniel Schulte

GSI, TU Darmstadt, CERN

*Classification:* A-2

Beam instabilities caused by impedances and electron clouds potentially limit the intensity and luminosity in the proposed Future Circular Collider (FCC-hh). Scaling of the observed instability thresholds from the LHC to the FCC using simulation tools is also one goal of the studies. Compared to the LHC the inner FCC beam screen radius is smaller and has two openings for the synchrotron radiation. The complex beam pipe is the dominant contribution for beam instabilities. Using an impedance solver in the frequency domain the pipe impedance is obtained and instability growth rates are estimated. Besides the foreseen broad-band damper system, the resistive wall induced transverse instabilities should be stabilized by conventional and eventually also advanced Landau damping concepts, which are studied using particle tracking. Electron cloud buildup should be mitigated in the FCC by either carbon or laser coating of the screen. Simulations of electron cloud buildup including realistic secondary emission yield (SEY) data and the detailed screen design are performed and the resulting heat load and tune spreads are analyzed.

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## BEAM DYNAMICS SIMULATIONS AND CHALLENGES FOR THE FAIR SIS100 SYNCHROTRON

Oliver Boine-Frankenheim, Vera Chetvertkova, Vladimir Kornilov, Stefan Sorge, Yuan Yaoshuo

GSI, TU Darmstadt

*Classification:* D-1

The SIS100 synchrotron is the central accelerator of the upcoming FAIR project at GSI, Darmstadt, Germany. The major challenges for the design studies and the later operation are related to high-intensity, low beam loss operation for a wide range of ion species and charge states, for different operational cycles and extraction schemes. We focus our simulation studies on the long (up to 1 s) accumulation plateau and on the final bunch compression before extraction. During accumulation emittance growth and beam loss due to transverse space charge in combination with the magnet field errors has to be well controlled. We use different simulation approaches with frozen and self-consistent "symplectic" space charge solvers to identify optimum working point areas, including realistic field error models for the superconducting, superferric SIS100 dipole and quadrupole magnets.

## POLARIZED PROTON BEAMS FROM LASER-INDUCED PLASMAS

Markus Buescher, Anna Huetzen, Andreas Lehrach,  
Johannes Thomas

Forschungszentrum Juelich, Heinrich-Heine University  
Duesseldorf

*Classification:* B-2, D-1, D-2, F-1

Laser-driven particle acceleration has undergone impressive progress in recent years. Nevertheless, one unexplored issue is how the particle spins are influenced by the huge magnetic fields inherently present in the plasmas. In the framework of the JuSPARC (Juelich Short-Pulse Particle and Radiation Center) facility and of the ATHENA consortium, the laser-driven generation of polarized particle beams in combination with the development of advanced target technologies is being pursued. In order to predict the degree of beam polarization from a laser-driven plasma accelerator, particle-in-cell simulations including spin effects have been carried out for the first time. For this purpose, the Thomas-BMT equation, describing the spin precession in electromagnetic fields, has been implemented into the VLPL (Virtual Laser Plasma Lab) code. A crucial result of our simulations is that a target containing pre-polarized hydrogen nuclei is needed for producing highly polarized relativistic proton beams. For the experimental realization, a polarized HCl gas-jet target is under construction the Forschungszentrum Juelich where the degree of hydrogen polarization is measured with a Lamb-shift polarimeter. The final experiments, aiming at the first observation of a polarized particle beam from laser-generated plasmas, will be carried out at the 10 PW laser system SULF at SIOM/Shanghai.

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## SPARSE GRIDS PARTICLE IN CELL SCHEME FOR NOISE REDUCTION IN BEAM SIMULATIONS

Antoine Cerfon

Courant Institute of Mathematical Sciences, New York  
University

*Invited Talk*

*Classification:* D-1, D-2, A-2

Kinetic simulations of intense charged particle beams are subject to the curse of dimensionality: the run-time complexity of standard solvers grows exponentially with the number of dimensions of the underlying equations. This issue is particularly acute for continuum solvers, which need to discretize the six-dimensional phase-space distribution function, and whose run times are consequently large even for a moderate number of grid points for each dimension. Particle-in-Cell (PIC) schemes are a popular alternate approach to continuum methods, because they only discretize the three-dimensional physical space and are therefore less subject to the curse of dimensionality. Even if so, PIC solvers still have large run times, because of the statistical error which is inherent to particle methods and which decays slowly with the number of particles per cell. In this talk, we will present a new scheme to address the curse of dimensionality and at the same time reduce the numerical noise of PIC simulations. Our

PIC scheme is inspired by the sparse grids combination technique, a method invented to reduce grid based error when solving high dimensional partial differential equations [1]. The technique, when applied to the PIC method, has two benefits: 1) it almost eliminates the dependence of the grid based error on dimensionality, just like in a standard sparse grids application; 2) it lowers the statistical error significantly, because the sparse grids have larger cells, and thus a larger number of particles per cell for a given total number of particles. We will analyze the performance of our scheme for standard test problems in beam physics. We will demonstrate remarkable speed up for a certain class of problems, and less impressive performance for others. The latter will allow us to identify the limitations of our scheme and explore ideas to address them. [1] Griebel M, Schneider M and Zenger C 1990 A combination technique for the solution of sparse grid problems *Iterative Methods in Linear Algebra* ed R Bequwens and P de Groen (Amsterdam: Elsevier) pp 263-81

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## HIGH FIDELITY THREE-DIMENSIONAL SIMULATIONS OF THERMIONIC ENERGY CONVERTERS

Nathan Cook, Jon Edelen, Chris Hall, Mike Keilman,  
Paul Moeller, Rob Nagler

RadiaSoft LLC

*Classification:* E-1

Thermionic energy converters (TEC) are a class of thermoelectric devices, which promise improvements to the efficiency and cost of both small- and large-scale electricity generation. A TEC is comprised of a narrowly-separated thermionic emitter and an anode. Simple structures are often space-charge limited as operating temperatures produce currents exceeding the Child-Langmuir limit. We present results from 3D simulations of these devices using the particle-in-cell code Warp, developed at Lawrence Berkeley National Lab. We demonstrate improvements to the Warp code permitting high fidelity simulations of complex device geometries. These improvements include modeling of non-conformal geometries using mesh refinement and cut-cells with a dielectric solver. We also consider self-consistent effects to model Schottky emission near the space-charge limit for arrays of shaped emitters. The efficiency of these devices is computed by modeling distinct loss channels, including kinetic losses, radiative losses, and dielectric charging. We demonstrate many of these features within an open-source, browser-based interface for running 3D electrostatic simulations with Warp, including design and analysis tools, as well as streamlined submission to HPC centers.

## UNCERTAINTY QUANTIFICATION FOR THE FUNDAMENTAL MODE SPECTRUM OF THE EUROPEAN XFEL CAVITIES

Niklas Georg (1), Jacopo Corno (2), **Herbert De Gersem** (3), Shahnam Gorgi Zadeh (4), Ulrich Römer (1), Sebastian Schöps (2), Alexey Sulimov (5), Ursula van Rienen (4)

(1) Institute of Dynamics and Vibrations, TU Braunschweig; (2) Centre for Computational Engineering, TU Darmstadt; (3) TEMF, TU Darmstadt; (4) Theoretical Electrical Engineering, Universität Rostock; (5) DESY

*Classification:* E-2, C-2

The fundamental mode spectrum of superconducting cavities is sensitive to small geometry deformations introduced by the manufacturing process. In this work we consider variations in the equatorial and iris radii of the 1.3 GHz TESLA cavities used at the European XFEL. The cavities with slightly perturbed geometry are simulated using a finite element based eigenvalue solver. Employing uncertainty quantification methods such as sparse-grids, statistical information about the fundamental mode spectrum can be efficiently calculated. Moreover, using global sensitivity analysis, in particular Sobol indices, the impact of the individual geometry parameters on the quantities of interest, i.e. resonance frequencies, field-flatness and the cell-to-cell coupling coefficient, can be computed. We will explain important aspects of the uncertainty quantification methodology and give numerical results for illustration.

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## HIGH-PRECISION LOSSY EIGENFIELD ANALYSIS BASED ON THE FINITE ELEMENT METHOD

Wolfgang Ackermann, Vinh Pham-Xuan, **Herbert De Gersem**

TEMF, TU Darmstadt, Germany

*Classification:* C-2

A proper eigenanalysis of resonating particle accelerator components is particularly advantageous to characterize structures with high quality factors. While in former times eigenmode calculations have been concentrating on the lossless cases only, meanwhile also lossy structures with finite-conductive materials or with absorbing boundary conditions like PML or ports even with low quality factors are routinely available. In the lossless case where no damping is present, all eigenvalues are located along the real axis. If damping has to be modeled instead, the corresponding eigenvalues are distributed within the first quadrant of the complex plane that renders their determination much more expensive. One of the critical issues is that no resonance should be missed so that all desired eigenvalues in a given region of the complex plane can be precisely determined. We implemented two different eigenvalue solvers based on a distributed-memory architecture. While the first one is a classical Jacobi-Davidson eigenvalue solver which has been adopted to be used also within a complex-arithmetic environment, the second

one is based on the contour-integral method which enables to determine all eigenvalues within a given closed contour in the complex plane. Both solvers are attached to a FEM processor with second-order edge elements on curved tetrahedra and can be used together in order to improve the computational efficiency. In the presentation a selection of successful real-world applications of the implemented parallel eigenvalue solvers will be given.

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## SIXTRACK PROJECT: STATUS, RUNNING ENVIRONMENT AND NEW DEVELOPMENTS

**R. De Maria**, J. Andersson, V.K. Berglyd Olsen, L. Field, M. Giovannozzi, P.D. Hermes, N. Høimyr, S. Kostoglou, G. Iadarola, E.H. Maclean, E. McIntosh, A. Mereghetti, J. Molson, D. Pellegrini, T. Persson, M. Schwinzerl, K. Sjobak, I. Zacharov, S. Singh

CERN, Geneva, Switzerland; EPFL, Lausanne, Switzerland; IIT Madras, India

*Classification:* D-1

SixTrack is a single-particle tracking code for high-energy circular accelerators routinely used at CERN for the Large Hadron Collider (LHC), its luminosity upgrade (HL-LHC), the Future Circular Collider (FCC), and the Super Proton Synchrotron (SPS) simulations. The code is based on a 6D symplectic tracking engine, which is optimized for long-term tracking simulations and delivers fully reproducible results on many platforms. It also includes several scattering engines for beam-matter interactions studies, as well as facilities to run integrated simulations with FLUKA and GEANT4. These features differentiate SixTrack from general-purpose, optics-design software like MAD-X. The code recently underwent a major restructuring to merge advanced features in a single branch such as multiple ion species, interface with external codes and high-performance input/output (XRootD, HDF5). In the process, the code moved from Fortran 77 to Fortran 2018 standard, achieving also a better modularization. Physics models (beam-beam effects, rf-multipoles, current carrying wires, solenoid, electron-lenses) and methods (symplecticity check) have also been reviewed and refined to offer more accurate results. The SixDesk running environment allows the user to manage the large batches of simulations required for accurate predictions of the dynamic aperture. SixDesk supports CERN LSF and HTCondor batch systems, as well as the BOINC infrastructure in the framework of the LHC@Home volunteering computing project. SixTrackLib is a new library aimed at providing a portable and flexible tracking engine for single- and multi-particle problems using the models and formalism of SixTrack. The tracking routines are implemented in a parametrized C code that is specialized to run vectorized in CPUs and GPUs using SIMD intrinsics, OpenCL 1.2, and CUDA. This contribution presents the status of the code and an outlook of future developments of SixTrack, SixDesk and SixTrackLib.

## BRAGG DIFFRACTION MODELING BETWEEN X-RAY FREE-ELECTRON LASER AND CRYSTALS

Nanshun Huang, Kai Li, **Haixiao Deng**

Shanghai Institute of Applied Physics

*Classification:* B-1

In pursuit of fully coherent X-ray free-electron laser (FEL) [1], high reflective Bragg crystals have being and will be used as high selective spectral filter in the hard X-ray self-seeding FELs [2] and X-ray FEL oscillators (XFEL) [3], respectively. However, currently in the self-seeding FEL and XFEL simulations, the three-dimensional effect of Bragg diffraction is not fully considered. In this paper, we derive comprehensive solution for the response function of crystal in Bragg diffraction. And a three-dimensional X-ray crystal Bragg diffraction code named BRIGHT is introduced [4], which could collaborate closely with other FEL related code, e.g., GENESIS [5] and OPC [6]. The performance and feasibility are evaluated by two numerical examples, i.e., self-seeding experiment for LCLS [7] and XFEL options for Shanghai high repetition rate XFEL and extreme light facility (SHINE) [8]. The results indicate BRIGHT provides a new and useful tool for three-dimensional FEL simulation. [1] R. Bonifacio, C. Pellegrini, and L. M. Narducci, Collective instabilities and high-gain regime in a free electron laser, *Opt. Commun.* 50, 373 (1984). [2] J. Amann, et al., "Demonstration of self-seeding in a hard-x-ray free-electron laser," *Nat. Photonics* 6, 693–698 (2012). [3] K. J. Kim, Y. Shvydko, and S. Reiche, "A proposal for an x-ray free-electron laser oscillator with an energy-recovery linac," *Phys. Rev. Lett.* 100, 244802 (2008). [4] N. Huang, K. Li, H. Deng, BRIGHT: the three-dimensional X-ray crystal Bragg diffraction code (In preparation) [5] S. Reiche, "Genesis 1.3: A fully 3d time-dependent FEL simulation code," *Nucl. Instrum. Methods Phys. Res., Sect. A* 429, 243–248 (1999). [6] P. J. M. van der Slot, H. P. Freund, W. H. Miner, Jr., S. V. Benson, M. Shinn, and K.-J. Boller, "Time-dependent, three-dimensional simulation of free-electron-laser oscillators," *Phys. Rev. Lett.* 102, 244802 (2009). [7] P. Emma, R. Akre, J. Arthur, R. Bionta, C. Bostedt, J. Bozek, A. Brachmann, P. Bucksbaum, R. Coffee, F.-J. Decker et al., "First lasing and operation of an ångstrom-wavelength free-electron laser," *Nat. Photonics* 4, 641–647 (2010). [8] K. Li, H. Deng, Systematical design and three-dimensional simulation of X-ray FEL oscillator for the Shanghai coherent light facility, *Nucl. Instr. and Meth. A*, 895 (2018) 40-47.

## UPGRADE OF MAD-X FOR HL-LHC PROJECT AND FCC STUDIES

**Laurent Deniau**, Helmut Burkhardt, Massimo Giovannozzi, John M. Jowett, Andrea Latina, Tobias Persson, Frank Schmidt, and Piotr Krzysztof Skowronski

CERN

*Classification:* A-2, D-1, F-1

The design efforts for the High Luminosity upgrade of the Large Hadron Collider (HL-LHC) and for the FCC-ee project required significant extensions of the MAD-X code widely used for designing and simulating particle accelerators. The modelling of synchrotron radiation effects has recently been reviewed, improved and tested on the lattices of ESRF, LEP and CLIC Final Focus System. The results were cross checked with the codes AT, PLACET, Geant4, and MAD8. The implementation of space charge has been drastically restructured in a modular design. The linear coupling calculation has been completely reviewed and improved, from the theory to the implementation in MAD-X code to ensure its correctness in the presence of strong coupling as in the HL-LHC studies. The slicing module has been generalised to allow for thick slices of bending magnets, quadrupoles and solenoids. The SBEND element has been extended to support difference between bending angle and integrated dipole strength. Patches have been added to the list of supported elements. MAD-X PTC has also been extended to track resonance driving terms along layouts, and to support AC dipoles to simulate beams during optics measurements.

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## SURROGATE MODELS FOR BEAM DYNAMICS IN CHARGED PARTICLE ACCELERATORS

**Auralee Edelen**, Andreas Adelman, Nicole Neveu, Matthias Frey, Dinesh Acharya

SLAC, PSI, ANL, PSI, PSI

*Classification:* E-2, F-2, D-1

High-fidelity, PIC-based beam dynamics simulations are time and resource intensive. Consider a high dimensional search space, that is far too large to probe with such a high resolution simulation model. We demonstrate that a coarse sampling of the search space can produce surrogate models, which are accurate and fast to evaluate. In constructing the surrogate models, we use artificial neural networks [1] and multivariate polynomial chaos expansion [2]. The performance of both methods are demonstrated in a comparison with high-fidelity simulations, using OPAL, of the Argonne Wakefield Accelerator [3]. We claim that such surrogate models are good candidates for accurate on-line modeling of large, complex accelerator systems. [1] A. L. Edelen et al., arXiv:1610.06151[physics.acc-ph] [2] A. Adelman, arXiv:1509.08130v6[physics.acc-ph] [3] N. Neveu et al., 2017 J. Phys.: Conf. Ser. 874 012062

## NORMAL FORM APPROACH TO AND NONLINEAR OPTICS ANALYSIS OF THE IOTA RING

**Bela Erdelyi**

Northern Illinois University

*Invited Talk*

*Classification:* D-1, A-2

The IOTA ring is the realization as an accelerator system of a nonlinear, completely integrable Hamiltonian. Normal form methods allow analysis of one-turn maps of rings, exposing global information about the dynamics, including amplitude dependent tune shifts and resonance strengths. Since mapping the phase space of particle dynamics in IOTA is important to gain insight and offer practical ways to optimize for intensity frontier beam physics, this talk will summarize our group's results, the advantages, difficulties, and limitations of normal form analysis of the IOTA nonlinear optics.

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## ELECTRON BEAM LONGITUDINAL PHASE SPACE RESTORATION FROM THE IMAGE AFTER BEAM PASS DEFLECTOR CAVITY AND SPECTROMETER ARM

**Mikhail Fedurin**

Brookhaven National Laboratory, Accelerator Test Facility

*Classification:* D-2

Recently commissioned X-band deflector cavity at Brookhaven National Laboratory Accelerator Test Facility (BNL ATF) is used for electron bunch longitudinal profile measurements in both - at zero-degree beamline and at spectrometer arm directions to measure the e-beam longitudinal phase space profile. The deflector cavity induces energy distortions on the off-axis particles and corrupt real picture of the beam energy profile at spectrometer screen. A special computational phase space restoration technique which is under development at BNL ATF to reveal undistorted e-beam parameters will be discussed.

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## COMPUTATION OF EIGENMODES IN LONG AND COMPLEX ACCELERATING STRUCTURES BY MEANS OF CONCATENATION STRATEGIES

**Thomas Flisgen**

Helmholtz-Zentrum Berlin

*Invited Talk*

*Classification:* C-2

The computation of eigenmodes in chains of superconducting cavities with asymmetric couplers is a demanding problem. This problem typically requires the use of high-performance computers in combination with dedicated software packages. Alternatively, the eigenmodes of chains of superconducting cavities can be determined by the so-called State-Space Concatenation (SSC)

approach that has been developed at the University of Rostock. SSC is based on the decomposition of the full chain into individual segments. Subsequently, the RF properties of every segment are described by reduced order models. These reduced order models are concatenated to a reduced order model of the entire chain by means of algebraic side constraints arising from continuity conditions of the fields across the decomposition planes. The constructed reduced order model describes the RF properties of the complete structure so that the field distributions, the coupling impedances and the external quality factors of the eigenmodes of the full cavity chain are available. In contrast to direct methods, SSC allows for the computation of the eigenmodes of cavity chains using desktop computers. The current contribution discusses theoretical aspects of the scheme. Moreover, a set of application examples is presented such as eigenmode computations for cavity chains of the European XFEL, Berlin Pro, and BESSY VSR. Furthermore, an outlook is presented to include surface losses into the formulation by using perturbation approaches.

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## TRIMCOIL OPTIMISATION USING MULTI-OBJECTIVE OPTIMISATION TECHNIQUES AND HPC

**Matthias Frey, Jochem Snuverink, Andreas Adelman**

Paul Scherrer Institut (PSI)

*Classification:* D-1, E-2, A-2, F-1, F-2

Uncertainties in the bunch injection (i.e. energy, radius, radial momentum and angle) as well as magnet inaccuracies harm the isochronicity of the PSI 590 MeV Ring Cyclotron. An additional magnetic field provided by trim coils is an effective solution to restore this condition. Therefore, an accurate description of trim coils is essential to match the turn pattern of the machine in simulations. However, due to the high-dimensional search space consisting of 21 design variables and more than 180 objectives the turns cannot be matched in a straightforward manner and without sufficient HPC resources. In this talk we present a realistic trim coil model for the PSI 590 MeV Ring Cyclotron implemented in OPAL that was used together with its built-in multi-objective optimisation algorithm to find the 4 injection parameters and the magnetic field strengths of 17 trim coils. The optimisations were performed on Piz Daint (currently 3rd fastest supercomputer world-wide) with more than 1000 cores per job.

## COMPUTER ARCHITECTURE INDEPENDENT ADAPTIVE GEOMETRIC MULTIGRID SOLVER FOR AMR-PIC

Matthias Frey, Andreas Adelman

Paul Scherrer Institut (PSI)

*Classification:* F-2, F-1, D-1, D-2

The accurate and efficient simulation of neighboring bunch effects in high intensity cyclotrons requires to solve large-scale N-body problems of  $O(10^9 \dots 10^{10})$  particles coupled with Maxwell's equations. In order to capture the effects of halo creation and evolution of such simulations with standard particle-in-cell models an extremely fine mesh with  $O(10^8 \dots 10^9)$  grid points is necessary to meet the condition of high resolution. This requirement represents a waste of memory in regions of void, therefore, the usage of block-structured adaptive mesh refinement algorithms is more suitable. The N-body problem is then solved on a hierarchy of levels and grids using geometric multigrid algorithms. We show benchmarks of a new implementation of an adaptive geometric multigrid algorithm using 2nd generation Trilinos packages that ran on Piz Daint with  $O(10^4 \dots 10^5)$  cores.

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## RECENT DEVELOPMENTS IN WAKE FIELD AND BEAM DYNAMICS COMPUTATION

Erion Gjonaj, David A. Bizzozero, Steffen Schmid,  
Herbert De Gersem

Darmstadt University of Technology, Computational  
Electromagnetics Laboratory

*Plenary Talk*

*Classification:* C-2, F-1, D-1, B-1

Wake potentials and beam coupling impedances can be calculated analytically only for simple structures and special limiting cases. For the calculation of wake fields in "real-world" 3D accelerator structures, one has to rely on numerical field computations. Among the most successful numerical techniques for wake field calculations in the time domain are dispersion-free methods in the moving window. These techniques are particularly useful for short-range wake field calculations. Recently, this class of methods has been extended to include Surface Impedance Boundary Conditions (SIBC) based on the Auxiliary Differential Equation (ADE) technique. These boundary conditions allow the computation of resistive wall wake fields for 3D structures with arbitrary frequency dependent conductivity. An important application of this method is the calculation resistive wall wake fields in novel accelerator chambers with NEG and amorphous carbon coatings. Other developments to be discussed include the calculation of CSR-wakes in bunch compressors and undulator structures for x-ray sources. This task is computationally very difficult because of the curved bunch trajectory that leads to extremely high frequency and long-range wake fields. Time domain as well as frequency domain methods based on high order DG and FE discretization techniques for the electromagnetic fields computation in such structures will be presented.

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## EXPERIENCE WITH CBETA ONLINE MODELING TOOLS

C. Gulliford, D. Sagan, A. Bartnik, J. Dobbins, J.S. Berg

Cornell University

*Classification:* A-2, B-1, D-1, E-1, D-2, E-2, F-1

The CBETA machine is a four pass Energy Recovery Linac (ERL) with an Fixed-Field Alternating Gradient (FFAG) arc currently being developed as a joint project between the Cornell Laboratory for Accelerator-Based Sciences And Education (CLASSE) and Brookhaven National Lab. For online modeling of CBETA, a customized version of the Tao program, which is based upon the Bmad toolkit, is used along with the GPT program for low energy space charge calculations. The customized version of Tao, called CBETA-V, is interfaced to python for communication with the EPICS control system. This paper describes the online modeling system and initial experience during machine running.

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## SIMULATIONS OF BEAM CHOPPING FOR POTENTIAL UPGRADE OF THE SNS LEBT CHOPPER

B.X. Han, R.F. Welton, V. Peplov, R. Saethre, S.N.  
Murray Jr., T.R. Pennisi, C.M. Stinson, and M.P. Stockli

Spallation Neutron Source, Oak Ridge National  
Laboratory, Oak Ridge, TN 37831, USA

*Classification:* D-1, A-2, E-2

The Spallation Neutron Source (SNS) accelerator system includes a 65 keV H<sup>-</sup> injector, a 2.5 MeV RFQ, a 1 GeV linac chain (DTL-CCL-SCL), and an accumulator ring. The H<sup>-</sup> injector consists of a RF-driven, Cs-enhanced H<sup>-</sup> ion source and a two-lens electrostatic low energy beam transport (LEBT) that feed the RFQ accelerator with 1 ms H<sup>-</sup> beams pulsed at 60 Hz. To facilitate the multi-turn beam stacking in the ring and to create a gap for clean beam extraction from the ring, the H<sup>-</sup> beams are chopped in the LEBT section in front of the RFQ at the ring revolution frequency ( $\sim 1$  MHz). The second lens of the LEBT is azimuthally split into four segments to allow applications of various transverse electric fields for beam steering, chopping or blanking. Currently, the four segments are pulsed independently by four bipolar high voltage pulse generators and the four pulse generators are powered simultaneously at a time to chop the beam with  $\sim 1$  MHz repetition rate and toward the four different diagonal directions sequentially. In addition to a plan for upgrading the nearly obsolete high voltage pulse generators, different timing configurations for beam chopping are being proposed to improve the pulse generator performance by reducing switching frequency and power dissipation in the high voltage pulse generators. New chopping configurations where only two segments or even only one segment is used at a time are proposed. This paper presents simulations of the beam behavior under these new

chopping configurations to evaluate the beam chopping performance including the required high voltage amplitudes to deflect the beam out of the RFQ acceptance in phase-space, and the distributions of the deflected beams on the LEBT chopper target.

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## DESIGN STUDY OF A FAST KICKER MAGNET APPLIED TO THE BEAMLINE OF A PROTON THERAPY FACILITY

Wenjie Han, Bin Qin, Jun Yang, Kaifeng Liu, Zhikai Liang, Xu Liu

Huazhong University Of Science And Technology

*Classification:* C-1

A proton therapy facility based on isochronous superconducting cyclotron is under development in HUST (Huazhong University of Science and Technology). A fast kicker magnet will be installed at the upstream of the degrader to perform the beam switch function by kicking the proton beam to the downstream beam stop. The rising and falling time of the kicker is about 100us and the maximum repetition rate is 500Hz. This paper introduces simulation and optimization of the eddy current and dynamic magnetic field of the fast kicker, by using FEM code OPERA-3D. For kicker materials, laminated steel and ferrite are compared and the MnZn ferrite was chose. Design considerations including the eddy current effect, field hysteresis and mechanical structure of the kicker will also be introduced with multiphysics analysis.

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## SPIN DYNAMICS IN MODERN ELECTRON STORAGE RINGS: COMPUTATIONAL AND THEORETICAL ASPECTS

Klaus Heinemann, Daniel Appelo, Desmond P. Barber, Oleksii Beznosov, James A. Ellison

University of New Mexico, University of Colorado Boulder, Deutsches Elektronen Synchrotron, University of New Mexico, University of New Mexico

*Plenary Talk*

*Classification:* D-2, D-1, F-1, F-2, A-2

In this talk we present some numerical and analytical results from our work on the spin polarization in high energy electron storage rings. Our work is based on the initial value problem of what we call the full Bloch equations (FBEs). The solution of the FBEs is the polarization density which is proportional to the spin angular momentum density per particle in phase space and which determines the polarization vector of the bunch. The FBEs take into account spin diffusion effects and spin-flip effects due to synchrotron radiation including the Sokolov-Ternov effect and its Baier-Katkov generalization. The FBEs were introduced by Derbenev and Kondratenko in 1975 as a generalization of the Baier-Katkov-Strakhovenko equations from a single orbit to the whole phase space. The FBEs are a system of three uncoupled Fokker-Planck equations plus two coupling terms, i.e., the T-BMT term and the Baier-Katkov term. Neglecting the spin

flip terms in the FBEs one gets what we call the reduced Bloch equations (RBEs). The RBEs are sufficient for computing the depolarization time. The conventional approach of estimating and optimizing the polarization is not based on the FBEs but on the so-called Derbenev-Kondratenko formulas. However, we believe that the FBEs offer a more complete starting point for very high energy rings like the FCC-ee and CEPC. The issues for very high energy are: (i) Can one get polarization, (ii) are the Derbenev-Kondratenko formulas satisfactory at very high energy? If not, what are the theoretical limits of the polarization? Item (ii) will be addressed both numerically and analytically. Our numerical approach has three parts. Firstly we approximate the FBEs analytically using the method of averaging, resulting in FBEs which allow us to use large time steps (without the averaging the time dependent coefficients of the FBEs would necessitate small time steps). The minimum length of the time interval of interest is of the order of the orbital damping time. Secondly we discretize the averaged FBEs in the phase space variables by applying the pseudospectral method, resulting in a system of linear first-order ODEs in time. The phase space variables come in  $d$  pairs of polar coordinates where  $d=1,2,3$  is the number of degrees of freedom allowing for a  $d$ -dimensional Fourier expansion. The pseudospectral method is applied by using a Chebychev grid for each radial variable and a uniform Fourier grid for each angle variable. Thirdly we discretize the ODE system by a time stepping scheme. The presence of parabolic terms in the FBEs necessitates implicit time stepping and thus solutions of linear systems of equations. Dealing with  $2d+1$  independent variables poses a computational challenge due to the extreme size of the ODE system if the Fourier modes are coupled extensively. However, thanks to having used averaged FBEs, the Fourier modes are uncoupled in the Fokker-Planck terms. Hence the parabolic terms are separated from the mode coupling terms. We take advantage of this separation by using an implicit/explicit time stepping scheme so that we end up with a large system of only locally coupled ODEs. Since the Fourier mode couplings are local, a parallel implementation with only local communication is possible. Some numerical results will be shown. Details and more results will be presented in the talk by O.Beznosov.

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## OPTIMIZATION OF HADRON THERAPY BEAMLINES USING A NOVEL FAST TRACKING CODE FOR BEAM TRANSPORT AND BEAM-MATTER INTERACTIONS

Cédric Hernalsteens (1,2), Kévin André (1), Vincent Collignon (1), Quentin Flandroy (1), Baptiste Herregods (1), Raphaël Jungers (2), Robin Tesse (3), Zheming Wang (2)

(1) Ion Beam Applications (IBA) (2) Université Catholique de Louvain (3) Université Libre de Bruxelles

*Classification:* E-2, F-1, A-2, E-1

The optimization of proton therapy beamlines challenges the traditional approach used in beam optics due to the very strict constraints on beam quality, especially for Pencil Beam Scanning, despite the large losses induced by the emittance increase coming from the energy degrader. In order to explore the perfor-

mances of proton therapy beamlines, we proceed using a new fast beam tracking Python library coupled with a genetic algorithm. Global optimization algorithms such as the genetic algorithm or basin hopping schemes require numerous evaluations of the model and their practical implementations are limited by the computation time at each iteration. To overcome this limitation, while at the same time allowing an open-box user experience, a Python library has been developed, including transport models for the typical hadron therapy beamlines elements, as well as models for the computation of multiple Coulomb scattering. The Multi-Objective Genetic Algorithm (MOGA) allows to explore the parameter space in a global sense. This multi-objective algorithm enables the simultaneous optimization of complex constraints specific to proton therapy beamlines. Results for the IBA Proteus One system are presented and discussed in detail.

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### **NOVEL, FAST, OPEN-SOURCE CODE FOR SYNCHROTRON RADIATION COMPUTATION ON ARBITRARY 3D GEOMETRIES**

**Dean Andrew Hidas**

Brookhaven National Laboratory

*Classification:* B-1, C-2

Open Source Code for Advanced Radiation Simulation (OS-CARS) is an open-source project (<https://oscars.bnl.gov>) developed at Brookhaven National Laboratory for the computation of synchrotron radiation from arbitrary charged particle beams in arbitrary and time-dependent magnetic and electric fields on arbitrary geometries in 3D. Computational speed is significantly increased with the use of built-in multi-GPU and multi-threaded techniques which are suitable for both small scale and large scale computing infrastructures. OSCARS is capable of computing spectra, flux, and power densities on simple surfaces as well as on objects imported from common CAD software. It is additionally applicable in the regime of high-field acceleration. The methodology behind OSCARS calculations will be discussed along with practical examples and applications to modern accelerators and light sources.

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### **DESIGN AND SIMULATION OF HIGH MOMENTUM ACCEPTANCE GANTRIES FOR ION BEAM THERAPY**

**Anthony Huggins, Weishi Wan, Lucas Brouwer**

Varian Medical Systems, University of Duesseldorf,  
LBNL, PSI

*Invited Talk*

*Classification:* A-2, D-1

One challenge of proton beam therapy is the shear size of its equipment. A proton gantry that rotates a beamline about a patient is typically about 10 meters in diameter, heavy and expensive. One approach to reduce size and cost of gantries is their miniaturization by the application of superconducting (SC) magnets in the beamline. SC magnets, however, have difficulties

to quickly adapt their field when the beam energy is changed. Achromatic beamline designs with high momentum acceptance based on superconducting magnets can lead to compact gantries that still allow rapid beam application which is an important clinical requirement. In a collaborative effort LBNL, Varian Medical Systems and PSI have developed the Alternating Gradient Canted-Cosine-Theta (AG-CCT), a curved version of the CCT design that includes alternating quadrupole and sextupole components to build an achromat. The AG-CCT reaches a momentum acceptance of approx. 20 % dp/p while preserving beam profiles within clinical specification. Another design, conceived by LBNL and Varian, achieves momentum acceptance over the entire clinical beam energy range (70-225 MeV), called the fixed-field achromat. The beam optics principles of the two achromats and an optimized associated gantry beamline design is the main focus of the presented work, as well as putting these in context of clinical requirements and economic constraints.

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### **FEL SIMULATION USING THE LIE METHOD**

**Kilean Hwang, Ji Qiang**

Lawrence Berkeley National Lab

*Invited Talk*

*Classification:* B-1

Advances in numerical methods for free-electron-laser (FEL) simulation under wiggler period averaging (WPA) are presented. First, WPA is generalized using perturbation Lie map method. The conventional WPA is identified as the leading order contribution. Next, shot-noise model under WPA is improved along with a particle migration scheme across the numerical mesh. The artificial shot noise arising from particle migration across numerical mesh is suppressed. The improved model also allows using arbitrary mesh size, slippage resolution, and integration step size. These advances will improve modeling of longitudinal beam profile evolution for fast FEL simulation.

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### **ANALYSIS OF THE BEAM LOSS MECHANISM DURING THE ENERGY RAMP-UP AT THE SAGA-LS**

**Yoshitaka Iwasaki**

SAGA Light Source

*Classification:* B-1

The accelerator of the SAGA Light Source consists of 255 MeV injector linac and 1.4 GeV storage ring. The accumulated electron beam current of the storage ring is about 300 mA. The energy of the electrons are raised up to 1.4 GeV in 4 minutes in the storage ring. At the moment of the beam acceleration (the beam energy is lower than 300 MeV), the electron beam is lost like the step function. The lost beam current is normally about 5 mA to 30 mA. The beam loss at the energy ramp-up is not observed, when the beam current is lower than 200 mA. To understand the beam loss mechanism, which depend on the beam current, we developed high-speed logging system of 100 kHz for

monitoring the beam current and the magnets power supplies using National Instruments PXI. We investigated the relationship between the beam loss and the betatron tune shifts. The tune shifts during the beam acceleration were analyzed from the measured data of the output current of the magnets power supplies by using beam tracking code of TRACY2. By adopting the new high-speed logging system, the time structure of the beam loss process was clearly observed. We will present the high-speed logging system developed for monitoring the beam current and the power supplies at this meeting. The results of the investigation to find the relationship of the beam loss and the tune shifts will be also shown.

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### **SINGLE OBJECTIVE GENETIC OPTIMIZATION OF AN 85% EFFICIENT KLYSTRON**

**Aaron Jensen**, John Petillo, Lawrence Ives, Michael Read, Jeff Neilson

Leidos, Calabazas Creek Research, SLAC National Accelerator Laboratory

*Classification:* E-2, C-2, E-1

Overall efficiency is a critical priority for the next generation of particle accelerators as they push to higher and higher energies. In a large machine, even a small increase in efficiency of any subsystem or component can lead to a significant operational cost savings. The Core Oscillation Method (COM) and Bunch-Align-Compress (BAC) method have recently emerged as a means to greatly increase the efficiency of the klystron RF source for particle accelerators. The COM and BAC methods both work by uniquely tuning klystron cavity frequencies such that more particles from the anti-bunch are swept into the bunch before power is extracted from the beam. The single objective genetic algorithm from Sandia National Laboratory's Dakota optimization library is used to optimize both COM and BAC based klystron designs to achieve 85% efficiency. The COM and BAC methods are discussed. Use of the Dakota optimization algorithm library from Sandia National Laboratory is discussed. Scalability of the optimization approach to High Performance Computing (HPC) is discussed. The optimization approach and optimization results are presented.

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### **ADVANCED DESIGN AND SIMULATION OF FIXED-FIELD ACCELERATORS**

**Carol Johnstone**, Martin Berz, Kyoko Makino, Pavel Snopok

Particle Accelerator Corp., Michigan State Univ.,  
Michigan State Univ., Illinois Institute of Technology

*Classification:* A-2, F-1

The development of new types of accelerators that allow wide choices of parameters, promote complicated fields, and often need to efficiently handle very large emittance beams requires the availability of new simulation environments to design and

accurately predict operation. This is particularly true of Fixed-field accelerators, FFAs, which apply arbitrary-order fields - both alternating gradient, strong focusing - but also weak-focusing cyclotrons. This is especially applicable at medium-to-high energy combined with high intensity (mA currents). Synchrotron and cyclotron codes are generally inadequate to simulate accurately the performance of these strong-focusing fixed-field accelerators, particularly the new breed of non-scaling machines which have difficult, high-order fringe-field and edge-angle effects. One well-supported code, COSY INFINITY (COSY) is particularly suitable for accurate, high-order descriptions of accelerators. New tools have been developed in COSY INFINITY to address and accurately represent complex fixed-field machines in both a sector and spiral sector footprint. A description, application, and comparison of these tools with fields from magnet lattice design is presented.

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### **S-BASED MULTI-PARTICLE SPECTRAL SIMULATION OF AN ELECTRON GUN**

**Paul M. Jung**, Thomas Planche, Rick Baartman

TRIUMF

*Classification:* A-2, D-1, D-2

We derive a Hamiltonian description of a continuous particle distribution and its electrostatic potential from the Low Lagrangian. The self consistent space charge potential is discretized according to the spectral Galerkin approximation. The particle distribution is discretized using macro-particles. We choose a set of initial and boundary conditions to model the TRIUMF 300keV thermionic DC electron gun. The field modes and macro-particle coordinates are integrated self-consistently using map methods. The results are compared to results obtained from ASTRA simulations and experimental data.

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### **HOM-MITIGATION FOR FUTURE SPS 33-CELL 200 MHZ ACCELERATING STRUCTURES**

**P. Kramer**, C. Vollinger

CERN

*Classification:* C-2, A-2, E-1

The CERN SPS 200 MHz travelling wave (TW) accelerating structures pose an intensity limitation for the planned high luminosity (HL-) LHC upgrade. Higher-order modes (HOMs) around 630 MHz have been identified as one of the main sources of longitudinal multi-bunch instabilities. Improved mitigation of these HOMs with respect to today's HOM-damping scheme is therefore an essential part of the LHC injectors upgrade (LIU) project. The principles of HOM-couplers in cavities and the present damping scheme are reviewed, before illustrating the numerous requirements an improved damping scheme for the future 33-cell structures must fulfil. These are, amongst others, the mitigation of HOMs situated in the lower part of the structure where there are no access ports for extraction, a sufficient overall damping performance and an acceptable influence on the fundamental

accelerating passband (FPB). Different approaches tackling these challenges are investigated by 3D electromagnetic (EM) simulations and their performance, advantages and pitfalls are evaluated. The most promising solution involves slight changes of the accelerating structure, e.g. by the insertion of metallic perturbors in the bottom part of the cavity. Their behaviour is confirmed by lab measurements and its compatibility with the travelling-wave FPB is further examined.

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### **CONSTRAINED MULTI-OBJECTIVE SHAPE OPTIMIZATION OF SUPERCONDUCTING RF CAVITIES TO COUNTERACT DANGEROUS HIGHER ORDER MODES**

**Marija Kranjcevic**, Shahnam Gorgi Zadeh, Andreas Adelmann, Peter Arbenz, Ursula van Rienen

ETH Zurich, University of Rostock, Paul Scherrer Institut (PSI), ETH Zurich, University of Rostock

*Classification:* C-2, F-2, E-2

High current storage rings, such as the Z operating mode of the FCC-ee, require accelerating cavities that are optimized with respect to both the fundamental mode and the dangerous higher order modes (HOMs). In such cavities, monopole and dipole modes are the major sources of beam instability and have to be sufficiently damped. In addition to the damping method, optimizing the shape of the superconducting radio frequency (RF) cavity can help lower the effect of dangerous HOMs. In order to optimize the shape of the RF cavity we solve a constrained multi-objective optimization problem using a massively parallel implementation of an evolutionary algorithm. Focusing on axisymmetric RF cavities, we parameterize and mesh their cross section, and then use a fast 2D Maxwell eigensolver to solve time-harmonic Maxwell's equations. For each cavity, after the Fourier expansion in the azimuthal direction, we need to solve the eigenproblems corresponding to the few lowest Fourier modes. We investigate various approaches to parallelize this and implement a repair method to deal with the constraint on the frequency of the fundamental mode. Finally, we show the computed Pareto front approximation and individuals with good objective function values, i.e. the RF cavity shapes with desired properties.

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### **START-TO-END SIMULATIONS OF THZ SASE FEL PROOF-OF-PRINCIPLE EXPERIMENT AT PITZ**

**Mikhail Krasilnikov**, Prach Boonpornprasert

DESY, Zeuthen, Germany

*Classification:* B-1, D-1

The Photo Injector Test facility at DESY in Zeuthen (PITZ) develops high brightness electron sources for modern linac-based Free Electron Lasers (FELs). The PITZ accelerator has been proposed as a prototype for a tunable, high power THz source for pump and probe experiments at the European XFEL. A Self-Amplified Spontaneous Emission (SASE) FEL is considered to generate the THz pulses. High radiation power can be achieved

by utilizing high charge (4 nC) shaped electron bunches from the PITZ photo injector. THz pulse energy of up to several mJ is expected from preliminary simulations for 100 um radiation wavelength. For the proof-of-principle experiments a re-usage of LCLS-I undulators at the end of the PITZ beamline is under studies. One of the challenges for this setup is transport and matching of the space charge dominated electron beam through the narrow vacuum chamber. Start-to-end simulations for the entire experimental setup - from the photocathode to the SASE THz generation in the undulator section - have been performed by combination of several codes: ASTRA, SC and GENESIS-1.3. The space charge effect and its impact onto the output THz radiation have been studied. The results of these simulations will be presented and discussed.

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### **REVIEW OF SPECTRAL MAXWELL SOLVERS FOR ELECTROMAGNETIC PARTICLE-IN-CELL: ALGORITHMS AND ADVANTAGES**

**Remi Lehe**

LBNL

*Invited Talk*

*Classification:* C-2, B-2, F-2

Electromagnetic Particle-In-Cell codes have been used to simulate both radio-frequency accelerators and plasma-based accelerators. In this context, the Particle-In-Cell algorithm often uses the finite-difference method in order to solve the Maxwell equations. However, while this method is simple to implement and scales well to multiple processors, it is liable to a number of numerical artifacts that can be particularly serious for simulations of accelerators. An alternative to the finite-difference method is the use of spectral solvers, which are typically less prone to numerical artifacts. In this talk, I will review recent progress in the use of spectral solvers for simulations of plasma-based accelerators. This includes techniques to scale those solvers to large number of processors, extensions to cylindrical geometry, and adaptations to specific problems such as boosted-frame simulations.

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### **ESS ACCELERATOR LATTICE DESIGN STUDIES AND AUTOMATIC SYNOPTIC DEPLOYMENT**

**Y. Levinsen**, M. Eshraqi, T. Grandsaert, A. Jansson, H. Kocevar, O. Midttun, N. Milas, R. Miyamoto, C. Plostinar, A. Ponton, R. de Prisco, T. Shea, H. D. Thomsen

European Spallation Source ERIC, Sweden & Aarhus University, Denmark

*Classification:* D-1

The European Spallation Source (ESS) is currently under construction in south of Sweden. A highly brilliant neutron source with a 5 MW proton driver will provide state of the art experimental facilities for neutron science. A peak proton beam power in the accelerator of 125 MW means that excellent control over the beam losses becomes essential. The beam physics design of

the ESS accelerator is in a TraceWin format, for which we have developed revision control setup, automated regression analysis and deployment of synoptic viewer and tabulated spreadsheets. This allows for an integrated representation of the data that are always kept synchronized and available to other engineering disciplines. The design of the accelerator lattice has gone through several major and minor iterations which are all carefully analysed. In this contribution we present the status of the latest studies which is the first time a complete end-to-end study beginning from the ion source has been performed.

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### GENETIC ALGORITHM ENHANCED BY MACHINE LEARNING FOR DYNAMIC APERTURE OPTIMIZATION

Yongjun Li, Weixing Cheng, Li Hua Yu, and Robert  
Rainer

Brookhaven National Laboratory

#### *Invited Talk*

*Classification:* E-2

With the aid of machine learning techniques, the genetic algorithm has been enhanced and applied to the multi-objective optimization problem presented by the dynamic aperture of the NSLS-II Ring. During the evolution employed by the genetic algorithm, the population is classified into different clusters. The clusters with top average fitness are given elite status. Intervention is implemented by repopulating some potentially competitive candidates based on the accumulated data. These candidates replace randomly selected candidates among the original data pool. The average fitness of the population is improved while diversity is not lost. The quality of the population increases and produces more competitive descendants accelerating the evolution process significantly. When identifying the distribution of optimal candidates, they appear to be located in isolated islands within the search space. Some of these optimal candidates have been experimentally confirmed at the NSLS-II storage ring. The machine learning techniques that exploit the genetic algorithm can also be used in other population-based optimization problems such as particle swarm algorithm.

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### PYAOPT OPTIMIZATION SUITE AND ITS APPLICATION ON ASTRA-SIMULATED SRF MEV GUN DESIGN FOR UEMS

Ao Liu, Chunguang Jing

Euclid Techlabs

*Classification:* B-2

In order to achieve sharp, high resolution real-time imaging, electrons in a MeV UEM (ultrafast electron microscope) beamline need to minimize instabilities. The Superconducting RF (SRF) photocathode gun is a promising candidate to produce highly stable electrons for UEM/UED applications. It operates in an ultrahigh Q, CW mode, and dissipates a few watts of RF power,

which make it possible to achieve a 10s ppm level of beam stability by using modern RF control techniques. In order to find the best performance of the gun design, an optimization procedure is required. pyaopt is a Python-based optimization suite that supports multi-objective optimizations using advanced algorithms. In this paper, the novel SRF photogun design and its optimizations through pyaopt and Astra's beam simulations will be discussed.

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### URGENT NEED OF START-TO-END SIMULATIONS FOR SHANGHAI CW HARD X-RAY FEL PROJECT

Bo Liu, Qiang Gu, Zhen Wang, Meng Zhang, Si Chen,  
Haixiao Deng, Chao Feng, Dong Wang, Zhentang Zhao

Shanghai Institute of Applied Physics

*Classification:* A-1, B-1

Shanghai has started to construct the X-ray FEL facility SHINE (Shanghai high repetition rate XFEL and extreme light facility), which is based on a 8 GeV CW-SRF linac and will build three undulator lines in the first stage. Designs of the gun, the injector, the linac, the distribution section and the FEL lines have already been done and will be presented here. Preliminary study shows that comprehensive study of the beam and FEL properties with start-to-end simulations is really necessary.

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### BEAM ALIGNMENT SIMULATION ON THE BEAMLINE OF A PROTON THERAPY FACILITY

Xu Liu, Qushan Chen, Bin Qin, Guangyao Feng

Huazhong University of Science and Technology

*Classification:* D-1

Proton therapy is now recognized as one of the most effective radiation therapy methods for cancers. A proton therapy facility with multiple gantry treatment rooms is under development in HUST (Huazhong University of Science and Technology). Misalignments of magnets and beam diagnostics instruments induce the offset of the beam trajectory, which will influence the clinical therapeutic effect. This paper describes the beam alignment simulations based on response matrix and this technology is applied to the design of the HUST-PTF beamline. To perform this study, we use the simulation code ELEGANT, and utilize the global correction method. By optimizing the layout of correctors and beam position monitors, we completed the beam correction calculation. The results show that the accuracy of center beam trajectory in the iso-center is better than 0.5 mm, meeting physical and clinical requirements.

## STATISTICAL ANALYSIS OF THE EIGENMODE SPECTRUM IN THE SRF CAVITIES WITH MECHANICAL IMPERFECTIONS

A. Lunin, T. Khabiboulline, N. Solyak, A. Sukhanov and V. Yakovlev

Fermilab

*Classification:* C-2

The SRF technology is progressing rapidly over last decades toward high accelerating gradients and low surface resistance making feasible the particle accelerators operation with high beam currents and long duty factors. However, the coherent RF losses due to HOM radiation becomes a limiting factors for these regimes. In spite of the operating mode, which is tuned separately, the parameters of HOMs vary from one cavity to another due to finite mechanical tolerances during cavities fabrication. It is vital to know in advance the spread of HOM parameters in order to predict unexpected cryogenic losses, overheating of beam line components and to keep stable beam dynamics. In this paper we present the method of generating the unique cavity geometry with imperfections while preserving operating mode frequency and field flatness. Based on the eigenmode spectrum calculation of series of randomly generated cavities we can accumulate the data for the evaluation the HOM statistics. Finally we describe the procedure for the estimation of the probability of the resonant HOM losses in the SRF resonators. The study of these effects leads to specifications of SC cavity and cryomodule and can significantly impact on the efficiency and reliability of the machine operation.

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## SIMULATION CHALLENGES FOR ERHIC BEAM-BEAM STUDY

Y. Luo, Y. Hao, J. Qiang, Y. Roblin

Brookhaven National Laboratory

*Classification:* A-1, A-2, D-1

The 2015 Nuclear Science Advisory Committee Long Rang Plan identified the need for an electron-ion collider facility as a gulo microscope with capabilities beyond those of any existing accelerator complex. To reach the required high energy, high luminosity, and high polarization, the eRHIC design based on the existing heavy ion and polarized proton collider RHIC adopts a very small beta-function at the interaction point, a high collision repetition rate, and a novel hadron cooling scheme. Collision with a full crossing angle of 22 mrad and crab cavities for both electron and proton rings are required. In this article, we will present the high priority R&D items related to beam-beam interaction for the current eRHIC design, the simulation challenges, and our plans to address them.

## SIMULATIONS OF COHERENT ELECTRON COOLING WITH FREE ELECTRON LASER AMPLIFIER AND PLASMA-CASCADE MICRO-BUNCHING AMPLIFIER

Jun Ma, Gang Wang, Vladimir N. Litvinenko

Brookhaven National Laboratory

*Classification:* D-1

SPACE is a parallel, relativistic 3D electromagnetic Particle-in-Cell (PIC) code used for simulations of beam dynamics and interactions. An electrostatic module has been developed with the implementation of Adaptive Particle-in-Cloud method. Simulations performed by SPACE are capable of various beam distribution, different types of boundary conditions and flexible beam line, as well as sufficient data processing routines for data analysis and visualization. Code SPACE has been used in the simulation studies of coherent electron cooling experiment based on two types of amplifiers, the free electron laser (FEL) amplifier and the plasma-cascade micro-bunching amplifier.

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## PLASMA WAKEFIELD START TO END ACCELERATION SIMULATIONS, FROM PHOTOCATHODE TO FEL WITH SIMULATED DENSITY PROFILES

Alberto Marocchino

INFN Laboratori Nazionali di Frascati, Frascati, Italy

*Invited Talk*

*Classification:* A-2

Plasma Wakefield acceleration is a promising new acceleration technique that profit by a charged bunch, e.g. an electron bunch, to break the neutrality of a plasma channel to produce a wake where a trailing bunch is eventually accelerated. The quest to achieve extreme gradient conserving high brightness has prompted to a variety of new approaches and techniques. Most of the proposed schemes are however limited to the only plasma channel, assuming in the vast majority of cases, ideal scenarios (e.g. ideal bi-gaussian bunches and uniform density plasma channels). Realistic start-to-end simulations from the photocathode to a FEL via a plasma accelerating section are a fundamental step to further investigate realistic scheme possibilities, the underlying physics, and future applications. To remove ideal simplifications, the SPARC.LAB simulation team is simulating bunches from the photo-cathode and tracking them all the way to the plasma. Similarly, the density profiles, where bunches evolve and accelerate, are calculated with a magneto-hydrodynamic code. The density profile is imported into the particle in cell codes used to calculate the particle evolution within the plasma section. The use of a multitude of codes, involving different architectures, physical units, and programming languages, made necessary the definition of code interfacing and pipe-processes to ensure a proper pipeline of tools that are traditionally used in different fields are do not often come across. By combining the different numerical codes (particle tracker, particle in cell, magneto-hydrodynamics and FEL codes) we could propose a first realistic start-to-end

simulation from the photo-cathode to a FEL laser for a possible upcoming Italian PWFA-FEL facility. Such a work is conducted with a great focus on code reliability and data reproducibility. The Italian PWFA experimental team uses a capillary to control and tailor the plasma density profile, we could perform preliminary code comparison and validation against experimental data. Code validation has also been possible for passive plasma lens experiments, where the detailed experimental six-dimensional phase space reconstruction had allowed a direct comparison with the numerical tools.

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### **EFFICIENT MODELING OF LASER WAKEFIELD ACCELERATION THROUGH THE PIC CODE SMILEI IN CILEX PROJECT**

**Francesco Massimo** (1), Arnaud Beck (1), Julien Derouillat (2), Mickael Grech (3), Frédéric Pérez (3), Imen Zemzemi (1), Arnd Specka (1)

(1) Laboratoire Leprince-Ringuet - École Polytechnique, CNRS-IN2P3, Palaiseau 91128, France - (2) Maison de la Simulation, CEA, CNRS, Université Paris-Sud, UVSQ, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France - (3) Laboratoire d'Utilisation des Lasers Intenses, CNRS, École Polytechnique, CEA, Université Paris-Saclay, UPMC Université Paris 06: Sorbonne Universités, F-91128 Palaiseau Cedex, France

*Classification:* B-2, F-1

The design of plasma acceleration facilities requires considerable simulation effort for each part of the machine, from the plasma injector and/or accelerator stage(s), to the beam transport stage, from which the accelerated beams will be brought to the users or possibly to another plasma stage. The urgent issues and challenges in simulation of multi-stage acceleration with the Apollon laser of CILEX facility will be addressed. To simulate the beam injection in the second plasma stage, additional physical models have been introduced and tested in the open source Particle in Cell collaborative code Smilei. The efficient initialisation of arbitrary relativistic particle beam distributions through a Python interface allowing code coupling and the self consistent initialisation of their electromagnetic fields will be presented. The comparison between a full PIC simulation and a simulation with a recently developed envelope model, which allows to drastically reduce the computational time, will be also shown for a test case of laser wakefield acceleration of an externally injected electron beam.

### **DESIGN OF A COMPACT PERMANENT MAGNET SPECTROMETER FOR CILEX/APOLLON**

M. Khojayan (1), J. Prudent (1), A. Cauchois (1), **F. Massimo** (1) and A. Specka (1)

(1) Laboratoire Leprince-Ringuet - École Polytechnique, CNRS-IN2P3, Palaiseau 91128, France

*Classification:* C-1, C-2, D-1

Laser wakefield acceleration experiments make extensive use of small permanent magnets or magnet assemblies for diagnostic and focusing of electron beams produced in plasma accelerators. This choice is motivated by the ease of operation inside vacuum chambers, absence of power-supplies and feedthroughs, and potentially lower cost. Indeed, in these experiments space is at premium, and compactness is frequently required. At the same time, these magnets need to have a large angular acceptance for the divergent electron beams, which imposes constraints on the gap size. We will present the optimized design and characterization of a 100 mm long, 2.1 Tesla permanent magnet dipole. Furthermore, we will present the implementation of this magnet in a spectrometer that will measure the energy spectrum of electrons of [60-2000] MeV with a few percent resolution in the CILEX/APOLLON 10PW laser facility in France.

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### **LIGHTSOURCE UNIFIED MODELING ENVIRONMENT (LUME), A START-TO-END SIMULATION FRAMEWORK FOR ELECTRONS AND PHOTONS.**

**Christopher Mayes**, Paul Fuoss, Chuck Yoon

SLAC National Accelerator Laboratory

*Invited Talk*

*Classification:* A-2, D-1

Since first light at LCLS, there has been continuous invention of new operating modes, introduction of new optical elements, and rapid improvement in detectors. While these improvements have led to new experiments with much greater scientific impacts, their transfer to user operations has often taken several experimental runs (many months to years). The integration of these technical advances into scientific programs would be greatly accelerated by a modeling tool that allowed for quantitative assessment of the impact on scientific programs of facility improvements. To this end, SLAC is developing the Lightsource Unified Modeling Environment (LUME) for unified modeling of X-ray free electron laser (XFEL) performance. This modeling tool will be built in several stages with an initial focus on quantitative prediction of critical parameters of the X-ray pulses delivered to experimental stations. This initial development will be followed by incorporation of X-ray-sample interaction and detector performance. This project will take a holistic approach starting with the simulation of the electron beams, to the production of the photon pulses and their transport through the optical components of the beamline, their interaction with the samples and the simulation of the detectors, followed by the analysis of simulated data. LUME will leverage existing, well-established codes [Astra, Bmad, Elegant, Genesis, Impact for electrons, Genesis

1.3 for FEL simulation, and the “Synchrotron Radiation Workshop” (SRW) for X-ray optics] that will be driven and configured by a coherent high-level framework. The high-level framework will build on the Simex platform being developed by the European Cluster of Advanced Laser Light Sources (EUCALL). The platform will be built with an open, well-documented architecture so that science groups around the world can contribute specific experimental designs and software modules, advancing both their scientific interests and a broader knowledge of the opportunities provided by the exceptional capabilities of X-ray FELs. LUME will be the first platform in the world for unified modeling of XFEL performance. LUME’s optimization capabilities will guide SLAC accelerator physicists in developing world leading XFEL performance. LUME will identify performance bottlenecks, both in the accelerator and photon transport, and enhance operational efficiency and reliability. The complete integration of electron and X-ray processes will allow LCLS scientists to invent instruments that optimally use those unique X-ray beams. Finally and most importantly, the ability to simulate experiments will stimulate the development of new approaches to the scientific and technological challenges facing the country, maximizing the impact of DoE’s investment in cutting-edge X-ray sources.

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**A FULL FIELD-MAP MODELING OF  
CORNELL-BNL CBETA 4-PASS ENERGY  
RECOVERY LINAC**

**F. Meot, S. Brooks, J. Crittenden, D. Trbojevic, N.  
Tsoupas**

BNL and Cornell

*Classification:* A-2

The Cornell-BNL Electron Test Accelerator (CBETA) is a four-pass, 150 MeV energy recovery linac (ERL), now in construction at Cornell. A single fixed-field alternating gradient (FFAG) beam line recirculates the four energies, 42, 78, 114 and 150 MeV. The return loop is comprised of 107 quadrupole-doublet cells, built using Halbach permanent magnet technology. Spreader and combiner sections (4 independent beam lines each) connect the 36 MeV linac to the FFAG loop. We present here a start-to-end simulation of the 4-pass ERL, entirely, and exclusively, based on the use of magnetic field maps to model the magnets and correctors. There are paramount reasons for that and this is discussed, detailed outcomes are presented, together with comparisons with regular beam transport (mapping based) techniques.

**POLARIZATION LIFETIME IN AN ELECTRON  
STORAGE RING, AN ERGODIC APPROACH IN  
ERHIC EIC**

**Francois Meot**

Brookhaven National Laboratory

*Classification:* D-2

Electron polarization in a storage ring is subject to two very long term effects: Sokolov-Ternov polarization and depolarization by diffusion. This leads to an equilibrium state, over a very long time scale, and, simulation-wise, is highly CPU time and memory consuming. Simulations aimed at determining optimal ring storage energy in an electron-ion collider are always tracking bunches with thousands of particles, and in addition for too short time scales due to HPC limitations. Based on considerations of ergodicity of electron bunch dynamics in the presence of synchrotron radiation, and on the very slow depolarization aimed at in a collider, tracking a single particle instead is investigated. This saves a factor of more than 2 orders of magnitudes in the parameter CPU-time x Memory-allocation, it allows much longer tracking and thus accuracy on the evaluation of polarization and time constants. The concept is illustrated with polarization lifetime and equilibrium polarization simulations at the eRHIC electron-ion collider.

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**SPACE CHARGE AND TRANSVERSE  
INSTABILITIES AT THE CERN SPS AND LHC**

**Elias Metral**

CERN

*Invited Talk*

*Classification:* D-1

At the CERN accelerator complex, only the highest energy machine in the sequence, the LHC, with space charge parameter close to one, sees a beneficial effect of space charge on transverse coherent instabilities. In the other circular machines of the LHC injector chain (PSB, PS and SPS), where the space charge parameter is much bigger than one, space charge does not seem to play a major role. All the measurements and simulations performed so far in both the SPS and LHC will be reviewed and analyzed in detail.

## ANALYSIS OF EMITTANCE GROWTH DUE TO COLLISIONAL PARTICLE NOISE IN A GRIDLESS SPECTRAL POISSON SOLVER FOR FULLY SYMPLECTIC MULTIPARTICLE TRACKING

Chad Mitchell, Ji Qiang

Lawrence Berkeley National Laboratory

*Classification:* D-1, D-2, F-1

Gridless spectral methods for self-consistent space charge modeling possess several advantages over traditional momentum-conserving particle-in-cell methods, including the absence of numerical grid heating and the presence of an underlying multiparticle Hamiltonian. Nevertheless, evidence of collisional particle noise remains. For a class of such 2D algorithms, we provide analytical models of the numerical field error, the optimal choice of spectral mode cutoff, and the numerical emittance growth per timestep. We compare these results with the emittance growth models of Struckmeier, Hoffman, Kesting, and others.

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## BEAMLINE MAP COMPUTATION FOR PARAXIAL OPTICS

Boaz Nash

RadiaSoft LLC

*Classification:* B-1, C-2

Modeling of radiation transport is an important topic tightly coupled to many charged particle dynamics simulations for synchrotron light sources and FEL facilities. The radiation is determined by the electron beam and magnetic field source, and then passes through beamlines with focusing elements, apertures and monochromators, in which one may typically apply the paraxial approximation of small angular deviations from the optical axis. The radiation is then used in a wide range of spectroscopic experiments, or else may be recirculated back to the electron beam source, in the case of an FEL oscillator. The Wigner function representation of electromagnetic wavefronts has been described in the literature and allows a phase space description of the radiation, similar to that used in charged particle dynamics. It can encompass both fully and partially coherent cases, as well as polarization. Here, we describe the calculation of a beamline map that can be applied to the radiation Wigner function, reducing the computation time. We discuss the use of ray tracing and wave optics codes for the map computation and benchmarking. We construct a four crystal 1:1 imaging beamline that could be used for recirculation in an XFEL oscillator, and benchmark the map based results with SRW wavefront simulations.

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## COMPARISON OF MODEL BASED AND HEURISTIC OPTIMIZATION ALGORITHMS APPLIED TO PHOTOINJECTORS USING LIBENSEMBLE

Nicole Neveu, Jeffrey Larson, Stephen Hudson, Linda Spentzouris

Illinois Institute of Technology, Argonne National Laboratory

*Classification:* E-2, F-2

Genetic algorithms are common and often used in the accelerator community. They require large amounts of computational resources and empirical adjustment of hyperparameters. Model based methods are significantly more efficient, but often labeled as unreliable for the nonlinear or unsmooth problems that can be found in accelerator physics. We investigate the behavior of both approaches using a photoinjector operated in the space charge dominated regime. All optimization runs are coordinated and managed by the Python library libEnsemble, which is developed at Argonne National Laboratory.

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## CHALLENGES IN SIMULATING BEAM DYNAMICS OF DIELECTRIC LASER ACCELERATION

Uwe Niedermayer

TEMF TU Darmstadt

*Plenary Talk*

*Classification:* B-2, D-1

Dielectric Laser Acceleration (DLA) achieves highest gradients in non-plasma accelerators by using the inverse Smith-Purcell effect on a dielectric grating, which is almost lossless at the respective laser wavelength. The use of dielectrics increases the breakdown field strength, and thus the achievable gradient, by a factor of at least 10 in comparison to metals. Experimental breakthroughs in DLA led to the Accelerator on a Chip (ACHIP) project, funded by the Gordon and Betty Moore Foundation from 2015 till 2020. In ACHIP, our main goal is to build an accelerator on a silicon chip, which can accelerate electrons from below 100keV to above 1MeV with a gradient of at least 100MeV/m. For stable acceleration on the chip, magnet-only focusing techniques are insufficient to compensate the strong acceleration defocusing. Thus higher spatial harmonic and Alternating Phase Focusing (APF) laser based focusing techniques have been developed. We have also developed the simplified symplectic tracking code DLATrack6D, which makes use of the periodicity and applies only one kick per DLA cell, which is calculated by the Fourier coefficient of the synchronous spatial harmonic. Due to the coupling of the cells, the Fourier coefficients are not flat but a field flatness optimization (similarly as in multi-cell cavities) needs to be performed. The effect of the APF-drifts and the end cells need to be studied and mitigated by individual design. Moreover, fabrication tolerances and misalignment need investigation and mitigation by improving the beam dynamics robustness. The simulation of the entire accelerator on a chip by a PIC code is possible, but not practical for optimization purposes since

a cluster computer is already required for a single run. Finally, we also outline the treatment of wake field effects at attosecond bunches in the grating by DLTrack6D, where the wake field is computed by an external solver.

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**PARTICLE-IN-CELL SIMULATION OF A BUNCHED ELECTRONS BEAM ACCELERATION IN A TE113 CYLINDRICAL CAVITY AFFECTED BY A STATIC INHOMOGENEOUS MAGNETIC FIELD**

**Eduardo A. Orozco** (1), Victor E. Vergara (2), Jesús D. González (2) and Jesús R. Beltrán (2)

(1) Universidad Industrial de Santander, Bucaramanga, Colombia; (2) Universidad del Magdalena, Santa Marta, Colombia.

*Classification:* B-2, C-2, D-1

The results of the relativistic full electromagnetic Particle-in-cell (PIC) simulation of a bunched electrons beam accelerated in a cylindrical cavity mode TE113 in the presence of a static inhomogeneous magnetic field are presented. This type of acceleration is known as Spatial AutoResonance Acceleration (SARA) [1]. The magnetic field profile is such that it keeps the electrons beam in the acceleration regime along their trajectories. Numerical experiments of bunched electrons beam with the concentrations in the range  $10^8$ - $10^{11}$  cm<sup>-3</sup> in a linear TE113 cylindrical microwave field of a frequency of 2.45GHz and an amplitude of about 14kV/cm show that it is possible to accelerate the bunched electrons up to energies of the order of 300keV without serious defocalization effect. A comparison between the data obtained from the full electromagnetic PIC simulations and the results derived from the relativistic Newton-Lorentz equation in a single particle approximation [2] is carried out. This acceleration scheme can be used to produce hard x-ray [3]. [1] Dugar-Zhabon, V. D., & Orozco, E. A. (2009). Cyclotron spatial autoresonance acceleration model. Physical Review Special Topics-Accelerators and Beams, 12(4), 041301. [2] Vergara, V. E., González, J. D., Beltrán, J. R., & Orozco, E. A. (2017, December). Electrons acceleration in a TE113 cylindrical cavity affected by a static inhomogeneous magnetic field. In Journal of Physics: Conference Series (Vol. 935, No. 1, p. 012076). IOP Publishing. [3] Dugar-Zhabon, V. D., & Orozco, E. A. (2017). Compact self-resonant x ray source. (USA Patent: 9,666,403 )

**COMPUTATIONAL BEAM DYNAMICS REQUIREMENTS FOR FRIB**

**Peter Ostroumov**

MSU, FRIB

*Plenary Talk*

*Classification:* A-1, D-1, E-2

The Facility for Rare Isotope Beams (FRIB) being built at Michigan State University moved to the commissioned stage in the summer of 2017. There were extensive beam dynamics simulations in the FRIB driver linac during the design stage. Recently, we have used TRACK and IMPACT simulation codes to study dynamics of ion beam contaminants extracted from the ECR together with main ion beam. The contaminant ion species can produce significant losses after the stripping. These studies resulted in development of beam collimation system at relatively low energy of 16 MeV/u and room temperature bunchers instead of originally planned SC cavities. Commissioning of the Front End and the first 3 cryomodules enabled detailed beam dynamics studies experimentally which were accompanied with the simulations using above-mentioned beam dynamics codes and optimization code FLAME. There are significant challenges in understanding of beam dynamics in the FRIB linac. The most computational challenges are in the following areas: (1) Simulation of the ion beam formation and extraction from the ECR; (2) Development of the virtual accelerator model available on-line both for optimization and multi-particle simulations. The virtual model should include realistic accelerator parameters including device misalignments; (3) Large scale simulations to support high-power ramp up of the linac with minimized beam losses; (4) Interaction of the beam with the gas stripper which is the backup option for high power operation of the linac. Work supported by the U.S. Department of Energy Office of Science under Cooperative Agreement DE-SC0000661 and the National Science Foundation under Cooperative Agreement PHY-1102511, the State of Michigan and Michigan State University.

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**STUDY OF ELECTRON CYCLOTRON RESONANCE ACCELERATION BY CYLINDRICAL TE011 MODE**

**Oswaldo Otero Olarte**(1), Eduardo Alberto Orozco (1), Ana María Herrera (2)

(1) Universidad Industrial de Santander, Bucaramanga, Colombia, (2) Heidelberg Institute for Theoretical Studies, Heidelberg, Germany

*Classification:* B-2

In this work, we present results from analytical and numerical studies of the electron acceleration by a TE011 cylindrical microwave mode in a static homogeneous magnetic field under electron cyclotron resonance (ECR) condition. The stability of the orbits is analyzed using the particle orbit theory. In order to get a better understanding of the interaction wave-particle we decompose the azimuthally electric field component as the superposition of right and left hand circular polarization standing waves. The trajectory, energy and phase-shift of the electron are found

through a numerical solution of the relativistic Newton-Lorentz equation in a finite difference method by the Boris method. It is shown that an electron longitudinally injected with an energy of 7 keV in a radial position  $r=Rc/2$ , being  $Rc$  the cavity radius, is accelerated up to energy of 90 keV by an electric field strength of 14 kV/cm and frequency of 2.45 GHz. This energy can be used to produce X-ray for medical imaging. These results can be used as a starting point for the study the acceleration of electrons in a magnetic field changing slowly in time (GYRAC), which has some important applications as the electron cyclotron resonance Ion proton accelerator (ECR-IPAC) for cancer therapy and to control plasma bunches with relativistic electrons.

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## MULTIPASS SIMULATIONS OF SPACE CHARGE COMPENSATION USING ELECTRON COLUMNS AT IOTA RING

**Chong Shik Park**, Moses Chung, Ben Freemire, Chad Mitchell, Greg Penn, Giulio Stancari, Eric Stern

Korea University, UNIST, NIU, LBNL, Fermilab

*Classification:* D-1

Defocusing repulsive forces due to self space charge fields leads to degradation of high-intensity particle beams. Being of particular concern for low- and medium-energy proton beams, they result in the emittance growth, beam halo formation, and beam losses. They set stringent limits on the intensity frontier accelerators, therefore, the mitigation of space charge effects is a crucial challenge to improve the proton beam intensity. The space charge effects in the positively charged proton beams can be effectively compensated by using negatively charged electron columns. In this paper, we present the key parameters of the electron columns for the space charge compensation (SCC) and discuss results of the Warp3D numerical simulations for the matching of the transverse and longitudinal charge distributions of electrons produced by the high intensity proton beam and accumulated in the column. In order to investigate the evolution of both the electron column and the proton beam over multi-passes, we track the proton beam further within in the IOTA ring using Synergia and IMPACT.

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## SYMPLECTIC PARTICLE-IN-CELL

**Thomas Planche**

TRIUMF

*Invited Talk*

*Classification:* D-1, D-2

This is a review talk on symplectic self-consistent algorithms for the study of space-charge effects in particle accelerators. Starting from the Low Lagrangian for collision-less plasmas, I will show how to derive a Hamiltonian for relativistic beams in particle accelerators. From this Hamiltonian one can derive the evolution of the particle distribution as well as the self-field. Having obtained a discretized version of this Hamiltonian, I will discuss the use of

map methods to achieve self-consistent symplectic multi-particle tracking.

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## LONGITUDINAL BEAM DYNAMICS IN FRIB AND REA LINACS

**A.S. Plastun**, P.N. Ostroumov, A.C.C. Villari, Q. Zhao

Facility for Rare Isotope Beams, Michigan State University, 48824, East Lansing, MI, USA

*Classification:* E-2

The Front-End and first three cryomodules of the Facility for Rare Isotope Beam (FRIB) at Michigan State University (MSU) has been commissioned in July, 2018. The paper describes procedures developed for the online tuning of the longitudinal beam dynamics through the FRIB linac. These procedures include (a) an automated simulation-based tuning of the multi-harmonic buncher, (b) measurements and simulations of the RFQ threshold voltage and longitudinal acceptance, (c) RF phase scans of the rebunchers and superconducting accelerating cavities. While FRIB is being commissioned, the reaccelerator (ReA3) for rare isotope beams (RIBs) is being upgraded. In order to match any ReA3 beam both to the following upgrade cryomodules and physics experiments' requirements, room temperature rebunchers/debunchers are being designed. The design procedure includes the electromagnetic, thermal and mechanical simulations and optimizations.

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## MAGNETIZED ELECTRON COOLING SIMULATIONS FOR JLEIC

**Ilya Pogorelov** (1), David Bruhwiler (1), Christopher Hall (1), Stephen Webb (1), Dan Abell (1), Yury Eidelman (1), Johan Carlsson (1), James Gerity (2), Peter McIntyre (2)

(1) RadiaSoft LLC, (2) Texas A&M U.

*Classification:* D-1, D-2, F-1, A-2

Relativistic magnetized electron cooling in untested parameter regimes is essential to achieve the ion luminosity requirements of proposed electron-ion collider (EIC) designs. Therefore, accurate calculations of magnetized dynamic friction are required, with the ability to include all relevant physics that might increase the cooling time, including space charge forces, field errors and complicated phase space distributions of imperfectly magnetized electron beams. We present simulations relevant to the JLEIC design, using the BETACOOOL and JSPEC codes. We also present recent work on Warp simulations of the electron beam through the solenoid field. Space charge neutralization is provided by impact ionization of a background hydrogen gas. For optimal cooling it is essential that space charge be sufficiently neutralized. We also present recent work on a new analytic treatment of momentum transfer from a single magnetized electron to a drifting ion, and its use for calculations of dynamic friction. This work is supported by the U.S. DOE Office of Science, Office of Nuclear Physics, under Award Number DE-SC0015212.

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## APPROACHES TO OPTIMIZING SPIN TRANSMISSION IN LATTICE DESIGN

Vahid Ranjbar

BNL

*Classification:* D-2, E-2, A-2

We present our experiences in optimizing the proposed Rapid Cycling Synchrotron (RCS) injector for the eRHIC Storage ring and the RHIC 2017 lattice. We have developed python code to drive lattice calculations in MADX which are then used to calculate spin resonances using the DEPOL algorithm. This approach has been used to minimize intrinsic spin resonances during the RCS acceleration cycle while controlling lattice parameters such as dispersion and beta functions. This approach has also been used to construct localized imperfection bumps using a spin response matrix and SVD. This approach has also been used to reduce interfering intrinsic spin resonances during the RHIC acceleration ramp.

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## MACHINE LEARNING FOR X-RAY FREE-ELECTRON LASERS

Daniel Ratner

SLAC

*Invited Talk*

*Classification:* B-1, E-2, F-2

X-ray Free Electron Lasers (XFELs) are among the most complex accelerator projects in the world today. With large parameter spaces, sensitive dependence on beam quality, huge data rates, and challenging machine protection, there are expanding opportunities to apply machine learning (ML) to XFEL operation. In this talk I will summarize some promising ML methods for XFELs, and highlight recent examples of successful applications.

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## SIMULATIONS OF LONGITUDINAL BEAM STABILITY IN THE CERN SPS WITH BLOND

J. Repond, K. Iliakis, I. Karpov, A. Lasheen, D. Quartulo,  
M. Schwarz, E. Shaposhnikova, H. Timko

CERN

*Classification:* D-1, F-1

The Super Proton Synchrotron (SPS) at CERN, the Large Hadron Collider (LHC) injector, is currently pushed to its limits for the production of the LHC proton beam while beam quality and stability in the longitudinal plane are influenced by many effects. Particle simulation codes become an essential tool to study the beam instabilities. BLOND, developed at CERN, is a 2D particle-tracking simulation code, modeling the phase space of single and multi-bunch beams in multi-harmonic RF systems. Computation of collective effects due to the machine impedance and space charge is available on a multi-turn basis. Various beam

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## EFFICIENT COMPUTATION OF LOSSY HIGHER ORDER MODES IN COMPLEX SRF CAVITIES USING REDUCED ORDER MODELS AND NONLINEAR EIGENVALUE PROBLEM ALGORITHMS

Hermann W. Pommerenke, Johann D. Heller, Ursula van Rienen

Institute of General Electrical Engineering, University of Rostock, Germany

*Invited Talk*

*Classification:* C-2

Superconducting radio frequency (SRF) cavities meet the demanding performance requirements of modern accelerators and high-brilliance light sources. For the operation and design of such resonators, a very precise knowledge of their electromagnetic resonances is required. The non-trivial cavity shape demands a numerical solution of Maxwell's equations to compute the resonant eigenfrequencies, eigenmodes, and their losses. For large and complex structures this is hardly possible on conventional hardware due to the high number of degrees of freedom required to obtain an accurate solution. Here, we propose a method which can solve the considered problems on workstation computers without extensive simplification of the structure itself. First, the State-Space Concatenation scheme (SSC) is applied to the complex, closed and thus lossless RF structure. SSC employs a combination of model order reduction and domain decomposition, greatly reducing the computational effort by effectively constraining the considered frequency domain. Next, a perturbation approach based on SSC is used to describe the resonances of the same geometry subject to external losses. Due to the boundary conditions this results in a nonlinear eigenvalue problem (NLEVP). The NLEVP can be solved efficiently by Newton's method, or in combination with a contour integral algorithm. We present the general workflow to compute the electromagnetic resonances with an emphasis given to the algorithm used to solve the arising NLEVP.

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## ADVANCES IN SIMULATION OF HIGH BRIGHTNESS/HIGH INTENSITY BEAMS

Ji Qiang

LBNL

*Plenary Talk*

*Classification:* D-1

Large-scale advanced modeling of high intensity/high brightness beams plays an important role in beam dynamics study and accelerator design. In this paper, we report on recent progress in start-to-end simulation of high brightness electron beam in x-ray FEL accelerator and progress in long-term tracking simulation of space-charge effects in high intensity proton beam.

control loops of the RF system are implemented (phase, frequency and synchro-loops, and one-turn delay feedback) as well as RF phase noise injection used for controlled emittance blow-up. The challenges of the longitudinal beam stability simulations during long SPS acceleration cycle (19.93 s) are the variety of effects impacting beam dynamics (beam loading, instabilities, particle losses, controlled blow-up, double RF system operation, low-level RF control, bunch distribution, etc.), the complicated SPS impedance model containing broad and narrow-band resonant modes between 50 MHz and 4 GHz, and the large number of bunches in the nominal LHC batch (288). This paper presents a selection of BLonD simulation studies addressing these challenges and with results substantiated, when possible, by beam measurement data.

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### OPTIMIZATION STUDIES FOR THE K12 BEAM LINE AT THE CERN NORTH AREA

M. Rosenthal (1), D. Banerjee (1), J. Bernhard (1), M. Brugger (1), N. Charitonidis (1), B. Döbrich (1), L. Gagnon (1), A. Gerbershagen (1), E. Montbarbon (1), B. Rae (1), T. Spadaro (2), **M. van Dijk** (1)

(1) CERN, 1211 Geneva 23, Switzerland, (2) Laboratori Nazionali di Frascati, I-00044 Frascati, Italy

*Classification:* A-2, F-1, A-1

The North Area at the Super Proton Synchrotron at CERN has a long history of fixed target experiments and R&D studies. The 400 GeV/c proton beam is extracted from the SPS and guided to two experimental halls (EHN1, EHN2) and an underground cavern (ECN3) located at the CERN Prévessin site. Currently, ECN3 hosts the NA62 experiment studying rare decays of positively charged kaons into pions and two neutrinos. The required high-intensity kaon beam is provided by a new secondary beam line, designated K12, which was constructed in 2012. At its start, the primary proton beam impinges on a beryllium target (T10) with a nominal intensity of  $3E12$  protons per burst. The momentum selection is performed by a massive dump collimator (TAX), which is surrounded by four bending magnets in an achromat configuration. A future proposal for NA62 within the Physics Beyond Colliders (PBC) framework suggests the search for dark sector particles such as heavy neutral leptons, dark photons and axions. For this purpose, the T10 target will be moved out, dumping the primary proton beam on the 3.2 m long TAX. Muons originating in these interactions are a severe background for this kind of experiment, demanding an effective magnetic sweeping along the beam line. The simulation of production and transport of this muon background is computationally highly expensive and requires precise magnetic field information of the entire beam line. Monte Carlo studies based on the program G4Beamline combined with analytical parametrisations are used to reduce the computational demands. In this contribution, benchmarking results with already recorded data as well as results from the optimization studies will be presented.

### NONLINEAR OPTICS AT UMER

**Kiersten Ruisard**, Brian Beaudoin, Irving Haber,  
Timothy Koeth

ORNL, University of Maryland

*Invited Talk*

*Classification:* D-1

Design of accelerator lattices with nonlinear optics to suppress transverse resonances is a novel approach and may be crucial for enabling low-loss high-intensity beam transport. Large amplitude-dependent tune spreads, driven by nonlinear field inserts, damp resonant response to driving terms. This presentation will focus on simulations of the UMER lattice operated as a quasi-integrable system (1 invariant of transverse motion) with a single strong octupole insert. We will discuss the evolution of simulation models, including the observation of losses associated with the original operating point near a fourth-order resonance. Other operating points farther from this resonance are considered and shown to be more promising.

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### CHALLENGES IN EXTRACTING PSEUDO-MULTIPOLES FROM MAGNETIC MEASUREMENTS

**Stephan Russenschuck**, Gianni Caiafa, Melvin Liebsch,  
Carlo Petrone

CERN, 1211 Geneva 23, Switzerland

*Classification:* C-1

Extracting the coefficients of the Fourier-Bessel series (known as pseudo-multipoles or generalized gradients) from magnetic measurements of accelerator magnets bears some technical and mathematical challenges. A novel design of a short, rotating-coil magnetometer is required that does not intercept any longitudinal field components. Moreover, displacing short magnetometers step-by-step along the axis of the magnet, delivers a signals for the transversal multipoles that are convolutions of the multipoles and the sensitivity of the induction coil. The deconvolution of the measured signals has then to deal with the (noisy) measurement data from the magnetometer. Moreover, the compensation schemes for the main component, as implemented in long coils used for the integrated harmonics, cannot be applied to the short magnetometers. The paper presents the theory of the data acquisition and deconvolution, as well as the design and production of a rotating-coil magnetometer that consists of four layers of flexible printed circuit mounted on a precision machined shaft. The design aimed at maximizing the sensitivity factors for field harmonics up to order 13 and at a compensation (bucking) ratio for the main component in the same range of what is achievable with standard rotating coils. The design, the uncertainty analysis (yielding the manufacturing tolerances), the manufacturing challenges, and the results of dipole and quadrupole field scans will be presented. Ref: [1] Berz, M.: Modern Map Methods in Particle Beam Physics, Academic Press, 1999. [2] Russenschuck, S.: Rotating- and translating-coil magnetometers for extracting pseudo-multipoles in accelerator magnets, COMPEL - The international journal for computation and mathematics in electrical

and electronic engineering, Vol. 36 Issue: 5, 2017 [3] Arpaia, P., Buzio, M., De Matteis, E., Russenschuck, S.: A rotating coil transducer for magnetic field mapping, Jinst, 2015.

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## COMPUTATIONAL ACCELERATOR PHYSICS: ON THE ROAD TO EXASCALE

**Robert D Ryne**

Lawrence Berkeley National Laboratory

*Plenary Talk*

*Classification:* F-2

The first conference in what would become the ICAP series was held in 1988. At that time the most powerful computer in the world was a Cray YMP with 8 processors and a peak performance of about 2 gigaflops. Today the fastest computer in the world has more than 2 million cores and a theoretical peak performance of nearly 200 petaflops. Compared to 1988, performance has increased by a factor of 100 million, accompanied by huge advances in memory, networking, big data management and analytics, etc. By the time of the next ICAP conference in 2021 we can expect to be living with the first exascale computers. In this talk I will describe the advances that have taken place in computational accelerator physics since this conference series began, with emphasis on current examples ranging from 1000's of cores up to the petascale, and describe what to expect in the exascale regime of the future.

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## REPTIL - A RELATIVISTIC 3D SPACE CHARGE PARTICLE TRACKING CODE BASED ON THE FAST MULTIPOLE METHOD

**Steffen Schmid, Erion Gjonaj, Herbert De Gerssem**

TU Darmstadt, TEMF

*Classification:* D-1

Modern free electron lasers and high current energy recovery linacs accelerate electron beams with particle bunch charges reaching up to several nanocoulombs. Especially in the low energy sections, such as the photoinjector of the accelerator, space charge interaction forces are the dominating effect influencing the dynamics of the electron beam. A direct computation of space charge forces is numerically very expensive. Commonly used simulation codes typically apply mesh based particle-in-cell methods (PIC) to solve this problem. Our simulation tool, REPTIL, is a relativistic, three-dimensional space charge tracking code, which computes the interaction forces based on a meshless fast multipole method (FMM). The FMM based space charge solver is more flexible regarding the choice of the interaction model and yields maximum accuracy for the near field forces between particles. For this reason, the FMM is very suitable for the simulation of the influence of space charge on the particle emission process in high current photoinjectors. In this contribution, we present a numerical study of the efficiency and the accuracy of the method. Therefore, we perform a case study for the PIZ

photoinjector used for the European XFEL at DESY. Furthermore, we compare the performance of REPTIL with commonly used PIC codes like e.g. ASTRA. Finally, we investigate a hybrid approach by using the FMM on a mesh. The latter method makes further increases in the particle number possible, which translates to a higher resolution in the phase space of the electron bunch.

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## UPDATE ON THE STATUS OF LINAC PART OF THE PYORBIT CODE

**Andrei Shishlo**

Oak Ridge National Lab

*Classification:* F-1

The structure and capabilities of the linac beam dynamics part of the PyORBIT code are presented. The PyORBIT is an open source code, a descendant of the original ORBIT code that was developed at the Spallation Neutron Source (SNS) for design, commissioning, and studies of the ring. The linac part was started 8 years ago to utilize PyORBIT classes and infrastructure for the SNS linac simulations. The PyORBIT linac model has its own lattice description that is necessary to include lattice elements significantly different from the PyORBIT ring elements. The most important among them are accelerating RF structures. The five different RF gap models recently implemented in PyORBIT are discussed. Some benchmarks of the PyORBIT with Parmila, the XAL Online Model, and TraceWin code are presented.

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## MUON G-2: AN INTERPLAY OF BEAM DYNAMICS AND HEP

**Michael Syphers**

Northern Illinois University

*Classification:* A-2, D-1

The Fermilab experiment E989, Muon g-2, unites particle beam physics with a high energy physics experiment in a unique way. The close interplay of the understanding of particle beam dynamics and the preparation of the beam properties with the experimental measurement is tantamount to the reduction of systematic errors in the determination of the anomalous magnetic moment of the muon to unprecedented precision. The precision of the g-2 measurement will be increased by a factor of two over the most recent case (BNL, E821) mostly due to the increased statistics offered by the higher proton flux delivered by the Fermilab accelerators. However, it is possible that even further gains can be made through a better understanding of the muon beam being delivered to the g-2 Storage Ring. Several effects come into play that can contribute to systematic errors and for which detailed calculations and modeling of the incoming muon beam properties will aid in interpreting the results. Various correlations of spin and momentum, spin and position along the bunch, etc., will become important to understand during the analysis of the experiment's data sets. While orders of magnitude of these types of effects are

straightforward to estimate, detailed calculations and experimental verification of beam properties will be necessary to contribute to the sub-ppm accuracy of the g-2 measurement.

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## BEAM DYNAMICS SIMULATIONS OF THE MUON G-2 EXPERIMENT BEAMLINES AT FERMILAB

David Tarazona, Martin Berz, Kyoko Makino

Michigan State University

*Classification:* D-1, D-2, A-2

The main goal of the Muon g-2 Experiment (g-2) at Fermilab is to measure the muon anomalous magnetic moment to unprecedented precision. This new measurement will allow to test the completeness of the Standard Model (SM) and to validate other theoretical models beyond the SM. Simulations of the beamlines from the pion production target to the entrance of the g-2 Storage Ring using COSY INFINITY have contributed to the understanding of several factors that affect the systematics and statistical uncertainties of the anomaly measurement. Nonlinearities, spin dynamics, muon production, are some of the beam properties analyzed from high-order simulations that consider fringe fields, misalignments, and other errors intrinsic to the beamlines.

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## SEAMLESS BEAM AND RADIATION TRANSPORT SIMULATIONS OF IBA PROTEUS SYSTEMS USING BDSIM

Robin Tesse (1), Stewart Boogert (2), Alain Dubus (1), Eustache Gnacadja (1), Cédric Hernalsteens (3), Laurence J. Nevay (2), Nicolas Pauly (1), William Shields (2)

(1) Université libre de Bruxelles (2) John Adams Institute at Royal Holloway, University of London (3) Ion Beam Applications (IBA)

*Classification:* A-2

The precise modeling of proton therapy systems is challenging and requires simulation tools that have capabilities in both beam transport and in the detailed description of particle-matter interactions. Current separate simulations such as those of optical codes or Monte-Carlo transport through discrete elements show their limitations due to the very strict requirements on beam quality at the isocenter. This is particularly relevant with the development of compact systems where the coupling between the components is dominant. For such systems the design of the concrete shielding, which has a large impact on the total cost of the system, is of primary importance. Beam Delivery Simulation (BDSIM) allows the seamless simulation of the transport of particles in a beamline and its surrounding environment. A complete 3D model is built using Geant4, CLHEP and ROOT to provide an extensive insight into beam loss, its interaction and subsequent radiation. This capability is applied to the IBA eye treatment proton therapy machine and to the IBA Proteus One compact system. We discuss the validation of both models against experimental data. In particular, we use it to predict lateral profiles and energy spectra using a detailed geometry of the eye-treatment

beam forming nozzle. For the Proteus One system, we present results on the activation of the concrete shielding of the system estimated after a period of 20 years of operation obtained for the first time using end-to-end simulations of the transport of protons in the beamline and their interactions with the environment.

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## MULTI PASS ERL DESIGN WITH A SINGLE FIXED FIELD MAGNET RETURN LINE

Dejan Trbojevic, Stephen Brooks, Francois Meot, Nick Tsoupas, J. Scott Berg, William Lou(2)

BNL and Cornell University

*Classification:* A-2

We present a new approach of the Energy Recovery Linac Design for the future projects: PERLE (Powerful Energy Recovery Linac for Experiments), LHeC/FCCeH and eRHIC. The concept uses superconducting linacs and a single fixed field beam lines with multiple energy passes of electron beams. This represents an update to the existing CBETA (Cornell University Brookhaven National Laboratory ERL Test Accelerator) where the superconducting linac uses a single fixed field magnet beam line with four times in energy acceleration and four passes for the energy recovery through the same single structure. To match the single fixed field beam line to the linac the CBETA uses the spreaders and combiners on both sides of the linac, while the new concept eliminates them. The arc cells from the single fixed field beam line are connected to the linac with an adiabatic transition arcs where its cells increase in length. The orbits of different energies merge into a single orbit through the interleaved linac within the straight sections as in the CBETA project. The betatron functions from the arcs are matched to the linac and the time of flight of different electron energies is adjusted for the central orbits by added kicker controlled induced beam oscillations.

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## COMPUTATION AND MEASUREMENT OF ABERRATIONS FOR ABERRATION CORRECTED ELECTRON MICROSCOPY

Rudolf M. Tromp

IBM T.J. Watson Research Center

*Invited Talk*

*Classification:* A-2, E-2

Computation and measurement of geometric and chromatic aberrations is critical for the optimal design and use of aberration corrected electron microscopes, and for quantitative understanding of images obtained with such instruments. Here, I will focus on the correction of spherical and chromatic aberrations of a cathode lens instrument (i.e. Low Energy Electron Microscope -LEEM- or Photo Electron Emission Microscope -PEEM) using catadioptrics, i.e. a combination of electron lenses (dioptrics) and an electron mirror (catoptrics). First-order properties calculated with high precision using Munro's Electron Beam Software's MİRDA package are in excellent with detailed experimental results. Theoretical maps of C3 vs Cc as a function of

the applied potentials then provide a deterministic method to dial in the desired mirror properties at will. Now it is necessary to measure the resultant aberrations of the full system. Unfortunately, the experimental methods developed for TEM and STEM are not applicable in LEEM/PEEM for a variety of reasons. Spherical aberration (plus defocus and astigmatism) can be measured using so-called micro-spot real-space Low Energy Electron Diffraction, or by measuring image shift as a function of beam tilt. Measuring chromatic aberration is more troublesome as it conventionally requires that defocus be measured as a function of gun voltage. However, the use of magnetic prism arrays to separate in- and outgoing path in LEEM results in changing alignment conditions when gun voltage is changed. However, a novel method first demonstrated using ray-tracing simulations enables us to measure chromatic aberration, even at fixed gun voltage. The chromatically corrected system behaves like a simple (but adjustable) achromat, comparable to the crown/flint optical achromat invented by Chester Moore Hall around 1730.

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### CALCULATION OF THE AGS OPTICS BASED ON 3D FIELDS DERIVED FROM EXPERIMENTALLY MEASURED FIELD MAPS ON THE MEDIAN PLANE

N. Tsoupas†, J. S. Berg, S. Brooks, F. Méot, V. Ptitsyn, D. Trbojevic

Brookhaven National Laboratory

*Classification:* F-1

Closed orbit calculations of the AGS synchrotron were performed and the beam parameters at the extraction point of the AGS [1] were calculated using the RAYTRACE computer code [2] which was modified to generate 3D fields from the experimentally measured field maps on the median plane of the AGS combined function magnets. The algorithm which generates 3D fields from field maps on a plane is described in reference [3] which discusses the details of the mathematical foundation of this approach. In this presentation we will discuss results from studies [1,4] that are based on the 3D fields generated from the known field components on a rectangular grid of a plane. A brief overview of the algorithm used will be given, and two methods of calculating the required field derivatives on the plane will be presented. The calculated 3D fields of a modified Halbach magnet [5] of inner radius of 4.4 cm will be calculated using the two different methods of calculating the field derivatives on the plane and the calculated fields will be compared against the “ideal” fields as calculated by the OPERA computer code [6]. \*Work supported by the US Department of Energy †tsoupas@bnl.gov [1] N. Tsoupas et. al. “Closed orbit calculations at AGS and Extraction Beam Parameters at H13” AD/RHIC/RD-75 Oct. 1994 [2] S.B. Kowalski and H.A. Enge “The Ion-Optical Program Raytrace” NIM A258 (1987) 407 [3] K. Makino, M. Berz, C. Johnstone, Int. Journal of Modern Physics A 26 (2011) 1807-1821 [4] N. Tsoupas et. al. “Effects of Dipole Magnet Inhomogeneity on the Beam Ellipsoid” NIM A258 (1987) 421-425 [5] “The CBETA project: arXiv.org > physics > arXiv:1706.04245” [6] Vector Fields Inc. <https://operafea.com/>

### MAIN AND FRINGE FIELD COMPUTATIONS FOR THE ELECTROSTATIC QUADRUPOLES OF THE MUON G-2 EXPERIMENT STORAGE RING

Eremey Valetov and Martin Berz

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*Classification:* C-2

We consider semi-infinite electrostatic deflectors with plates of different thickness, including plates with rounded edges, and we calculate their electrostatic potential and field using conformal mappings. To validate the calculations, we compare the fringe fields of these electrostatic deflectors with fringe fields of finite electrostatic capacitors, and we extend the study to fringe fields of adjacent electrostatic deflectors with consideration of electrostatic induction, where field falloffs of semi-infinite electrostatic deflectors are slower than exponential and thus behave differently from most magnetic fringe fields. Building on the success with electrostatic deflectors, we develop a highly accurate and fully Maxwellian conformal mappings method for calculation of main fields of electrostatic particle optical elements. A remarkable advantage of this method is the possibility of rapid recalculations with geometric asymmetries and mispowered plates. We use this conformal mappings method to calculate the multipole terms of the high voltage quadrupole used in the storage ring of the Muon g-2 Experiment (FNAL-E-0989). Completing the methodological framework, we present a method for extracting multipole strength falloffs of a particle optical element from a set of Fourier mode falloffs. We calculate the quadrupole strength falloff and its effective field boundary (EFB) for the Muon g-2 quadrupole, which has explained the experimentally measured tunes, while simple estimates based on a linear model exhibited discrepancies up to 2%.

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### THE FAST/IOTA PROJECT AT FERMILAB

Alexander Valishev

Fermi National Accelerator Laboratory

*Plenary Talk*

*Classification:* A-1

The Fermilab Accelerator Science and Technology (FAST) facility is being developed as a fully-equipped accelerator chain intended to support research and development of accelerator technology for the next generation of particle accelerators. The primary focus of this effort is the Integrable Optics Test Accelerator (IOTA) ring, which will be able to circulate either electrons with the energy of up to 150MeV, or 2.5MeV protons. The FAST electron injector is a state of the art superconducting RF linac capable of full ILC beam parameters and beam energy of up to 300MeV. The FAST accelerator science program focuses on high-intensity and high-brightness issues in the future machines for high-energy physics research. This talk will describe the facility design and status, review key beam physics experiments, and discuss the computational needs associated with the IOTA/FAST research.

## PARALLEL ALGORITHMS FOR SOLVING NONLINEAR EIGENVALUE PROBLEMS IN ACCELERATOR CAVITY SIMULATIONS

Roel Van Beeumen

Lawrence Berkeley National Laboratory

### *Invited Talk*

*Classification:* F-2

We present an efficient and reliable algorithm for solving a class of nonlinear eigenvalue problems arising from the modeling of particle accelerator cavities. The eigenvalue nonlinearity in these problems results from the use of waveguides to couple external power sources or to allow certain excited electromagnetic modes to exit the cavity. We use a rational approximation to reduce the nonlinear eigenvalue problem first to a rational eigenvalue problem. We then apply a special linearization procedure to turn the rational eigenvalue problem into a larger linear eigenvalue problem with the same eigenvalues, which can be solved by existing iterative methods. By using a compact scheme to represent both the linearized operator and the eigenvectors to be computed, we obtain a numerical method that only involves solving linear systems of equations of the same dimension as the original nonlinear eigenvalue problem. We refer to this method as a compact rational Krylov (CORK) method. We implemented the CORK method in the Omega3P module of the Advanced Computational Electromagnetic 3D Parallel (ACE3P) simulation suite and validated it by comparing the computed cavity resonant frequencies and damping Q factors of a small model problem to those obtained from a fitting procedure that uses frequency responses computed by another ACE3P module called S3P. We also used the CORK method to compute trapped modes damped in an ideal eight 9-cell SRF cavity cryomodule. This was the first time it was possible to compute these modes directly. The damping Q factors of the computed modes match well with those measured in experiments and the difference in resonant frequencies is within the range introduced by cavity imperfection. Therefore, the CORK method is an extremely valuable tool for computational cavity design.

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## A NEW FINITE ELEMENT SOLVER FOR MOEVE PIC TRACKING

Ursula van Rienen<sup>1,2</sup>, Dawei Zheng<sup>1</sup>, Johann Heller<sup>1</sup>,  
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*Classification:* D-1

A relevant task in designing high-brilliance light sources based on high-current linear accelerators (e.g. Energy Recovery Linacs “ERLs”) consists in systematic investigations of ion dynamics in the vacuum chamber of such machines. This is of high importance since the parasitic ions generated by the electron beam turned out to be a current-limiting factor for many synchrotron

radiation sources. In particular, the planned high current operation at ERL facilities requires a precise analysis and an accurate development of appropriate measures for the suppression of ion-induced beam instabilities. The longitudinal transport of ions through the whole accelerator plays a key role for the establishment of the ion concentration in the machine. Using the Particle-in-Cell (PIC) method, we redesigned our code MOEVE PIC Tracking in order to allow for the fast estimation of the effects of ions on the beam dynamics. For that, we exchanged the previously used Finite Difference (FD) method for the solution of Poisson’s equation within the PIC solver by a solver based on the Finite Element Method (FEM). Employing higher order FEM, we expect to gain improved convergence rates and thus lower computational times. We chose the Open Source Framework FEniCS for our new implementation. With regard to a better performance, we also studied an adaptive grid refinement together with higher order approaches. We investigated certain strategies with regard to compromises between accuracy and performance in the need of further refinement in a certain time step. Aiming to apply again the Boris pusher for the update in particle position, we examined several possibilities for an efficient determination of the particle position.

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## BEAM DYNAMICS SIMULATIONS OF MEDICAL CYCLOTRONS AND BEAM TRANSFER LINES AT IBA

Jarno Van de Walle<sup>(1)</sup>, Willem Kleeven<sup>(1)</sup>, Vincent Nuttens<sup>(1)</sup>, Erik Van der Kraaij<sup>(1)</sup> Jerome Mandrillon<sup>(1)</sup>, Eric Forton<sup>(1)</sup>, Cedric Hernalsteens<sup>(1)</sup>

<sup>(1)</sup> Ion Beam Applications, Louvain-la-Neuve, Belgium

*Classification:* F-1, A-2, D-1

The company Ion Beam Applications (IBA), based in Belgium, is specialized in the design and fabrication of cyclotrons for medical applications since more than 30 years. Two main classes of cyclotrons can be distinguished : cyclotrons for radiopharma production (3 MeV up to 70 MeV proton beams) and cyclotrons used in proton therapy (230 MeV proton beam). In this contribution, the developments of computational tools to simulate beam dynamics in the variety of cyclotrons and associated beam lines will be described. The main code for simulating the cyclotron beam dynamics is the “Advanced Orbit Code” (AOC) [1]. Examples will be shown of beam dynamics studies in the newly designed Cyclone KIUBE (18 MeV proton cyclotron for PET isotope production), the Cyclone230 and the superconducting synchro-cyclotron (S2C2), both 230 MeV proton cyclotrons for proton therapy. Calculated beam emittances, resonance crossings and beam losses will be shown and their impact on the performance of the machine will be highlighted. A strong emphasis will be put on the beam properties from the S2C2 (proton therapy cyclotron), since unexpected extracted proton beam was discovered and explained by detailed simulations [2] and the beam properties serve as input to subsequent beam line simulation tools. Several tools have been developed to simulate and design transfer lines coupled to the cyclotrons. In radiopharma applications beam losses along the beamline and the beam size on the production target are crucial, since beam intensities are

high and radiation damage can be considerable. In proton therapy, beam intensities are very low but the constraints on the beam position, drift (in position, energy and intensity) and size at the patient level are very tight. In both cases a strong predictive power of the calculated beam properties in the transfer lines is needed. The compact proton gantry (CGTR) coupled with the S2C2 in the ProteusONE proton therapy system will be shown in detail. The CGTR is a spectrometer with sensitive beam diagnostics devices and enables us to detect small fluctuations of the extracted beam properties. Measurements and calculations of the proton beam in the CGTR will be used to illustrate the performance of the calculation tools. [1] W. Kleevan et al., IPAC 2016 proceedings, TUPOY002 [2] J. Van de Walle et al., Cyclotrons2016 proceedings, THB01

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### MODE-ANALYSIS METHODS FOR THE STUDY OF COLLECTIVE INSTABILITIES IN ELECTRON-STORAGE RINGS

**Marco Venturini**

LBNL

*Classification:* B-1, A-2, D-1

We report on recent progress on the application of mode analysis to the study of collective instabilities in electron storage rings including Higher Harmonic RF Cavities (HHCs). The focus is on transverse instabilities in the presence of a dominant resistive-wall impedance, a problem of particular relevance to the new generation of diffraction-limited light sources. The secular equation for the system eigenvalues is solved after applying a regularizing transformation, a key step to obtaining numerically accurate solutions. We provide a demonstration that for vanishing chromaticity and in the absence of radiation damping the beam motion is always unstable. This is in contrast to the more conventional Transverse-Mode-Coupling Instability (TMCI) without HHCs, which is known to exhibit a well defined instability threshold.

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### ANALYTICAL CALCULATIONS FOR THOMSON-BACKSCATTERING BASED-LIGHT SOURCES

**Paul Volz**, Atoosa Meseck

Helmholtz-Zentrum Berlin

*Classification:* F-1, A-2

There is a rising interest in Thomson-backscattering based-light sources, as scattering intense laser radiation on MeV electrons produces high energy photons that would require GeV or even TeV electron beams when using conventional undulators or dipoles. Particularly, medium energy high brightness beams delivered by LINACs or Energy Recovery LINACs, such as bERLinPro being built at Helmholtz-Zentrum Berlin, seem suitable for these sources. In order to study the merit of Thomson-backscattering-based light sources, we are developing an analytical code to simulate the characteristics of the Thomson scattered

radiation. The code calculates the distribution of scattered radiation depending on the incident angle and polarization of the laser radiation. Also the impact of the incident laser profile and the full 6D bunch profile, including microbunching, are incorporated. The Status of the code and first results will be presented.

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### A HOLISTIC APPROACH TO SIMULATING BEAM LOSSES IN THE LARGE HADRON COLLIDER USING BDSIM

**Stuart Walker**, Andrey Abramov, Stewart Boogert, Hector Garcia Morales, Stephen Gibson, Helena Pikhartova, William Shields, Laurie Nevay

Royal Holloway, University of London

*Classification:* F-1, A-2

To fully understand the beam losses, subsequent radiation, energy deposition and activation in particle accelerators, a holistic approach combining a 3-D model, physics processes and accelerator tracking is required. Beam Delivery Simulation (BDSIM) is a program developed to simulate the passage of particles, both primary and secondary, in particle accelerators and calculate the energy deposited by these particles via material interactions using the Geant4 physics library. A Geant4 accelerator model is built from an existing optical description of a lattice by procedurally placing a set of predefined accelerator components. These generic components can be refined to an arbitrary degree of detail with the use of user-defined geometries, detectors, field maps, and more. A detailed model of the Large Hadron Collider has been created in BDSIM, validated with existing tracking codes and applied to study beam loss patterns. The simulated beam loss monitor response is compared with data from individual BLMs placed around the LHC.

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### SHINE: SHANGHAI HIGH REP-RATE XFEL AND EXTREME LIGHT FACILITY

**Dong Wang** and Weishi Wan

Chinese Academy of Sciences/ShanghaiTech University

*Classification:* A-1

SHINE(Shanghai High Rep-rate XFEL and Extreme Light Facility) is a Free Electron Laser facility providing intense x-ray photons at soft and hard X-ray regimes with high repetition rate up to 1 MHz. This new facility is located at Zhangjiang National Comprehensive Science Center, Shanghai, where also hosts other large facilities on photon science including Shanghai Synchrotron Radiation Facility(SSRF) and Soft X-ray Free Electron Laser Facility(SXFEL). With an overall length of about 3.1km the SHINE facility consists a linear accelerator yielding up to 8 GeV electron beam, 3 long FEL undulator lines producing 0.4-25 keV coherent photons and 10 endstations for user experiments. The ground breaking of project took place in April, 2018. This talk will present the status of SHINE facility with an emphasis on accelerator machine.

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## THEORETICAL AND COMPUTATIONAL MODELING OF A PLASMA WAKEFIELD BBU INSTABILITY

**Stephen Webb**, David Bruhwiler, Alexey Burov, and  
Sergei Nagaitsev

RadiaSoft, LLC, RadiaSoft, LLC, Fermi National  
Accelerator Lab, Fermi National Accelerator Lab

**Invited Talk**

**Classification:** B-2, D-1

Plasma wakefield accelerators achieve accelerating gradients on the order of the wave-breaking limit,  $mc^2 k_p / e$ , so that higher accelerating gradients correspond to shorter plasma wavelengths. Small-scale accelerating structures, such as plasma and dielectric wakefields, are susceptible to the beam break-up instability (BBU), which can be understood from the Panofsky-Wenzel theorem: if the fundamental accelerating mode scales as  $b^{-1}$  for a structure radius  $b$ , then the dipole mode must scale as  $b^{-3}$ , meaning that high accelerating gradients necessarily come with strong dipole wake fields. Because of this relationship, any plasma-accelerator-based future collider will require detailed study of the trade-offs between extracting the maximum energy from the driver and mitigating the beam break-up instability. Recent theoretical work\* predicts the tradeoff between the witness bunch stability and the amount of energy that can be extracted from the drive bunch, a so-called “efficiency-instability relation”. We will discuss the beam break-up instability and the efficiency-instability relation and the theoretical assumptions made in reaching this conclusion. We will also present preliminary particle-in-cell simulations of a beam-driven plasma wakefield accelerator used to test the domain of validity for the assumptions made in this model. \* V. Lebedev, A. Burov, and S. Nagaitsev, “Efficiency versus instability in plasma accelerators”, Phys. Rev. Acc. Beams 20, 121301 (2017).

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## ADVANCES IN ACCELERATOR MODELING WITH PARALLEL MULTI-PHYSICS CODE SUITE ACE3P

**Liling Xiao**, Lixin Ge, Zenghai Li, Cho-Kuen Ng

SLAC National Accelerator Laboratory

**Classification:** C-2, E-1

ACE3P is a comprehensive set of parallel finite-element codes for multi-physics modeling of accelerator structures including integrated electromagnetic, thermal and mechanical effects. Recent advances of ACE3P have been focused on the development of multi-physics modeling capabilities, implementation of advanced numerical algorithms, and improvement of code performance on state-of-the-art high-performance computing (HPC) platforms for large-scale accelerator applications. A nonlinear eigensolver using the CORK algorithm [1] has been implemented in the eigensolver module Omega3P to enable accurate determination of damping factors of resonant modes above the

beampipe cutoff frequency. It has enabled the first-ever direct calculation of trapped modes in the TESLA TTF cryomodules, providing reliable damping factors that were validated against measurements. A newly developed mechanical eigensolver in the multi-physics module TEM3P has allowed the determination of mechanical modes in Fermilab PIP-II high beta 650 MHz cryomodule, demonstrating mode coupling between the 6 cavities in the cryomodule. To exploit multi-core computer architectures on supercomputers, a hybrid MPI+OpenMP parallel programming has been developed in the particle tracking module Track3P to speed up dark current simulation in multiple cavities for the LCLS-II linac. Highlights of these developments and their impacts on accelerator modeling using HPC will be presented. [1] R. Van Beeuman, Invited talk, this conference.

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## MEAN-FIELD DENSITY EVOLUTION OF BUNCHED PARTICLES WITH NON-ZERO INITIAL VELOCITY

**Brandon Zerbe**, Phil Duxbury

MSU

**Classification:** D-1

Reed(Reed 2006) presented a 1D mean-field model of initially cold pancake-beam expansion demonstrating that the evolution of the entire spatial distribution can be solved for all time where the 1D assumption holds. This model is relevant to ultra-fast electron microscopy as it describes the evolution of the distribution within the photoelectron gun, and this model is similar to Anderson’s sheet beam density time dependence(Anderson 1987) except that Reed’s theory applies to freely expanding beams instead of beams within a focussing channel. Our recent work(Zerbe 2018) generalized Reed’s analysis to cylindrical and spherical geometries demonstrating the presence of a shock that is seen in the Coulomb explosion literature under these geometries and further discussed the absence of a shock in the 1D model. This work is relevant as it offers a mechanistic explanation of the ring-like density shock that arises in non-equilibrium pancake-beams within the photoelectron gun; moreover, this shock is coincident with a region of high-temperature electrons providing an explanation for why experimentally aperturing the electron bunch results in a greater than 10-fold improvement in beam emittance(Williams 2017), possibly even resulting in bunch emittance below the intrinsic emittance of the cathode. However, this theory has been developed for cold-bunches, i.e. bunches of electrons with 0 initial momentum. Here, we briefly review this new theory and extend the cylindrical- and spherical-symmetric distribution to ensembles that have non-zero initial momentum distributions that are symmetric but otherwise unrestricted demonstrating how initial velocity distributions couple to the shocks seen in the less general formulation.

## FAST MULTIPOLE METHODS FOR MULTIPARTICLE SIMULATIONS

He Zhang

JLab

### *Invited Talk*

*Classification:* C-2, D-1, D-2

The fast multipole method (FMM) reduces the computation cost of the pairwise non-oscillating interaction between  $N$  particles from  $O(N^2)$  to  $O(N)$ . In the FMM, the contribution from a source particle is represented as a multipole expansion, while the contributions from multiple faraway sources can be combined into a local expansion around an objective particle. Without the dependence on a grid covering the whole domain under study, the FMM treats any charge distribution and geometry in a natural way. It avoids artificial smoothing due to the grid size and redundant computation on the free space grids. We will introduce the concept of the FMM using the Coulomb interaction as an example and then explain how the FMM can be extended to arbitrary non-oscillating interactions. Examples and discussions on how the FMM can be used in scientific simulations, especially in accelerator physics will also be provided.

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## GENERATION OF PARTICLE DISTRIBUTIONS AT RFQ EXIT AT SNS BEAM TEST FACILITY

Zhouli Zhang, A. Aleksandrov, S. Cousineau, A. Shishlo,  
A. Zhukov

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*Classification:* A-2, E-1

The first 6D phase space measurement are being conducted at the beam test facility (BTF) of SNS. Generation of 2D particle distributions are done first for preparation of reconstruction of 6D distributions. A back-tracking PIC simulation code is written and proved to be reliable. The concept of distribution discrepancy is proposed to evaluate the effects of fluctuations of beam parameters and uncertainties of quadrupole gradients on initial distributions at RFQ exit. Results suggest effects of fluctuations of beam parameters are very small, while initial particle distributions are mainly affected by quadrupole gradients. The initial particle distributions which are considered to be the closest to the real ones are generated when distribution discrepancies are very small in transverse phase spaces and are proved to be convincing by comparing measured distributions and distributions produced by tracking the initial distributions. The distribution discrepancy method in generation of initial particle distributions is confirmed to be practicable and can be used for reconstruction of 6D particle distributions.

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## NUMERICAL SIMULATIONS FOR GENERATING FULLY COHERENT SOFT X-RAY FREE ELECTRON LASERS WITH ULTRA-SHORT WAVELENGTH

Kaishang Zhou

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of Sciences

*Classification:* B-1

For the fully coherent, ultra-short and high power soft x-rays are becoming key instruments in different research fields, such as biology, chemistry or physics. However it's not easy to generate this kind of advantaged light source by conventional lasers, especially for the soft x-rays with ultra-short wavelength. The external seeded free electron laser (FEL) is considered as one feasible method. Here, we give an example to generate fully coherent soft x-rays with the wavelength 1nm by the two-stage cascaded FELs. The EEHG scheme is used in the first-stage while the HGHG scheme is used in the second-stage.

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