FINAL TECHNICAL REPORT

Department of Energy, Office of **Nuclear Physics**
Grant #: **DE-SC0008588**

STUDIES OF CONVENTIONAL AND ERL-BASED RE-CIRCULATOR ELECTRON COOLING FOR AN ELECTRON ION COLLIDER

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Grant period: **08/15/2012 – 08/14/2021**

Submission date: **January 3, 2023**

1. EXECUTIVE SUMMARY

The project developed the required tools and associated software framework that make possible, for the first time, microscopically correct modeling and simulations of electron cooling processes with a minimum number of assumptions. We did this by developing the most accurate, precise and efficient numerical algorithms for pair-wise charged particle interactions and propagation in time for large systems. We employed modern hardware solutions based on compute clusters combined with the state-of-the-art algorithms that scale well in parallel computations.

We performed the first electron cooling simulations based on first principles. The range of phenomena studied include low energy DC, as well as high energy coherent electron cooling. In addition, we proved the suitability of our new dynamical framework to be able to handle related beam physics processes such as Landau damping, conservative relaxation, beam echoes and the bump-on-tail of plasma physics.

As a consequence of these developments, we were able, also for the first time, to provide benchmarked results of our code against experimental data. The very good agreement with empirical results gives us the confidence to propose our numerical infrastructure to function as a de facto standard against any other electron cooling software that would employ further approximations to speed up time to solution. In sum, we now have proven that high fidelity electron cooling simulations and optimizations are starting to become feasible for future scientific endeavors, were these processes play a significant role in planned system performance, such as the future Electron-Ion Collider (EIC).

The software framework developed during the project is freely available for download along with documentation. Two physics Ph.D. were awarded at NIU based on research related to this project.

2. ACCOMPLISHEMENTS

Accomplishments are categorized according to the chronology of the final published products and described in the following subsections.

2.1. The Fast Multipole Method (FMM)

The first major accomplishment was the development of the best algorithmic structure for pair-wise particle-by-particle force computation [1]. It is well known that accurate and reliable electron cooling simulations need this, on one hand, and a naïve implementation would scale quadratically with the number of particles, on the other hand. Quadratic scaling makes impossible microscopic electron cooling simulations of systems with anything close to realistic size. The FMM has been shown to scale linearly, to be

highly parallelizable, possessing strong arithmetic intensity, and it compares advantageously with alternate force computation methods in the settings required by electron cooling.

A novel form of the fast multipole method is realized by the combination of adaptive data structures with implementation of the multipole expansions and their translations in Cartesian basis, and enabled by algorithmic differentiation. It may be possible to generalize it to any kernel that allows its formulation as a function of small quantities with respect to which they can be expanded. There is no hard and fast rule recipe that works for all cases. However, it is shown how to do it for the softened Coulomb kernel, which is different from the Coulomb kernel. The characteristics and performance of the method were mapped and shown to provide an attractive option for a generic fast multipole algorithm in a wide region of parameter space. The algorithm was illustrated with several beam dynamics applications, especially for electron cooling as related to this project.

2.2. The Picard Integrator

Motivated by the high accuracy requirements and the huge ratio of the largest to smallest time scales of Coulomb collision simulations of a considerable number of charges, we developed a novel numerical integration scheme, which uses algorithmic differentiation to produce variable, high-order integrators with dense output [2]. We showed that Picard iterations are not only a nice theoretical tool, but can also be successfully implemented to develop competitive integrators, especially when accuracies close to machine precision are required. The numerical integrators' performance and applications to the electrostatic n-body problem are illustrated. The latter application is again relevant to the electron cooling problem.

2.3. The Simo Integrator

Building on our success with the Picard integrator above, we also developed a novel collisional N-body numerical integrator, which we termed the Simò integrator [3], designed to model the electrostatic N-body problem of charged particle beams. It was proposed to accurately resolve close encounters and overcome efficiency challenges faced by other available N-body integrators, by provably achieving a prescribed accuracy with minimum computational effort. The Simò integrator utilizes Picard iterations combined with differential algebra to generate Taylor polynomials of the solutions of the equations of motion, as a base integrator. The integrator is adaptive and variable order with dense output. Our algorithm employs an automatic selection of the particles' individual optimal orders and optimal time step sizes. We described in detail the implementation of the Simò integrator along with our special approach in time stepping using time bins. We also provided some examples from beam physics to demonstrate the integrator's efficient

properties of adaptivity and variability for different cases and demonstrate its ability to achieve any given prescribed accuracy up to machine precision.

The FMM and the Simò integrator combined form the currently best available methodology for first principle level approach to electron cooling.

2.4. Particles' High-order Adaptive Dynamics (PHAD)

As we shown, high fidelity charged particle beam dynamics, especially if collisional, require specialized numerical methods. The challenges include the ability to deal with very large particle numbers, long-range electromagnetic forces, and vast spatial and timescales. We developed a novel algorithm to address these challenges [4]. The main characteristics of the algorithm are Strang splitting to separate near and far forces, the fast multipole method to lower the computational cost of the far region, and the Simò integrator to capture all close encounters efficiently in the near region. The algorithm is fully adaptive both in space and time, while maintaining symplecticity to machine precision. We illustrated its performance with two challenging examples from nonlinear multiparticle beam dynamics, including the first electron cooling simulations based on first principles.

2.5. Electron Cooling

As the culmination of the long term algorithmic, software, coding, and parallelization development, we finally were able to perform production runs and present the first microscopic electron cooling simulations from first principles with accurate prediction of cooling time [5]. These simulations were performed using our previously developed numerical method, PHAD, which is the first efficient large-scale collisional numerical method in beam physics. The simulation results were benchmarked with the experimental data of the low energy bunched electron cooling of ion beams at the storage ring CSRm at the IMP facility in China. We have accurately considered the nonlinear dynamics in the whole accelerator system in addition to the electron cooling section (also a first). As a result, our simulations correctly reproduced cooling times of the experiments from first principles and without any tuning or fitting parameters in the code.

In the case of coherent electron cooling, we performed PHAD simulations of the density modulations in the modulator section, which is a result of Debye shielding of the ion by the surrounding electrons. Our results support the possibility of obtaining modulations signals and show that better signals, and thus better cooling, is achieved when the ions are on-axis transversely. Longitudinally, the ions have to be within the core of the electron beam and without large variations of their velocities with respect to the electron beam. Modeling multiple ions suggests that these ions have to be well-separated (longitudinally) in order to obtain a clear, well-defined signal. If the ions are very close such that they are indistinguishable by the electron cloud, they cannot be cooled any

further. Moreover, we showed that the superposition principle has to be applied carefully to combine the signals due to individual ions as it might result in incorrect signals when ions are relatively close. Although we have shown that it is possible to extract the modulation signal using statistical averaging, the signal is very small with respect to the electron distribution and it is much straightforward to quantify it using the other approach of subtracting two simulations, one with the ions and one without them. The work on coherent electron cooling remains to be published in the near future [6].

Finally, we mention that recirculator-based cooling was dropped from our studies due to its neglect by the community in the aftermath of awarding the EIC to BNL instead of JLAB.

2.5. Other

For the final application we used the Simò integrator to study the relaxation of perturbed longitudinal momentum distributions of beams that are of importance to applications like beam echo in beam physics and the bump-on-tail problem in plasma physics. We showed how the relaxation time can be affected by different parameters such as the number of particles, the momentum spread, and the size of the perturbation. For the beam echo applications, our studies are important to select the time at which a second perturbation can be applied, and this time difference between the two applied perturbation can affect the resulting maximum echo amplitude. Also, our simulations provide a microscopic picture of the dynamics with clear finite N effects and importance of collisions which cannot be provided by the collisionless approach that considers the kinetic limit N tending to infinity, and neglects collisions ([6], to be published).

The development of our collisional methods, applying numerical and performance tests, and performing the simulations of the applications took a very long computational time. Conducted on the high-performance hybrid cluster Gaea at NIU [7], many jobs were launched, many nodes were utilized and CPU hours were consumed. Some statistics of utilization of Gaea are included in the table below.

It is worth noting that we operate a website dedicated to a repository of all our code frameworks, complete with downloadable software, manuals, examples, and associated publications. We also offer help to the community to use our code: the base code is called COSY Infinity, and it has 2500+ registered users. More information can be found here.

Throughout the lifetime of the project we had graduate research assistants working on the physics and computational issues, and also a postdoc on the mathematical and computational parts. The postdoc was funded from different sources. The two graduate assistants directly funded were both minority women, and obtained their Ph.D. based on work done for this project. One of them stayed in the field and continues to do research in beam physics.

CPU Hours per Job: The average CPU hours (number of CPU cores × wall time hours) per job	457.89
Total CPU Hours: The total CPU hours (number of CPU cores × wall time hours) used by all jobs	2,064,189.8
Max Job Size (Max Core Count): The maximum total number of processor cores used by a (parallel) job	360
Job Size per Job (Core Count): The average number of processor cores used by a (parallel) job per job	17.2
Job Size Weighted By CPU Hours (Core Count): The average job size weighted by CPU hours	43.9
Node Hours per Job: The average node hours (number of nodes × wall time hours) per job	65.56
Total Node Hours: The total node hours (number of nodes × wall time hours) used by all jobs	295,527.1
Gaea Utilization (%): The ratio of the total CPU hours consumed by jobs over a given time period divided by the maximum CPU hours that the system could deliver	6.09%
Number of Jobs Submitted: The total number of jobs that submitted/queued within the selected duration	4,422
Number of Jobs Ended: The total number of jobs that ended within the selected duration	4,508
Wall Hours per Job: The average time, in hours, a job takes to execute	20.82
Total Wall Hours: The total time, in hours, all jobs took to execute	93,869.4

3. PRODUCTS

Refereed publications:

[1] S. Abeyratne, A. Gee, and B. Erdelyi, "An adaptive fast multipole method in Cartesian basis, enabled by algorithmic differentiation," *Commun. Nonlinear Sci. Numer. Simul.*, vol. 72, pp. 294–317, 2019.

[2] H. D. Schaumburg, A. Al Marzouk, and B. Erdelyi, "Picard iteration-based variable-order integrator with dense output employing algorithmic differentiation," *Numer. Algorithms*, vol. 80, no. 2, pp. 377–396, 2019.

[3] A. A. Marzouk and B. Erdelyi, "Collisional N-body numerical integrator with applications to charged particle dynamics," *SIAM J. Sci. Comput.*, vol. 40, no. 6, pp. B1517–B1540, 2018.

[4] A. Al Marzouk, H. D. Schaumburg, S. Abeyratne, and B. Erdelyi, "Efficient algorithm for high fidelity collisional charged particle beam dynamics," *Phys. Rev. Accel. Beams*, vol. 24, no. 7, 2021.

[5] A. al Marzouk and B. Erdelyi, "First benchmarked electron cooling simulations from first principles", *NIM A*, accepted, 2022.

References

[6] Afnan Al Marzouk, Ph.D. Disseration, June 2021, "Collisional Methods with Applications to Charged Particle Beams".

[7] "NIU – Center for Research Computing and Data," *Northern Illinois University*. [Online]. Available: https://www.niu.edu/crcd. [Accessed: 30-Dec-2022].

Conference proceedings:

https://accelconf.web.cern.ch/IPAC2012/papers/moppc093.pdf
https://accelconf.web.cern.ch/IPAC2013/papers/mopwo074.pdf
https://accelconf.web.cern.ch/PAC2013/papers/mopba13.pdf
https://accelconf.web.cern.ch/PAC2013/papers/mopba14.pdf
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https://accelconf.web.cern.ch/napac2016/papers/thpoa68.pdf
https://accelconf.web.cern.ch/napac2016/papers/tupob14.pdf

Website (includes code):

[1] "NIU - Beam Physics Code Repository," *Northern Illinois University*. [Online]. Available: https://www.niu.edu/beam-physics-code/projects/index.shtml. [Accessed: 30-Dec-2022].

Dissertations:

[1] Sumana Abeyratne, Ph.D. Dissertation, October 2016, "New computational approaches to the N-body problem with applications to electron cooling of heavy ion beams".

[2] Afnan Al Marzouk, Ph.D. Dissertation, June 2021, "Collisional Methods with Applications to Charged Particle Beams".

4. PARTICIPANTS

1. **Name:** Bela Erdelyi
2. **Project Role:** Principal Investigator
3. **Nearest person months worked:** 1/year
4. **Contribution to Project:** technical leadership of full project

1. **Name:** Sumana Abeyratne
2. **Project Role:** Graduate Research Assistant
3. **Nearest person months worked:** 12/year for 5 years
4. **Contribution to Project:** developed the Fast Multipole Method and first PHAD version
5. **Ph.D.:** 2016

1. **Name:** Afnan al Marzouk
2. **Project Role:** Graduate Research Assistant
3. **Nearest person month worked:** 12/year for 5 years
4. **Contribution to Project:** developed the Simo integrator and performed the electron cooling simulations
5. **Ph.D.:** 2021

1. **Name:** Herman Schaumburg
2. **Project Role:** None (NIU postdoc)
3. **Nearest person month worked:** 0
4. **Contribution to Project:** synergistic research efforts on developing our coding framework PHAD for electron cooling