simulations to support the Electron Ion Collider design effort, including computational reproducibility

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Office of Science





Magnetized Electron Cooling –

RadiaSoft Vision

- Build a world class contract R&D organization
 - funded by the SBIR program in the near-term
 - develop non-federal customers & a reputation for excellence
 - near-term: charged particle beams, plasma and radiation
 - long term: diversify and grow (e.g. SAIC, now called Leidos)
- Scientific cloud computing services
 - the market is large & independent of any particular field
 - near-term: accelerator technology can provide initial users
 - 'Sirepo' is already a brand name in our community
 - <u>http://sirepo.com</u>
 - near term: Sirepo delivers software solutions to customers
 - soon: Sirepo is a freemium subscription-based product
- Long term: Sirepo subscriptions exceed contract R&D
 SBIR awards become a small fraction of total revenue
- Make computational reproducibility commonplace

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radiasoft Scholarship

RadiaSoft LLC consults regarding the simulation & design of particle beams, plasmas & radiation sources. We have 8 PhD physicists on staff, 3 PhD consultants & 1 COMSOL engineer.

- Helping teach 2 USPAS courses:
 - 1) Simulation of Beam and Plasma Systems, Winter 2018
 - 2) Classical Mechanics and Electromagnetism, Summer 2018
- Sirepo.com is a free scientific gateway for cloud-based particle accelerator codes.
 1) Accelerator Physics, Summer 2018
- **RadiaSoft LLC** scholarship this session:
- Pays for class registration and lodging

Fermilab

Recipient: Maria Simanovskaia (UC Berkeley)



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Core Competencies

- Contract R&D
 - particle accelerator modeling (ions, electrons, other)
 - lattice design, particle tracking, low-lever RF controls
 - x-ray optics, synchrotron radiation, FELs
 - ES and EM particle-in-cell (PIC) for beams and plasmas
 - hydrodynamics and charged fluids
 - machine learning, multi-objective genetic optimization (MOGA)
- Community physics codes
 - MAD-X, Synergia, elegant, Warp, Zgoubi, PTC
 - SRW, Shadow, Genesis, Flash
- Computer-aided engineering (CAE)
 - COMSOL Multiphysics
- GUI development
 - design and implement browser-based GUI for any code
- Computational reproducibility
 - archive full simulation environment for 6 months or 6 years
 - rerun previous simulations with same results to machine precision

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Non-SBIR revenue is up year over year



- Our customer base is diverse

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- Air Force Office of Scientific Research, DOE national labs
- high tech hardware companies (some funded by SBIR)
- medical technology; VC-funded hardware startups

Phase 2 SBIR project – Technical Objectives

- Integrate JSPEC cooling code into Sirepo platform
 - collaboration with He Zhang at JLab
 - <u>https://github.com/zhanghe9704/electroncooling</u>
 - <u>https://sirepo.com/#/jspec</u>
 - important alternative to BetaCool
- Develop and test a new conceptual design for both an accumulator ring and high current d.c. cooler
 - collaboration with P. McIntyre and J. Gerity at Texas A&M
- Incorporate new methods of dynamic friction calculation into a software package
 - risk reduction for high-energy magnetized e- cooling
 - target software package is JSPEC

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Task 1 – Develop browser-based GUI for e- cooling code

- Good progress has been made
 - He Zhang (JLab) is collaborating with us
 - <u>https://sirepo.com/#/jspec</u>
- I. Ben-Zvi (BNL) & M. Steck (GSI) have tested:
 - both provided good feedback
 - M. Steck simulated GSI cooler params with good results



JSPEC III Simulations I DC Cooling Example &	≁ Source 🗳 Visualization 🕸 - 🚱 - 🤱
Simulation Settings	Simulation Status
Total Simulation Time [s] 180 Total Number of Steps ① 180 Model BMS	Simulation Completed Start New Simulation
Simulate Electron Cooling Effect	
RMS Ion Beam Evolution	Cooling Rates 🖍 🏚 🖍 🔦
2.0e-6 1.5e-6	-0.02
1.0e-6 5.0e-7 0 20 40 60 80 100 120 140 160 180	
t [s] ● emit_x [m*rad] ● emit_y [m*rad]	t [s] • rx [1/s] - combined electron cooling and IBS heating rate (horizontal) • ry [1/s] - combined electron cooling and IBS heating rate (vertical) • ry [1/s] - combined electron cooling and IBS heating rate (vertical)

Task 2 – Preconceptual Design of a Cooling and Accumulator Ring

- JLEIC ion collider ring is a figure-8 layout
 - includes low-energy DC electron cooling
 - also, high-energy bunched electron cooling, using ERL
 - this includes significant technical risk
- consider e- cooling at intermediate energy: 6 GeV/u
 - less risky then high-energy cooling
 - new figure-8 design conforming to updated JLEIC design
 - the arc cells have twice the periodicity of those found in JLEIC ring
 - yields transition energy $\gamma_T \sim Q_X$ higher than collision ring, $\gamma_T = 12.46$
 - allows for acceleration after cooling, so beam can enter collision
 ring above transition
 - designed using MAD-X
 - basic lattice parameters:

\mathbf{B}_{dip}	1.0 T				
G_{quad}	7.02 T/m				
Q _x , Q _y	49.43, 48.83				
$\mathbf{B}_{solenoid}$	>1 T				



Task 2 – Preconceptual Design of a Cooling and Accumulator Ring

- Ongoing lattice improvements, using MAD-X
 - matching regions between arcs and straight sections
 - same matching conditions met with fewer magnets
- Particle tracking studies with 'elegant' code
 - initial results are consistent between the two codes



accepted phase space--input: run.ele lattice: lattice.lte

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accepted phase space--input: run.ele lattice: lattice.lte

Task 3 – Preconceptual design of a magnetized e- cooling system

- We consider parameters of Task 2 accumulator ring
- Consider space charge neutralization of ~1 A e- beam
 lower space charge forces means stronger dynamic friction
- Initial simulations have been run using Warp
 - space charge neutralization of the electron beam is observed
 - the neutralization time is $\sim 15 \ \mu s$
 - this requires 3.6 million simulation time steps

Quantity (Units)	Simulation Value					
Beam Energy (MeV)	3.2				→	
Beam Current (mA)	10		+2 kV		$B = (0, 0, B_z)$	+2 kV
Beam Density (cm^{-3})	6.75e + 5					
Gas Density (cm^{-3})	1.06e + 14	e⁻ Beam		\longrightarrow	H ₂ Gas	15.24 cm
Interaction Cross Section (Approx.) (cm^2)	1.8e-20			\rightarrow	2	13.21 cm
$H_2^+ T_p \ (\mu s)$	8.2					
$e^- \; T_p \; (\mu s)$	0.1				2.0 m	
$e^- T_{cycle} \ (ps)$	50					
Time step (ps)	5					

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Task 3 – Preconceptual design of a magnetized e- cooling system

Space charge neutralization is provided by impact ionization of the e- beam on residual H_2 :

The neutralization time depends on the interaction cross section, beam velocity and gas density as:

Calculated neutralization time of 17 μ s matches well with simulations:



 $e^{-} + H_{2} \rightarrow 2e^{-} + H_{2}^{+} + H_{2}^{+} + \frac{1}{\sigma_{c} v_{e} n_{H}}$

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Task 4 – Study equilibrium electron cooling rates

- Now that Task 2 and Task 3 are nearing completion, work on this task has recently begun.
- We'll use BETACOOL and JSPEC, with benchmarking
- BETACOOL: simulates long time (millions of turns) evolution of the ion beam phase space, including many physics models
 - developed in early 2000's at JINR (Dubna, Russia)
 - coupled ODEs for modeling RMS dynamics of 6D Gaussian distributions or Langevin-type simulation tacking a sample of ion macroparticles
 - particle loss (recombination) and multiple beam heating and cooling processes:
 - unmagnetized (Derbenev, Meshkov) and magnetized (Derbenev-Skrinsky-Meshkov, Parkhomchuk) asymptotic and/or parametrized electron cooling models
 - IBS (Bjorken-Mtingwa, Martini)
 - other effects (e.g., scattering on residual gas)
 - IBS calculation requires detailed knowledge of the optics structure of the ring

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Task 4 – Study equilibrium electron cooling rates

- The BETACOOL GUI (so-called Bolide Interface) is required to prepare input files and for postprocessing
 - a multi-window GUI, only available as a pre-compiled executable for Windows
 - difficult to set up (from scratch) the simulation of a new ring
 - it would be prohibitively difficult to add and use new capabilities without access to the GUI source code
 - far easier to work with JSPEC in this regard
 - Windows-only GUI necessitates working in a Windows VM, while most of our development and simulation cycle is on Linux and MacOS
- Benchmarking JSPEC and BETACOOL
 - we will understand and document the differences
 - new capabilities will be added to JSPEC

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Task 5 – Generalize dynamic friction calculations to include space charge and field errors

- JLEIC requires cooling at high energy
 - 100 GeV/n → $\gamma \approx 107$ → 55 MeV bunched electrons, ~1 nC
- Electron cooling at γ ~100 requires different thinking
 - friction force scales like $1/\gamma^2$ (Lorentz contraction, time dilation)
 - challenging to achieve the required dynamical friction force
 - not all of the processes that reduce the friction force have been quantified in this regime \rightarrow significant technical risk
 - normalized interaction time is reduced to order unity
 - $\tau = t \omega_{pe} >> 1$ for nonrelativistic coolers
 - $\tau = t \omega_{pe} \sim 1$ (in the beam frame), for $\gamma \sim 100$
 - violates the assumptions of introductory beam & plasma textbooks
 - breaks the intuition developed for non-relativistic coolers
 - as a result, the problem requires careful analysis

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Goals

- Simulate magnetized friction force
 - include all relevant real world effects
 - e.g. incoming beam distribution
 - include a wide range of parameters
 - cannot succeed via brute force
 - improved understanding is required



- Include key aspects of magnetized e- beam transport
 - imperfect magnetization
 - space charge
 - field errors



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from Zhang et al., MEIC design, arXiv (2012)

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Serious difficulties with dynamic friction calculations

- Can we quantify the required solenoidal field quality?
 - Parkhomchuk formula provides a parametric knob
 - Derbenev and Skrinsky do not offer quantitative guidance

– No

- Can we quantify the effects of space charge forces?
 No
- Can we quantify the effects of non-Gaussian e- beam phase space distributions?
 No
- New friction force calculations are important
 - Otherwise, technical risk will be high

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A new dynamical friction calculation is underway...

- We follow the approach described by Y. Derbenev
- However, we begin from a new starting point
 - analytic momentum transfer between ion and magnetized e-
 - proceed step by step with calculation
- Calculation is defined by the following considerations:

$$\vec{E}(\vec{r},\vec{v},t) = \langle \vec{E}^0 \rangle (\vec{r},t) + \langle \Delta \vec{E} \rangle (\vec{r},\vec{v},t) + \vec{E}^{fl}(\vec{r},\vec{v},t)$$
(1.1)

$$\vec{F} = -ze\langle\Delta\vec{E}\rangle(\vec{r},\vec{v},t)\big|_{\vec{r}=\vec{r}(t),\vec{r}(t)=\vec{v}}$$
(1.2)

Y. Derbenev, "Theory of Electron Cooling," arXiv (2017); https://arxiv.org/abs/1703.09735

THEORY OF ELECTRON COOLING

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*Translated from Russian by V.S. Morozov, Jefferson Lab, VA 23606, USA Translation supported by Jefferson Science Associates, LLC under U.S. DOE Contract No. DE-AC05-06OR23177. The U.S. Government retains a non-exclusive, paid-up, irrevocable, worldwide license to publish or reproduce this manuscript for U.S. Government purposes. The required steps are straightforward in principle:

- Calculate the perturbed e-velocities
 - due to a single ion
 - initially, we consider purely longitudinal motion
- Obtain time-derivative of perturbed E-field
 - via Poisson and continuity equations
- Integrate in time to get δE
 - initially, this is for only a single value of e-velocity
 - it is necessary to integrate over thermal e-velocities
- Integrate δE along ion trajectory to obtain <F> – hence, this is a 2nd-order effect, ~(Ze²)² xx
- Present efforts:
 - find best way to integrate <F> over e- distribution functions
 - consider transverse ion motion
 - numerical approaches, testing, etc.

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Hamiltonian for 2-body magnetized collision:

$$H(\overset{\mathcal{P}}{x_{ion}}, \overset{\mathcal{P}}{p}_{ion}, \overset{\mathcal{P}}{x_e}, \overset{\mathcal{P}}{p}_e) = H_0(\overset{\mathcal{P}}{p}_{ion}, y_e, \overset{\mathcal{P}}{p}_e) + H_C(\overset{\mathcal{P}}{x_{ion}}, \overset{\mathcal{P}}{x_e})$$
$$\overset{\mathcal{P}}{B} = B_0 \hat{z} \qquad \overset{\mathcal{P}}{A} = -B_0 y \hat{x} \qquad p_{e,x} = m_e(v_{e,x} - \Omega_L y_e)$$

$$H_0(p_{ion}, y_e, p_e) = \frac{1}{2m_{ion}} \left(p_{ion,x}^2 + p_{ion,y}^2 + p_{ion,z}^2 \right) + \frac{1}{2m_e} \left[\left(p_{e,x} + eB_0 y_e \right)^2 + p_{e,y}^2 + p_{e,z}^2 \right]$$

$$H_{C}(x_{ion}^{\rho}, x_{e}^{\rho}) = \frac{-Ze^{2}}{4\pi\varepsilon_{0}} / \sqrt{(x_{ion} - x_{e}^{\rho})^{2} + (y_{ion} - y_{e}^{\rho})^{2} + (z_{ion} - z_{e}^{\rho})^{2}}$$

D.L. Bruhwiler and S.D. Webb, "New algorithm for dynamical friction of ions in a magnetized electron beam," in *AIP Conf. Proc.* **1812**, 050006 (2017); <u>http://aip.scitation.org/doi/abs/10.1063/1.4975867</u>



After many steps we obtain an approximate friction force:

Let $z_e = v_{i,z}T$ and then integrate over T to obtain:

$$< F > = (n_0 e) \frac{n_0 (Z e^2)^2}{m_e v_{rel} T} \left\{ \frac{T}{v_{rel}} ln \left(\left[\rho_{gc}^2 + \left(v_{i,z} T \right)^2 \right]^{1/2} + v_{i,z} T \right) - \frac{v_{e,z}}{v_{i,z}^2 v_{rel}} \left(\left[\rho_{gc}^2 + \left(v_{i,z} T \right)^2 \right]^{\frac{1}{2}} - \rho_{gc} \right) \right\}$$

There is an integrable singularity for cold electrons. The challenge now is to integrate over thermal velocities



Task 6 – Develop software to perform dynamic friction calculations for e- distributions

• Now that Task 5 is nearing completion, work on this task will begin soon.



Enabling reproducibility for accelerator codes

- A single code with simple workflow
 - scientist #2 will initially get the same results as scientist #1
 - if simulation is properly archived, then many scientists can benefit
- What is required (assuming minimum effort from scientists)?
 - make community codes publicly available, pre-installed
 - provide a state-of-the-art GUI
 - ease of use (required for adoption)
 - constrain the workflow (always enable export to Python CLI)
 - cloud computing

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- control the execution environment
- minimize development and maintenance costs (sustainability)
- Advantages of using the browser as your scientific UI
 - enables "instantaneous collaboration" via URL sharing
 - the first sharing event corresponds to first bullet above
 - collaborative use case: multiple back-and-forth sharing events
 - cross-platform development pain is confined to JavaScript issues