Direct Simulation of Friction Forces for Heavy Ions Interacting with a Warm Magnetized Electron Distribution

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Abstract. A proposed luminosity upgrade to RHIC includes a novel electron cooling section [1], which would use ~55 MeV electrons to cool fully-ionized 100 GeV/nucleon gold ions. High-current bunched electron beams are required for the RHIC cooler, resulting in very high transverse temperatures and relatively low values for the magnetized cooling logarithm. The accuracy of analytical formulae in this regime requires careful examination. Simulations of the friction coefficient, using the VORPAL code [2], for single gold ions passing once through the interaction region, are compared with theoretical calculations [3,4]. Charged particles are advanced using a fourth-order Hermite predictor-corrector algorithm [5]. The fields in the beam frame are obtained from direct calculation of Coulomb's law, which is more efficient than multipole-type algorithms for less than ~10^6 particles. Because the interaction time is so short, it is necessary to suppress the diffusive aspect of the ion dynamics through the careful use of positrons in the simulations.

INTRODUCTION

The Relativistic Heavy Ion Collider (RHIC) [6] delivered the first collisions between gold nuclei in 2000 at then unprecedented energies of 100 GeV per nucleon [7]. RHIC is designed to accelerate a wide variety of ions, from protons to fully-stripped gold, Au^{+79}. A luminosity upgrade is being planned for RHIC [1], in order to improve the number and quality of collisions. A key component of the upgrade is an electron cooling section [8], which will significantly improve the ion beam luminosity and lifetime.

The RHIC electron cooler will be fundamentally different from existing facilities [1,9]. The electron energy must be ~55 MeV, requiring rf acceleration of a high-charge (~20 nC) magnetized electron bunch, with orders-of-magnitude larger temperatures then has been previously considered. Even with a solenoidal magnetic field as large as 5 T, the relevant Coulomb logarithm will be of order unity, so analytical models are only marginally applicable.

Analytical expressions for the friction force on a single ion moving through a magnetized electron distribution have been published by Derbenev and Skrinsky [3,10], Meshkov [11], Parkhomchuk [4] and Toepffer [12], among others. Parkhomchuk's formula is an empirical generalization of the theoretical friction force for unmagnetized electrons. The semi-numerical results of Toepffer, which have not yet been compared with others, will not be discussed further here.

These calculations implicitly assume a constant electron density, a uniform neutralizing background, the absence of any perturbation from other ion trajectories, and a constant longitudinal magnetic field. Parkhomchuk's formula includes an effective velocity which may help to remove some of these assumptions in a parametric fashion. The Derbenev-Skrinsky-Meshkov (DSM) and Parkhomchuk formulas disagree strongly in some parameter regimes, while showing approximate (roughly factor of two) agreement in other regimes. These formulas are applied in the beam frame, assuming nonrelativistic particle velocities and electrostatic particle-field dynamics.

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Order of magnitude calculations of the magnetized friction force has been acceptable for existing electron cooling facilities, because they operate in a regime where the friction force is strong enough by a large margin. In contrast, the proposed RHIC cooler will operate in a completely new regime, where the estimated friction force is expected to be adequate but with little margin for error.

Hence, we are developing a parallel 3D code capable of directly simulating from first principles the magnetized friction force and diffusion coefficients for parameters relevant to RHIC. This project is using molecular dynamics techniques (i.e. simulating every particle in the problem) to explicitly resolve close binary collisions and thus capture the friction force and the diffusion tensor with a bare minimum of physical assumptions [9,13].

These on-going simulations show great promise for resolving ambiguities in the theoretical understanding of the magnetized friction force under idealized conditions, and also for determining quantitatively the effect of complicating factors, such as the impact of errors in the solenoidal magnetic field.

NUMERICAL APPROACH

When all pairwise forces are computed directly for N particles, $\mathbf{O}(N^2)$ operations are required for each time step, making this approach numerically intensive. For biophysical applications like protein folding, where the charged particles remain well-separated and one can use a fixed time step, there are three types of tree-based algorithms [14] that dramatically improve this scaling: the Barnes-Hut algorithm [15], the fast multipole algorithm (FMA) [16,17], and the multipole tree algorithm [18].

For astrophysical applications, where stars are treated as gravitating point masses and very close binary collisions must be resolved, there is a need for aggressive variation of the time step for each "particle". It has been found that a specialized 4th-order predictor-corrector algorithm [19,5], used with the $\mathbf{O}(N^2)$ field calculation, is more efficient than a fixed-time-step multipole algorithm for less than 10^6 particles, in spite of the unfavorable scaling.

It is these close particle-to-particle interactions which are critical to correctly modeling the physics of electron cooling, especially in regimes where the relevant Coulomb logarithm is of order unity. Thus, we have generalized the 4th-order algorithm of Makino & Aarseth to accommodate charged particles in a magnetic field [13] and implemented it within the parallel simulation code VORPAL [2]. New positions and velocities for the i^{th} particle are predicted from a Taylor expansion in time, using the following acceleration and its time derivative:

$$\frac{m_i \mathbf{a}_i}{q_i} = \mathbf{v}_i \times \mathbf{B} + \frac{1}{4\pi\varepsilon_0}\sum_j \frac{q_j \mathbf{r}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{3/2}} \tag{1a}$$

$$\frac{m_i \dot{\mathbf{a}}_i}{q_i} = \mathbf{a}_i \times \mathbf{B} + \sum_j \frac{q_j}{4\pi\varepsilon_0}\left[\frac{\mathbf{v}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{3/2}} + \frac{3\left(\mathbf{v}_{ij}\cdot\mathbf{r}_{ij}\right)\mathbf{r}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{5/2}}\right] \tag{1b}$$

where $\mathbf{r}_{ij}$ and $\mathbf{v}_{ij}$ are the relative positions and velocities of particles i and j, and the "cloud radius" r_c is typically zero.

The more complicated "corrector" step follows Ref. [5], except that retaining 4th-order accuracy requires the $\mathbf{v}x\mathbf{B}$ force to be recalculated with the predicted velocity, and one of the coefficients must be changed for terms that include $\mathbf{B}$. Particles are binned in time step levels that differ by factors of two, and they are advanced in an order that minimizes the time separation between different populations. After each particle is pushed, a new time step is calculated and, if necessary, particles are moved to a new level. Whenever a corrector step is applied to one population of particles, all other populations are brought temporarily to the same time with a predictor step (i.e. no force calculation) and then the force is calculated only for those particles in the active population. These details are beyond the scope of the present paper and will be clarified in future work.

FRICTION & DIFFUSION FOR B=0

Our implementation of this algorithm was first applied to an ion moving through an unmagnetized plasma. The dynamical friction force due to the plasma electrons is given [20,21,22] by Eq. (2a):

$$\mathbf{F} = -\omega_{pe}^2 \frac{(Ze)^2}{4\pi\varepsilon_0}\ln\left(\frac{\rho_{\max}}{\rho_{\min}}\right)\frac{\mathbf{V}_{ion}}{V_{ion}^3}\Psi(\alpha) \tag{2a}$$

$$\rho_{\min} = \left(Ze^2/4\pi\varepsilon_0\right)/m_e V_{rel}^2 \qquad \rho_{\max} = V_{rel}/\max\left(\omega_{pe}, 1/\tau\right) \tag{2b}$$

$$V_{rel} = \max\left(V_{ion}, V_{e,rms}\right) \qquad \omega_{pe} = \sqrt{n_e e^2/\varepsilon_0 m_e} \tag{2c}$$

$$\Psi(\alpha) = \frac{2}{\sqrt{\pi}}\int_0^{\alpha} t^{1/2} e^{-t} dt \qquad \alpha = V_{ion}^2/2V_{e,rms}^2 \tag{2d}$$

Budker [23] first suggested that this friction could be used to cool heavy ions in a storage ring by having them co-propagate repeatedly with cold electrons.

For RHIC, the interaction time is $\tau = L/\gamma c \sim 0.4$ *ns*, where $L \sim 13$ m is the length of a solenoid magnet (for a

design with two solenoids of 13 m each [8]), γ~107 is the relativistic factor, and c is the speed of light. For a beam frame electron density of n_e~1x10^{15} cm^{-3}, the plasma frequency is ω_{pe}~1x10^9 rad/m. In this regime, the interaction time is smaller than a plasma period, so the electrons don't have time to screen the ion. Thus, we choose to neglect the e-/e- interactions, resulting in shorter simulation times that scale as **O**(N_{ion}*N_e).

For these very short interaction times, the rms spread in velocity due to diffusion is of the same order of magnitude as the velocity drag due to friction:

$$dV_f = -|\mathbf{F}|\tau / m_{ion} \qquad \delta V_{||,rms} = \sqrt{\tau D_{||}} \qquad (3)$$

where the parallel $D_{||}$ and perpendicular diffusion coefficients have different functional forms [20, 21, 22]. This is shown in Fig. 1, for an electron thermal velocity of $V_{e,rms}$=4x10^4 m/s, and a variety of initial ion velocities. This makes it difficult to accurately extract the friction force from simulated ion velocities. In the limit of millions of interactions, however, as will occur in RHIC, the diffusive dynamics becomes negligible, because it scales as the square root of the number of interactions, while friction scales linearly.

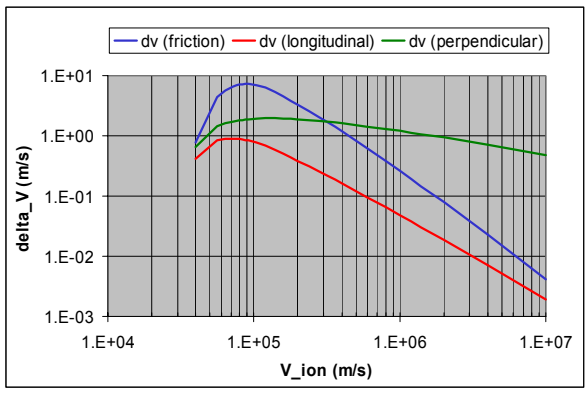

FIGURE 1. The rms spread of longitudinal (red) and perpendicular (green) velocity kicks are comparable to the dynamic velocity drag (blue) for brief interactions.

In the limit of an ideal plasma, Z<<N_D, where Z is the ion charge number and N_D is the number of electrons in a Debye sphere, the dynamical friction due to positrons is identical to that of electrons. If half of the electrons are replaced by positrons, the friction force is unchanged. Given a distribution of initially correlated e-/e+ pairs (same position and velocity), the diffusive kicks from each e- will be approximately cancelled by the corresponding e+.

Figure 2 shows the dynamics of a single Au^{+79} ion, with correlated e-/e+ pairs used to suppress diffusion. The velocity drag due to friction is seen in the bottom frame. Here, we have τ=0.935 ns (L=30 m); B=1 T; n_e=2x10^{15} m^{-3}; $V_{e,rms}$=4x10^4 m/s (same parameters as in Fig. 1), for initial ion velocity V_{ion}=6x10^5 m/s.

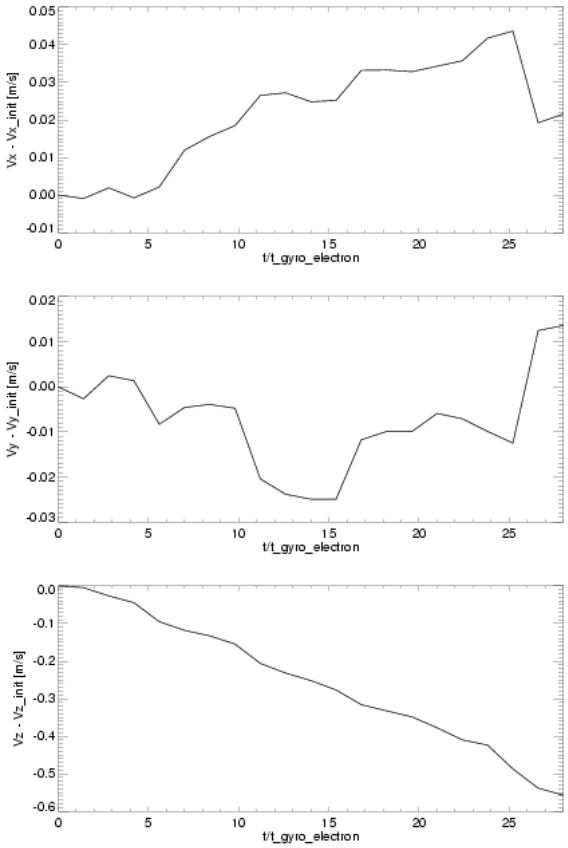

FIGURE 2. The change in transverse (V_x, V_y) and longitudinal (V_z) velocities for an Au^{+79} ion, with initial velocity V_z=6.5x10^4. The diffusive dynamics is artificially suppressed by using correlated e-/e+ pairs.

Table 1 shows a comparison of the frictional velocity drag as simulated by VORPAL and predicted by theory. The agreement is good when the Coulomb log is large, and poor when it is of order unity or smaller.

TABLE 1. Unmagnetized velocity drag due to friction

V_{ion} (m/s)	$ln(\rho_{max}/\rho_{min})$	dV_f (theory)	dV_f (VORPAL)
6.0 x10^5	8	-0.61	-0.62
2.0 x10^5	5	-3.3	-2.5
0.4 x10^5	0.2	-0.8	-0.02

MAGNETIZED FRICTION THEORY

The transverse rms electron velocity $V_{e,rms,\perp}$ in the proposed RHIC cooler will be much larger than the ion velocity, so dynamical friction will be negligible, unless the electrons are strongly magnetized. For ion velocities ranging from the longitudinal rms electron velocity $V_{e,rms,\|}$ up to $V_{e,rms,\perp}$, with impact parameters larger than the electron Larmor radius r_L, the ion effectively interacts with a ring of charge, rather than a fast electron. This results in a much stronger exchange of energy.

The formulas presented by Derbenev, Skrinsky and Meshkov (DSM) are relevant to this parameter regime:

$$F_{\|}^{DSM} = -\frac{3}{2}\omega_{pe}^2 \frac{(Ze)^2}{4\pi\varepsilon_0}\left[\ln\left(\frac{\rho_{\max}^{DSM}}{\rho_{\min}^{DSM}}\right)\left(\frac{V_\perp}{V_{ion}}\right)^2 + \frac{2}{3}\right]\frac{V_\|}{V_{ion}^3} \quad (4a)$$

$$F_{\perp}^{DSM} = -\omega_{pe}^2 \frac{(Ze)^2}{4\pi\varepsilon_0}\ln\left(\frac{\rho_{\max}^{DSM}}{\rho_{\min}^{DSM}}\right)\frac{\left(0.5V_\perp^2 - V_\|^2\right)}{V_{ion}^2}\frac{V_\perp}{V_{ion}^3} \quad (4b)$$

$$\rho_{\min}^{DSM} = \max\left(r_L, \rho_{\min}\right) \qquad r_L = V_{rms,e,\perp}/\Omega_L \quad (4c)$$

$$\rho_{\max}^{DSM} = V_{rel}^{DSM}/\max\left(\omega_{pe}, 1/\tau\right) \quad (4d)$$

$$V_{rel}^{DSM} = \max\left(V_{ion}, V_{e,rms,\|}\right) \qquad V_{ion}^2 = V_\|^2 + V_\perp^2 \quad (4e)$$

These results are valid in the limit that the magnetized Coulomb log is large. Hence, they are of limited value in the limit of poor magnetization, when the maximum impact parameter is not much larger than the Larmor radius.

In contrast, Parkhomchuk presents a parametric formula – a generalization of the unmagnetized result, which is predicted [4] to agree reasonably well with experiments for a wide range of parameters:

$$\mathbf{F}^P = -\frac{1}{\pi}\omega_{pe}^2 \frac{(Ze)^2}{4\pi\varepsilon_0}\ln\left(\frac{\rho_{\max}^P + \rho_{\min}^P + r_L}{\rho_{\min}^P + r_L}\right)\frac{\mathbf{V}_{ion}}{\left(V_{ion}^2 + V_{eff}^2\right)^{3/2}} \quad (5a)$$

$$\rho_{\min}^P = \left(Ze^2/4\pi\varepsilon_0\right)/m_e V_{ion}^2 \quad (5b)$$

$$\rho_{\max}^P = V_{ion}/\max\left(\omega_{pe}, 1/\tau\right) \quad (5c)$$

$$V_{eff}^2 = V_{e,rms,\|}^2 + \Delta V_{\perp e}^2 \quad (5d)$$

The subtle differences in the definitions of the min and max impact parameters, as compared to DSM or the unmagnetized case, lead to very different behavior. In the limit of weak magnetization, or small ion velocity, the ordering in size of the three impact parameters can change, while the log remains well defined. The new parameter $\Delta V_{\perp e}$, an effective transverse velocity of the charge rings, is used to capture the effects of transverse **E** and **B** fields.

Figure 3 compares the predictions of Parkhomchuk and DSM for purely longitudinal and transverse ion motion. One can see the unmagnetized contribution to friction is negligible. Here, we have τ=0.935 ns (L=30 m); B=5 T; n_e=2x10^{15} m^{-3}; $V_{e,rms,\perp}$=8x10^6 m/s; and $V_{e,rms,\|}$=1x10^5 m/s. The VORPAL simulations (red squares) show reasonable agreement with the DSM and Parkhomchuk formulas.

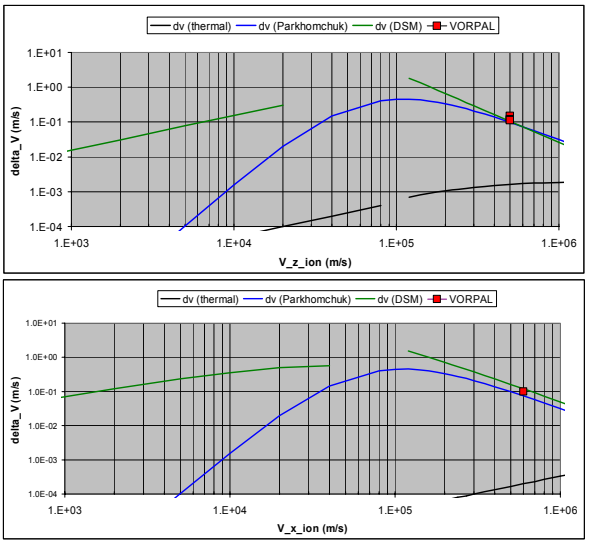

FIGURE 3. The velocity drag due to dynamical friction, according to DSM (green), Parkhomchuk (blue), unmagnetized theory (black) and VORPAL simulations (red), for the case of ion motion along the magnetic field (top) and perpendicular (bottom).

The parameter $\Delta V_{\perp e}$, which is zero in Fig. 3, can be chosen to model transverse velocity kicks of the charged electron rings driven by misalignments in the solenoidal fields. The Parkhomchuk model indicates that any field misalignments will reduce the friction force. Recent work [24] indicates that the effects are not so straightforward. The DSM model cannot include any effects due to misalignments.

Figure 4 shows the ion dynamics from a VORPAL simulation for these parameters, with perpendicular initial ion velocity V_{ion}=V_x=6x10^5 m/s. Other parameters are the same as in Fig. 3. Correlated e-/e+ pairs were used to suppress diffusion. The top frame shows the resulting velocity drag of the Au^{+79} ion.

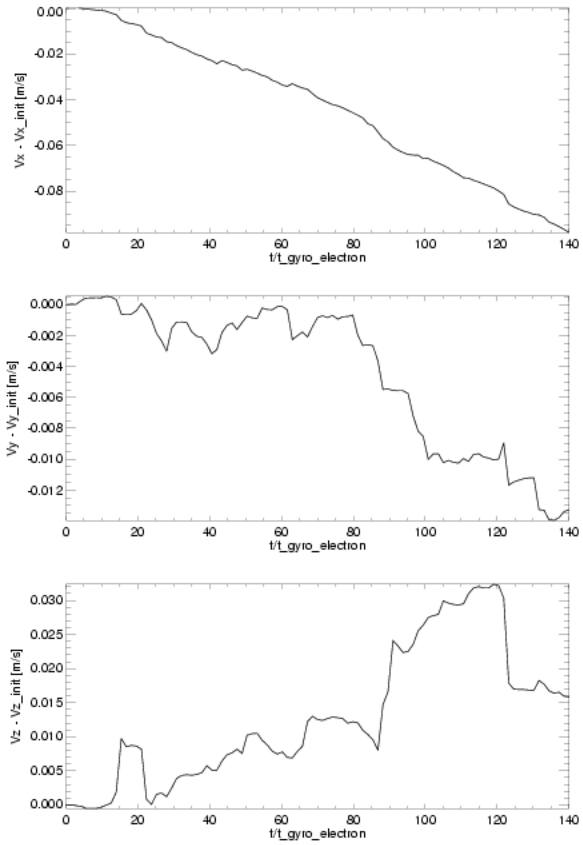

FIGURE 4. The change in transverse (V_x, V_y) and longitudinal (V_z) velocities for an Au^{+79} ion, with initial velocity V_x=6x10^5. The diffusive dynamics is artificially suppressed by using correlated e-/e+ pairs.

SUMMARY

A unique molecular dynamics algorithm has been implemented to study the dynamical friction and diffusion of ions moving through electrons and positrons. Binary coulomb collisions are explicitly resolved, in order to minimize the number of assumptions and approximations being made. Careful testing indicates that the algorithm is working well for magnetized and unmagnetized cases that are relevant to the proposed electron cooling section for RHIC.

Ongoing efforts are directed towards parameter studies to distinguish competing analytical formulas. Future work will address the critical issue of magnetic field errors and the extent to which these reduce the friction force and, hence, the effectiveness of the cooling. Efforts to reduce run time and improve parallel performance are also continuing.

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REFERENCES

1. I. Ben-Zvi *et al*., Proc. COOL'03 Workshop (2003).
2. C. Nieter & J.R. Cary, J. Comp. Phys. **196** (2004), p. 448.
3. Ya.S. Derbenev & A.N. Skrinskii, Sov. J. Plasma Phys. **4** (1978), p. 273.
4. V.V. Parkhomchuk, Nucl. Instr. Meth. in Phys. Res. A **441** (2000), p. 9.
5. J. Makino & S.J. Aarseth, Publ. Astron. Soc. Japan **44** (1992), p. 141.
6. See URL http://www.bnl.gov/RHIC/
7. B.B. Back *et al.* (PHOBOS collaboration), Phys. Rev. Lett. **85** (2000), p. 3100.
8. See URL http://www.agsrhichome.bnl.gov/eCool/
9. A. Fedotov *et al.*, these proceedings.
10. Ya.S. Derbenev & A.N. Skrinsky, Part. Accel. **8** (1978), p. 235.
11. I. Meshkov, Phys. Part. Nucl. **25** (1994), p.631.
12. Toepffer, Phys. Rev. A **66**, 022714 (2002).
13. R. Busby *et al.*, Bull. Am. Phys. Soc. **48**, no. 7 (2003), p. 117.
14. G. Blelloch & G. Narlikar, *Series in Discrete Math. and Theoretical Comp. Science* **30** (1997).
15. J.E. Barnes & P. Hut, Nature **4** (1986), p. 446.
16. L. Greengard & V. Rokhlin, J. Comp. Phys. **73** (1987), p. 325.
17. L. Greengard, *The rapid evaluation of potential fields in particle systems* (MIT Press, 1987).
18. J.A. Board *et al.*, Technical Report 94-002 (Duke University, 1994).
19. J. Makino, Astrophys. Journal **369** (1991), p. 200.
20. S. Chandrasekhar, *Principles of Stellar Dynamics* (U. Chicago Press, 1942).
21. B.A. Trubnikov, Rev. Plasma Physics **1** (1965), p. 105.
22. *NRL Plasma Formulary*, ed. J.D. Huba (2000).
23. G.I. Budker, At. Energ. **22** (1967), p. 346.
24. A. Burov, FERMILAB-TM-2213 (2003).