Parallel Simulation of Coulomb Collisions for High-Energy Electron Cooling Systems

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Proposed e-Cooler for RHIC II Luminosity Upgrade

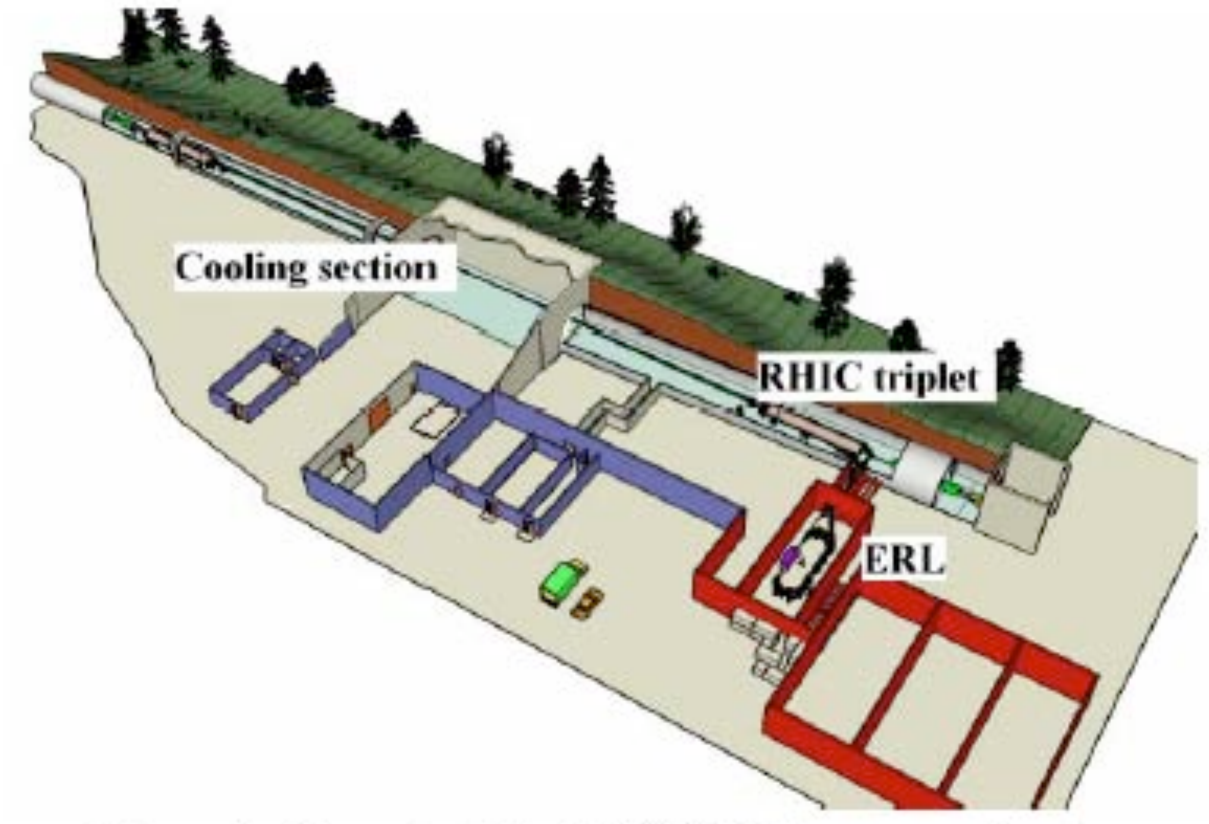


Figure taken from: I. Ben-Zvi, “The ERL High-Energy Cooler for RHIC,” Proc. EPAC (2004), p. 940.

See also http://www.bnl.gov/cad/ecooling/

Motivation & Background

- Need for high-fidelity simulations of dynamical friction
  - We are using the VORPAL code
    - C. Nieter and J.R. Cary, J. Comp. Physics **196** (2004), p. 448.
    - P. Messmer and D. Bruhwiler, Comp. Phys. Comm. **164** (2004), p. 118.
    - G.I. Bell *et al.*, J. Comp. Phys., in preparation
    - http://www.txcorp.com/products/VORPAL/
- Goals of the simulations
  - Resolve differences in theory, asymptotics, parametric models
  - Quantify the effect of wiggler magnets, general magnetic field errors
- Original numerical approach
  - use algorithm from astrophysical dynamics community
  - success w/ idealized case of magnetized cooling
    - Bruhwiler *et al.*, AIP Conf. Proc. **773** (2004)
    - Fedotov *et al.*, AIP Conf. Proc. **821** (2005).
    - Fedotov *et al.*, Phys. Rev. ST/AB **9**, 074401 (2006).
    - Fedotov *et al.*, New J. Phys. (2006), to appear.
- Recent efforts
  - Implementation of improved binary collision model
    - G.I. Bell *et al.*, AIP Conf. Proc. **821** (2005).
  - Effect of wiggler fields for “unmagnetized” approach

New simulation approach: Operator Splitting

- Numerical technique used for ODE's & PDE's
- Consider Lorentz force equations

$$\dot{\mathbf{x}} = \mathbf{v} \qquad \dot{\mathbf{v}} = \frac{q}{m}\mathbf{E}_{Coulomb} + \frac{q}{m}\left(\mathbf{E}_{ext} + \mathbf{v}\times\mathbf{B}_{ext}\right)$$

- Robust 2nd-order 'Boris' uses operator splitting
  - J. Boris, Proc. Conf. Num. Sim. Plasmas, (1970), p. 3.

$$\Delta\mathbf{x}(\Delta t/2);\ \Delta\mathbf{v}_{\mathbf{E}}(\Delta t/2);\ \Delta\mathbf{v}_{\mathbf{B}}(\Delta t);\ \Delta\mathbf{v}_{\mathbf{E}}(\Delta t/2);\ \Delta\mathbf{x}(\Delta t/2)$$

- Add external **E**, **B** fields via operator splitting
  - Hermite algorithm: drift + coulomb fields
  - Boris 'kick': all external **E**, **B** fields
- Benchmark w/ pure Hermite alg. for constant $B_{||}$

4^{th}-Order Predictor/Corrector Hermite Algorithm

- Algorithm developed and used extensively by galactic dynamics community
  - J. Makino, The Astrophysical Journal **369**, 200 (1991)
  - J. Makino & S. Aarseth, Publ. Astron. Soc. Japan **44**, 141 (1992)
- Predictor step:

$$\mathbf{v}_{p,j} = \frac{1}{2}(t - t_j)^2 \dot{\mathbf{a}}_j + (t - t_j)\mathbf{a}_j + \mathbf{v}_j$$

$$\mathbf{x}_{p,j} = \frac{1}{6}(t - t_j)^3 \dot{\mathbf{a}}_j + \frac{1}{2}(t - t_j)^2 \mathbf{a}_j + (t - t_j)\mathbf{v}_j + \mathbf{x}_j$$

- where

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

$$\mathbf{r}_{ij} = \mathbf{x}_{p,j} - \mathbf{x}_{p,i}$$

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

$$\mathbf{v}_{ij} = \mathbf{v}_{p,j} - \mathbf{v}_{p,i}$$

$r_c \to 0$ "cloud" radius

Hermite Algorithm – including a Magnetic Field

- The corrector step: $\mathbf{x}_i(t_i+\Delta t_i)=\mathbf{x}_{p,i}+\frac{1}{24}\Delta t_i^{\,4}\mathbf{a}_{0,i}^{(2)}+\frac{1}{120}\Delta t_i^{\,5}\mathbf{a}_{0,i}^{(3)}$

$$\mathbf{v}_i(t_i+\Delta t_i)=\mathbf{v}_{p,i}+\frac{1}{6}\Delta t_i^{\,3}\mathbf{a}_{0,i}^{(2)}+\frac{1}{24}\Delta t_i^{\,4}\mathbf{a}_{0,i}^{(3)}$$

  – where $\mathbf{a}_{0,i}^{(2)}$ and $\mathbf{a}_{0,i}^{(3)}$ are linear functions of $\mathbf{a}(t)$ and $\dot{\mathbf{a}}(t)$ evaluated at times t_i and $t_i+\Delta t_i$

- Adding B-field breaks 4th-order scaling, unless
  – Lab-frame B is purely longitudinal, constant in time
  – **v**x**B** force is evaluated again at the predicted positions
  – magnetic term in velocity correction (far right term above):
    - $\mathbf{a}_{0,i}^{(3)}$ is split into self-field $\mathbf{a}_{self-field,i}^{(3)}$ & magnetic $\mathbf{a}_{magnetic,i}^{(3)}$ terms
    - the coefficient in front of $\mathbf{a}_{magnetic,i}^{(3)}$ is changed from 1/24 to 5/72

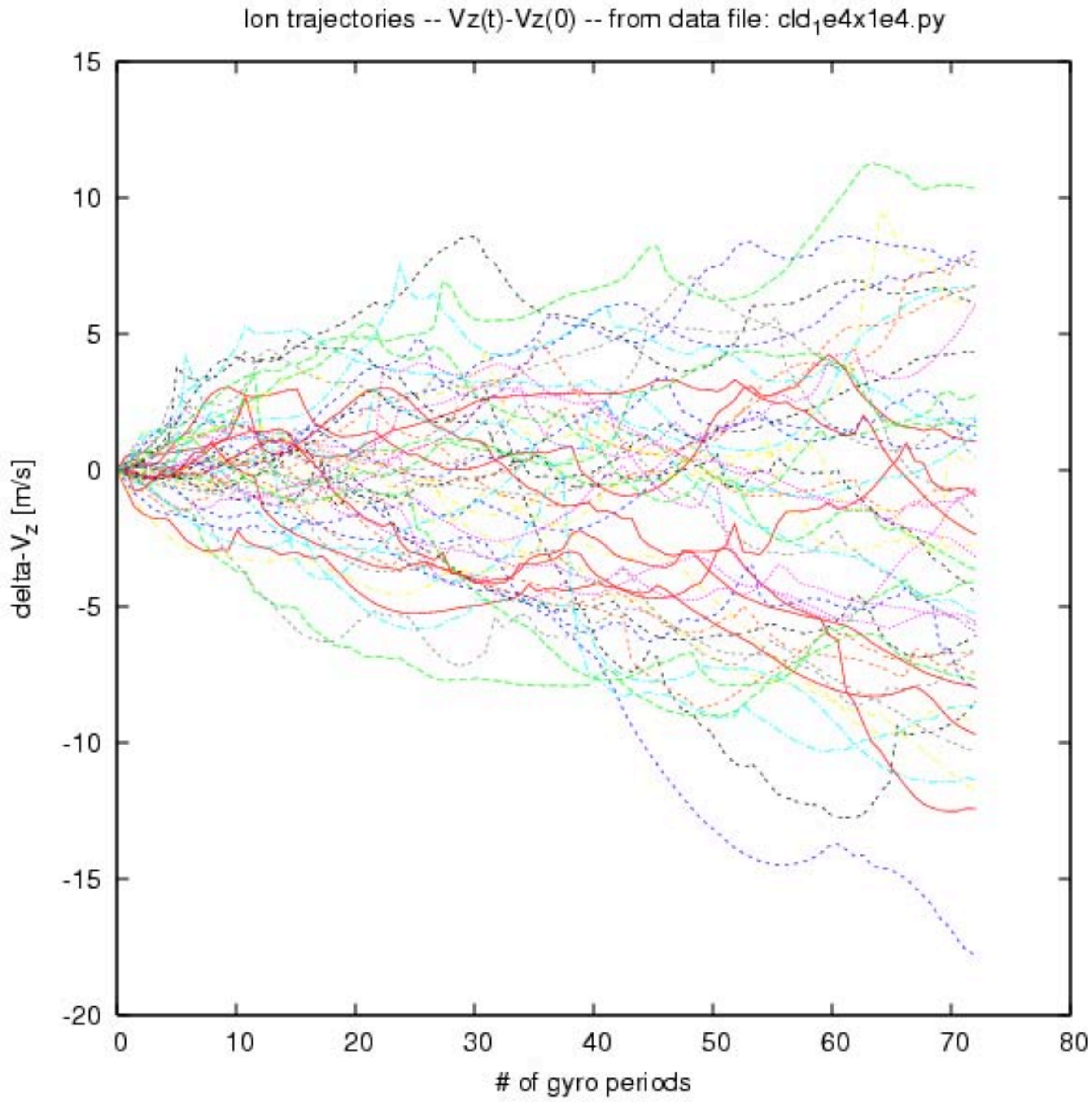
Diffusive dynamics can obscure friction/drag

- For a single pass through the cooler
  - Diffusive velocity kicks are larger than velocity drag
  - Consistent with theory
- For sufficiently large $\Delta_{e,||}$
  - numerical trick of e-/e+ pairs can suppress diffusion
- Only remaining tactic is to generate 100's of trajectories
  - Central Limit Theorem states that mean velocity drag is drawn from a Gaussian distribution, with rms reduced by $N_{traj}^{1/2}$ as compared to the rms spread of the original distribution
  - Hence, error bars are +/- 3 rms / $N_{traj}^{1/2}$
- Not practical to routinely generate 100's or 1000's of trajectories by hand, one at a time
  - run 8 trajectories simultaneously
  - use "task farming" approach to automate many runs

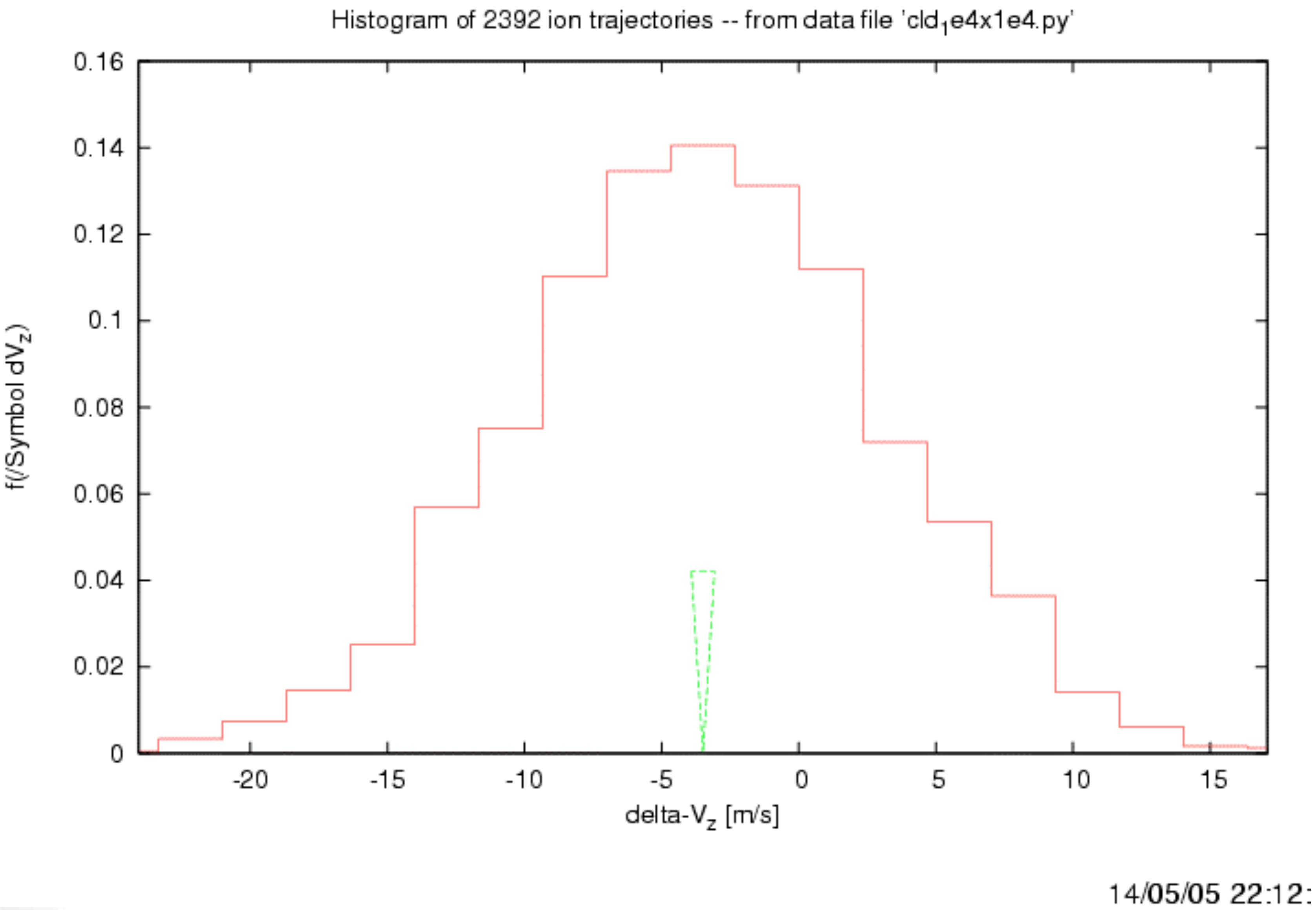
TaskDLish – Task Farming Parameter Scans

- Distributed “workers” are launched in an orderly fashion
  - works with cluster/super-computer scheduling software
  - shell scripts launch VORPAL sim.’s with different parameters
- A “tuple space” of independent tasks
  - made available to all processors
- Processors choose and independently execute tasks
- Efficient scheduling, load balancing, and fault tolerance
- Commercial version is available
  - http://www.txcorp.com/products/FastDL/

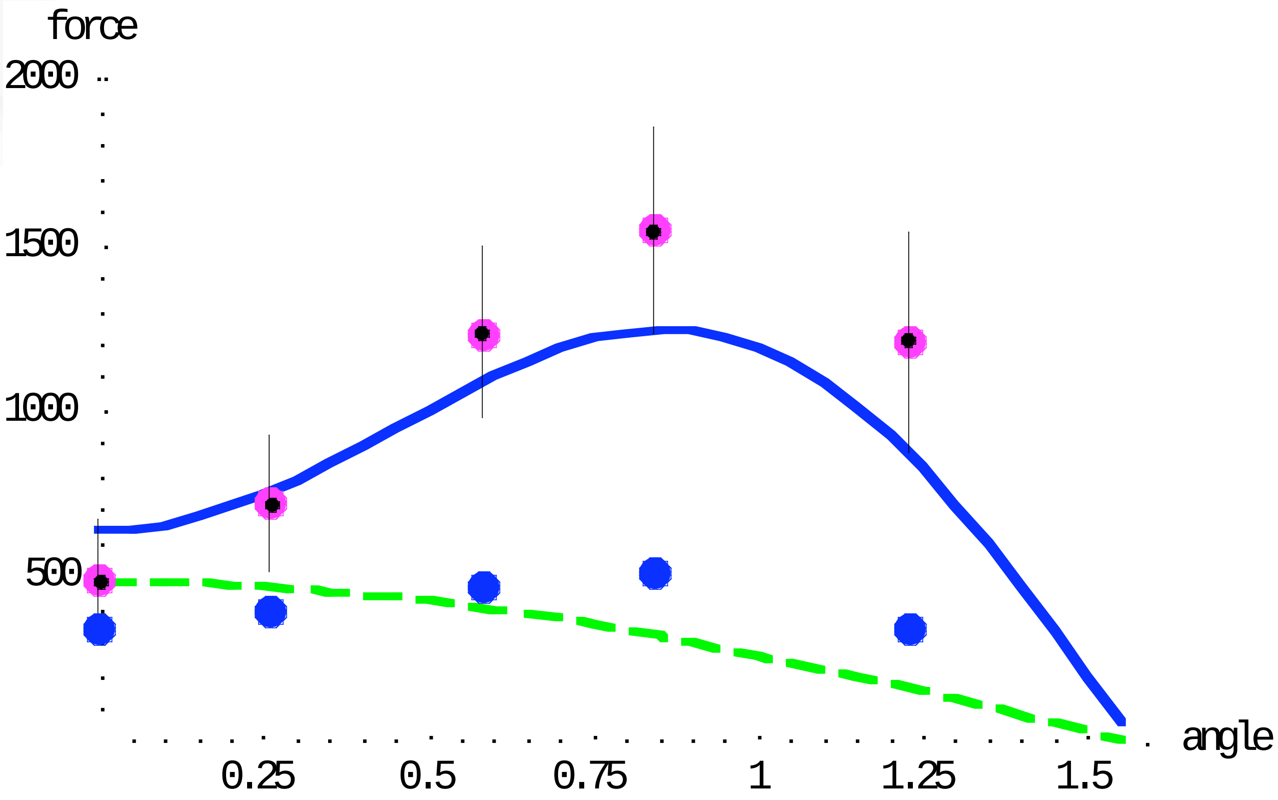
Task farming example: diffusion obscures friction



Task farming: central limit theorem extracts friction



VORPAL simulations of cooling physics have explained differences between competing analytical formulae



Dependence of longitudinal component of friction force [eV/m] on angle [rad] wrt magnetic field lines: solid blue line – Derbenev-Skrinsky asymptotics; dashed green line – empirical formula of Parkhomchuk empirical formula; pink dots with errors bars – VORPAL simulations of ultra-cold e- beam; blue dots without errors bars – VORPAL simulations of finite temperature electrons.

Fedotov, Bruhwiler, Abell & Sidorin, "Detailed Studies of Electron Cooling Friction Force," Proc. of COOL 05 Workshop (2005); Fedotov et al., PRSTAB (2006).

Wiggler approach to RHIC cooler

- Advantages of a wiggler
  - provides focussing for e- beam
  - suppresses recombination
    - Modest fields (~10 Gauss) effectively reduce recombination via 'wiggle' motion of electrons:

$$\rho_w = \frac{\Omega_{gyro}}{k_w^2 v_{beam}} \sim 1.4x10^{-3} \lambda_w^2[m] B_w[G] / \gamma$$

- Negative effects of 'wiggle' motion on cooling?
  - intuition suggests an increase of the minimum impact parameter in the Coulomb logarithm: $\rho_{\min} \to \rho_w$
  - this has now been confirmed via VORPAL simulations

Requirement to use Operator Splitting

- Hermite algorithm is highly specialized
  - strong external fields must be handled differently
  - operator splitting is standard for ODE's & PDE's
- Consider Lorentz force equations

$$\dot{\mathbf{x}} = \mathbf{v} \qquad \dot{\mathbf{v}} = \frac{q}{m}\mathbf{E}_{Coulomb} + \frac{q}{m}\left(\mathbf{E}_{ext} + \mathbf{v}\times\mathbf{B}_{ext}\right)$$

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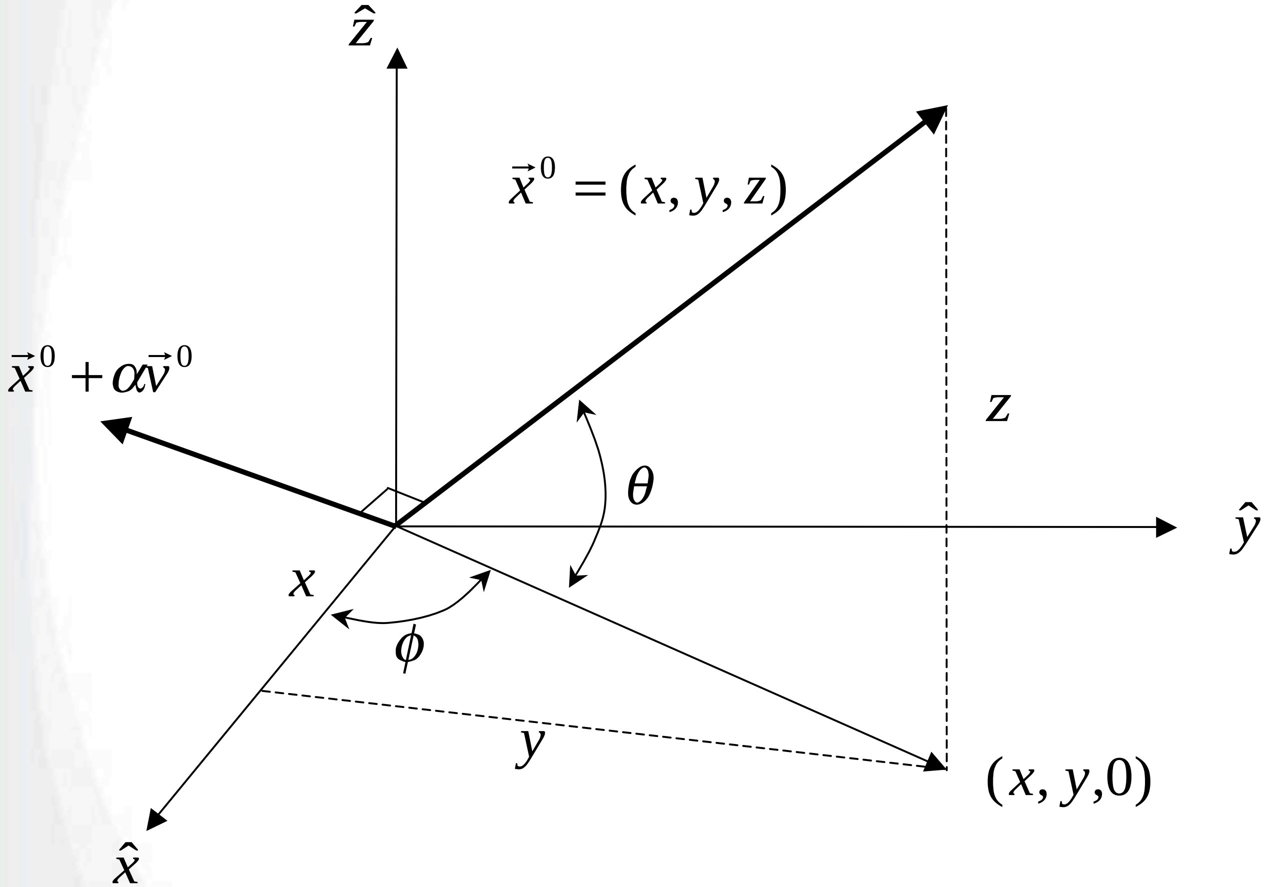
Operator splitting is implemented for 'reduced' model

- Hermite algorithm is problematic
  - difficult to parallelize
  - not well-suited for operator splitting
  - very "fussy", requiring careful choice of num. param.'s
- A new semi-analytical algorithm was developed
- Use two-body orbit theory for ion/e- pairs
  - handle each pair separately in center-of-mass frame
  - calculate initial orbit parameters in relevant plane
  - advance dynamics for a fixed time step
    - electron's new position and velocity are known
    - changes to ion position/velocity are small perturbations
  - total ion shift is sum of individual changes

Semi-analytic 'Reduced' Model for Binary Collisions

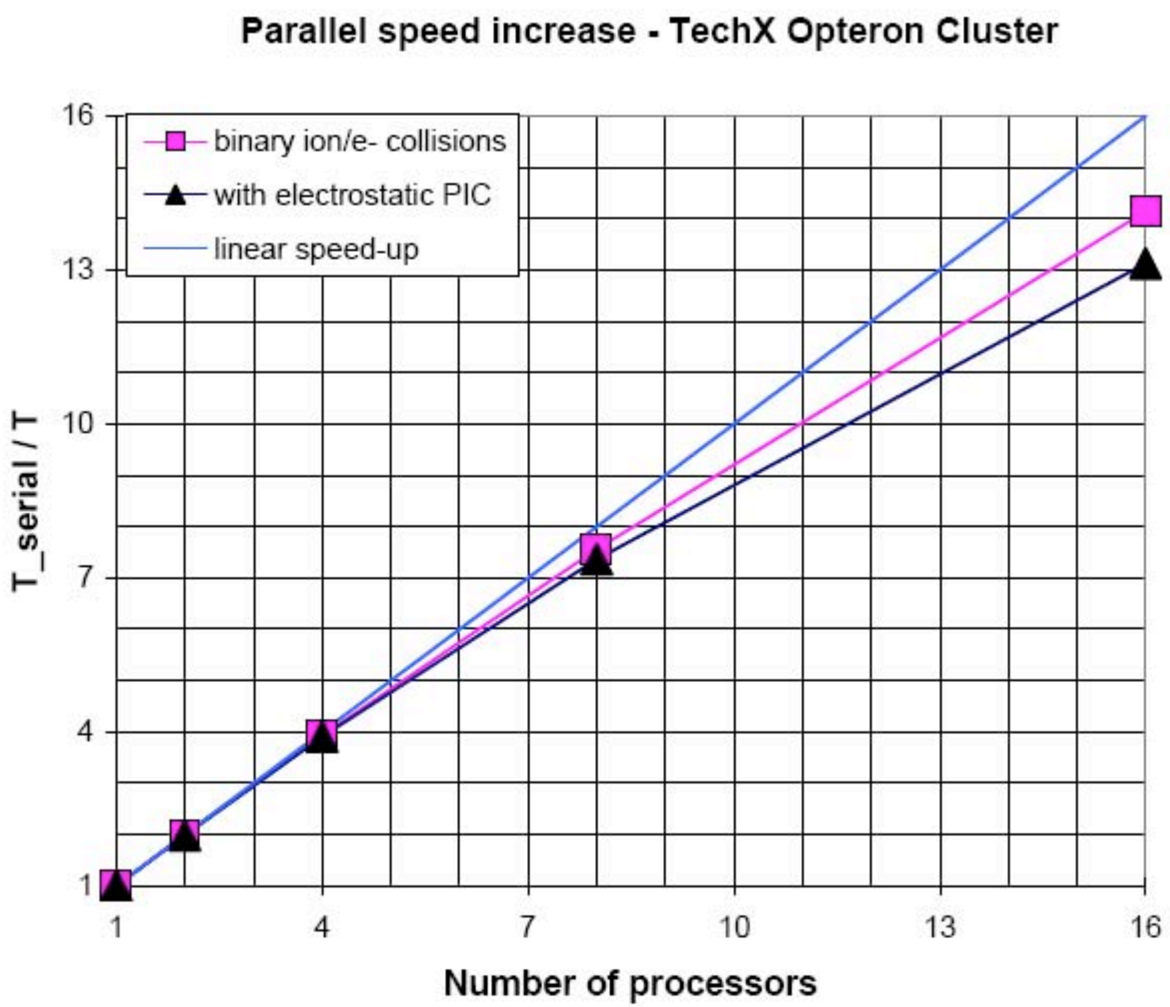
- Must find the plane in which partial orbit occurs
  - necessary rotations (yaw, pitch, roll) are complete
  - transformations are messy, but straightforward
  - "initial" positions & velocities obtained in this plane
- Then standard orbital parameters are calculated



$$R\vec{x}^0 = \begin{pmatrix} \left|\vec{x}^0\right| \\ 0 \\ 0 \end{pmatrix}$$

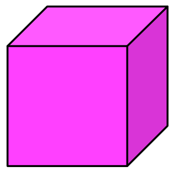
$$R^T(\Delta x)$$

Binary Collision Model works well in parallel



Baseline Parameters for RHIC-II Cooler

- e^- Beam parameters
  - Density: 9.5×10^{13} e^-/m^3
  - rms e- velocities [x,y,z]: 2.8×10^5, 2.8×10^5, 9.0×10^4 m/s
  - $\gamma = 108$
- Undulator parameters
  - Length: 80 m
  - Wavelength: 8 cm
  - Sections: 10
  - Field on axis: $B_0 = 10\,G = .001\,T$
  - Interaction time: 2.47 nanoseconds (beam frame)
- Problem setup in Vorpal
  - Domain size: 0.8 mm x 0.8 mm x 0.8 mm
  - Gold ions per domain: 8
  - Electrons per domain (actual): 4.86×10^4
  - Periodic domain

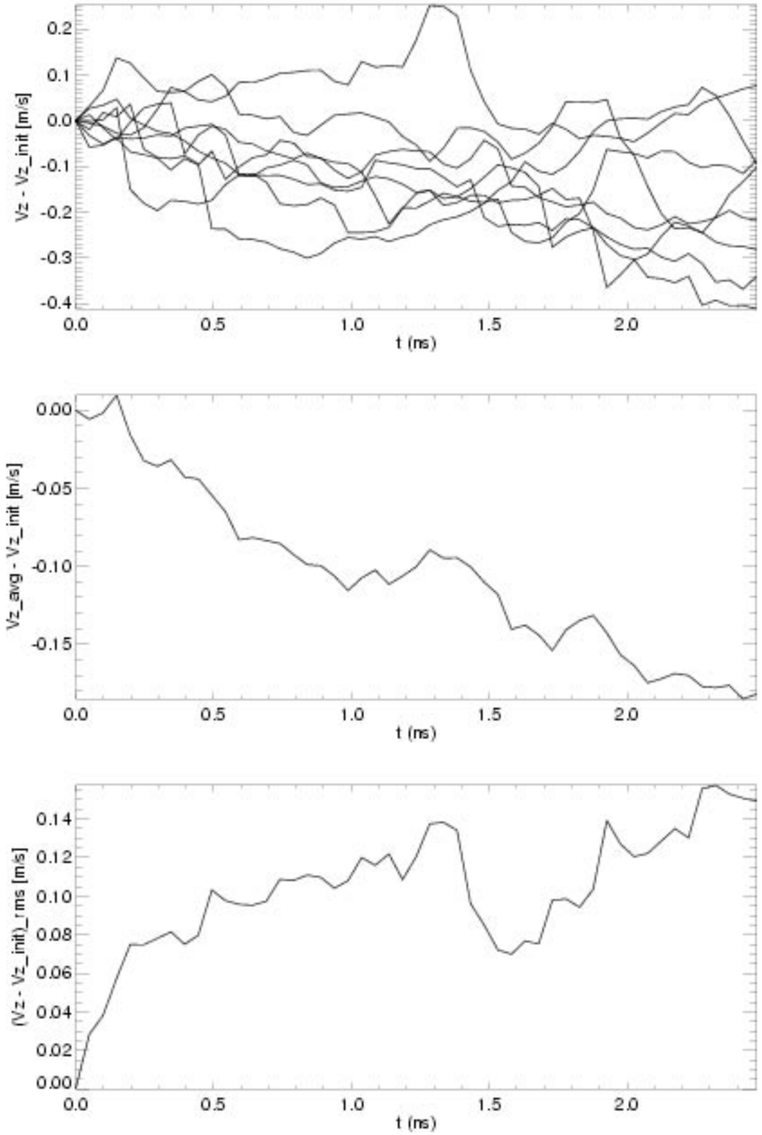


Suppressing diffusive dynamics, Part II

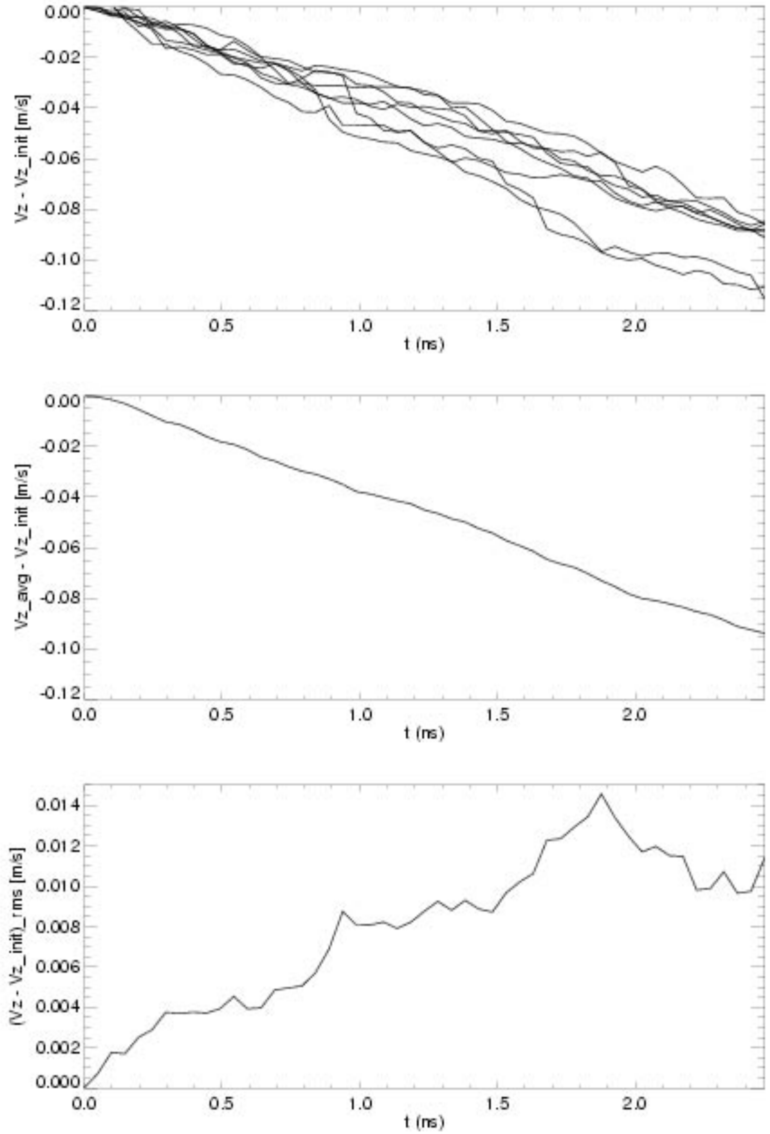
- For a single pass through the cooler
  - Diffusive velocity kicks are larger than velocity drag
  - Consistent with theory
- For sufficiently warm electrons…
  - numerical trick of e-/e+ pairs still works
- Better approach to generating 100's of traj.'s
  - "task farming" approach is no longer used
  - now we use "micro-particles" and parallel processing
    - each physical electron is divided into 100's of micro-particles
    - this is equivalent to averaging 100's of independent runs
    - parallel processing makes this practical in a single run
  - typically run 8 ion trajectories simultaneously

Noise reduction 1: splitting electrons

1 macroparticle per electron

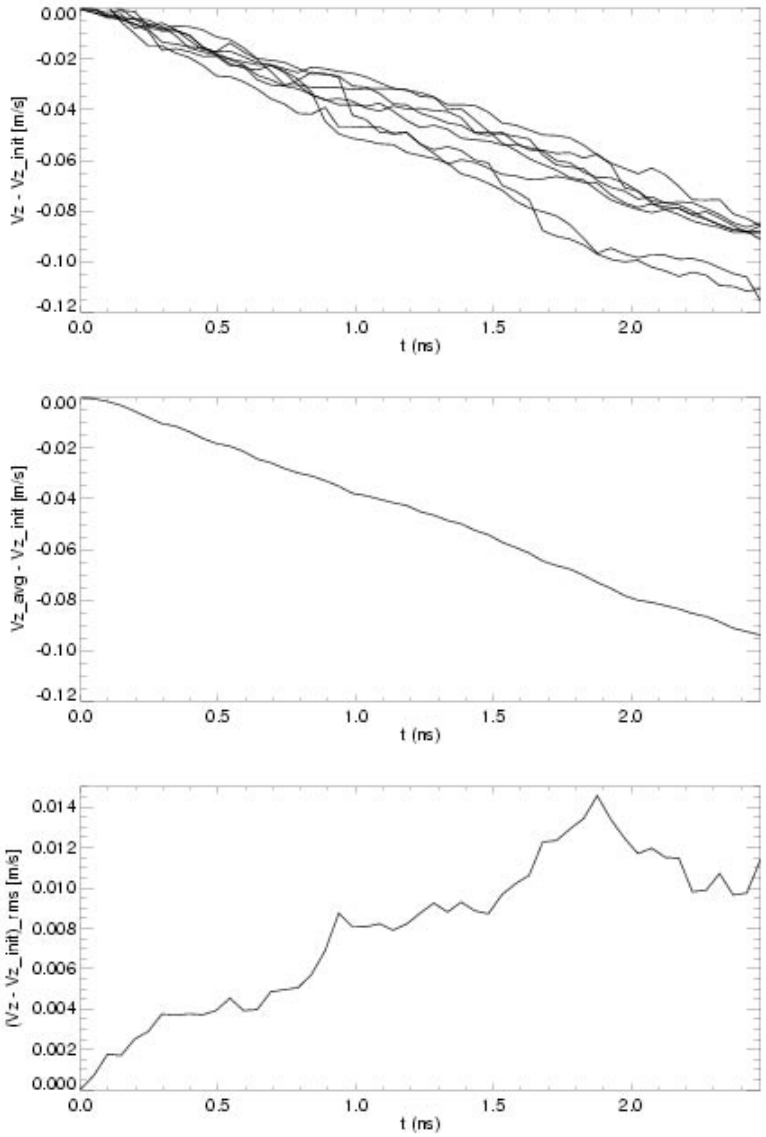


266 macroparticles per electron

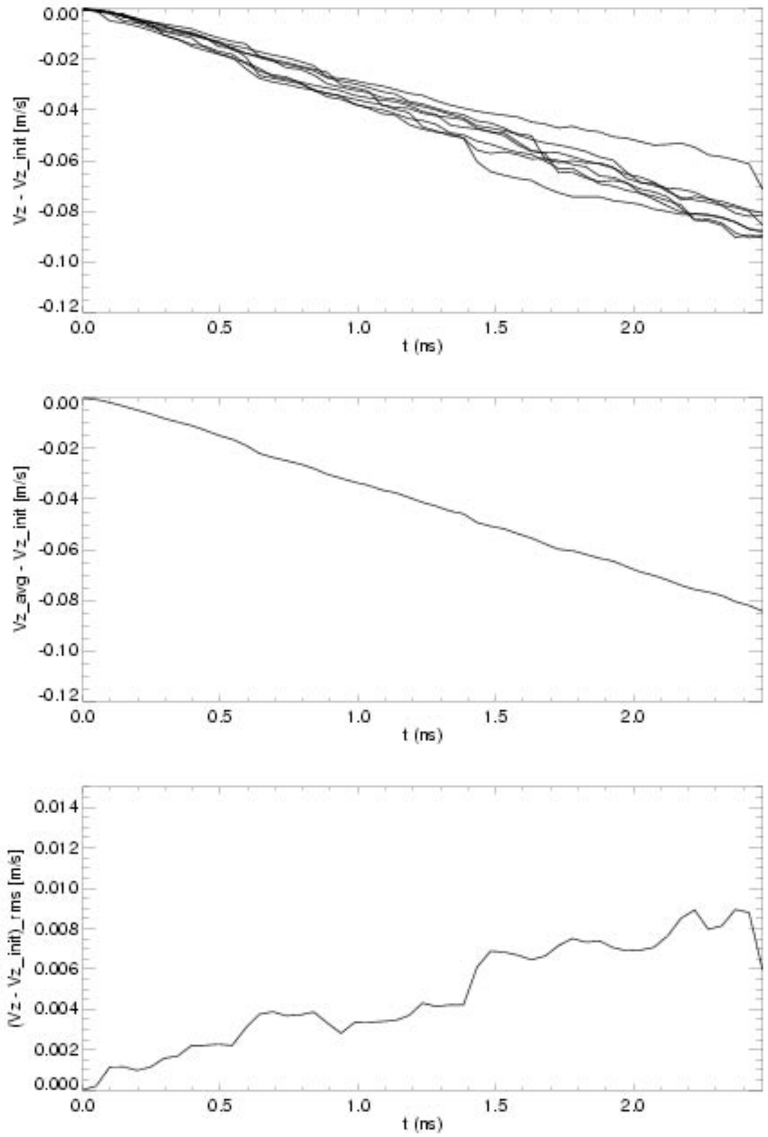


Noise Reduction 2: using positrons

266 macroparticles per electron



133 macroparticles per electron
133 macroparticles per positron



Field Expansion (courtesy A. Jain of BNL)

Harmonic Expansion

- Axial variation results in a 3-D field.
- A simple harmonic expansion results under the assumption of periodicity along the *Z*-axis with wavelength λ:

$$B_{r,\theta,z}(r,\theta,z) \equiv B_{r,\theta,z}(r,\tilde{\theta}); \quad \tilde{\theta} = \theta - kz$$

$$k = (d\alpha / dz) = \text{rate of change of dipole field angle} = 2\pi / \lambda$$

$$B_r(r,\tilde{\theta}) = B_0 \sum_{n=1}^{\infty} \left[\frac{2^n n!}{n^n (kR_{ref})^{n-1}} \right] I_n'(nkr) \left[\tilde{b}_n \sin(n\tilde{\theta}) + \tilde{a}_n \cos(n\tilde{\theta}) \right]$$

$$B_\theta(r,\tilde{\theta}) = B_0 \sum_{n=1}^{\infty} \left[\frac{2^n n!}{n^n (kR_{ref})^{n-1}} \right] \frac{I_n(nkr)}{kr} \left[\tilde{b}_n \cos(n\tilde{\theta}) - \tilde{a}_n \sin(n\tilde{\theta}) \right]$$

$$B_z(r,\tilde{\theta}) = -(kr) B_\theta(r,\tilde{\theta}) \qquad n = 1 \text{ is Dipole term, etc.}$$

Transforming fields to the beam frame

- A pure magnetic field in the lab frame

$$\vec{B} = \left(B_x(x,y,z), B_y(x,y,z), B_z(x,y,z)\right)$$

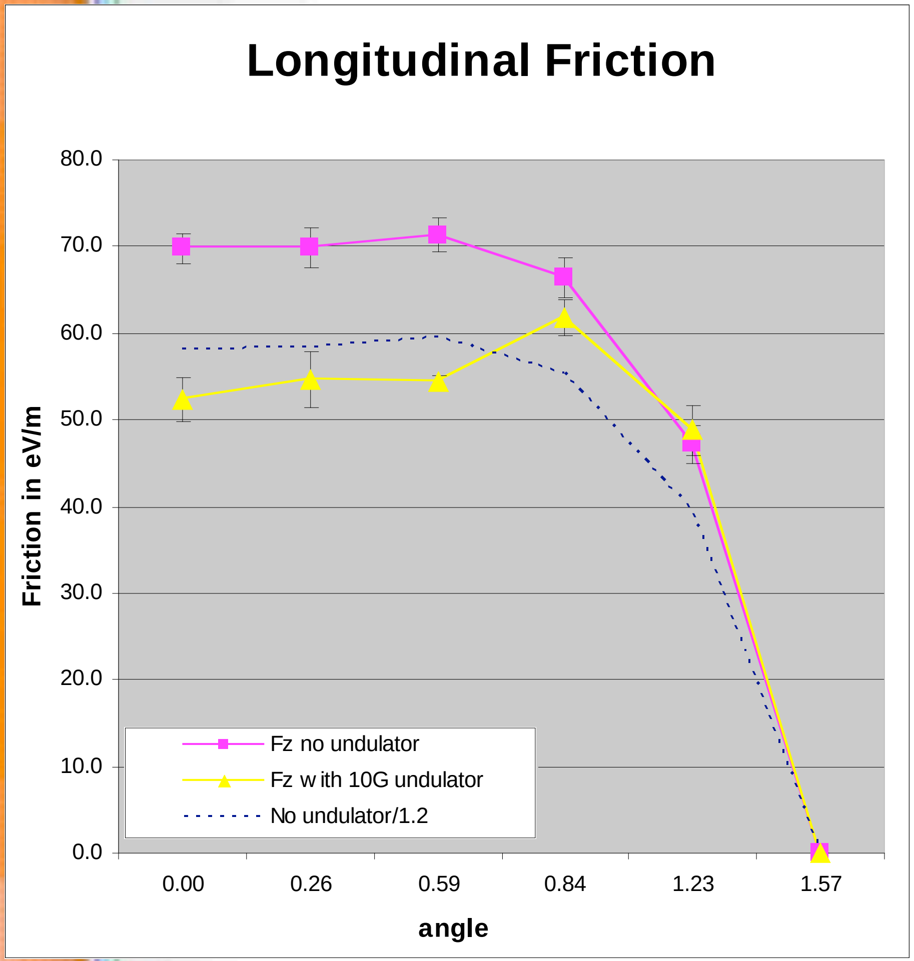
  in the beam frame becomes (via Lorentz transform):

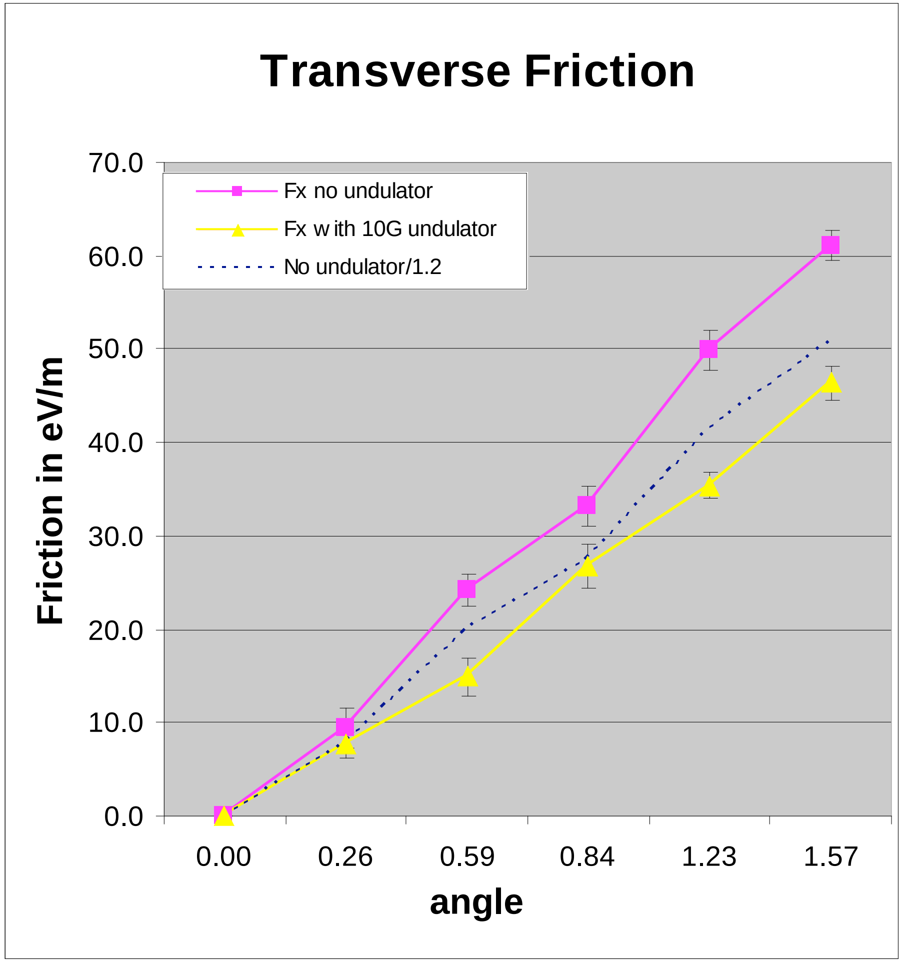
$$\vec{E}' = \gamma\vec{v}\times\vec{B} = \gamma\beta c\left(-B_y, B_x, 0\right)$$

$$\vec{B}' = \left(\gamma B_x, \gamma B_y, B_z\right)$$

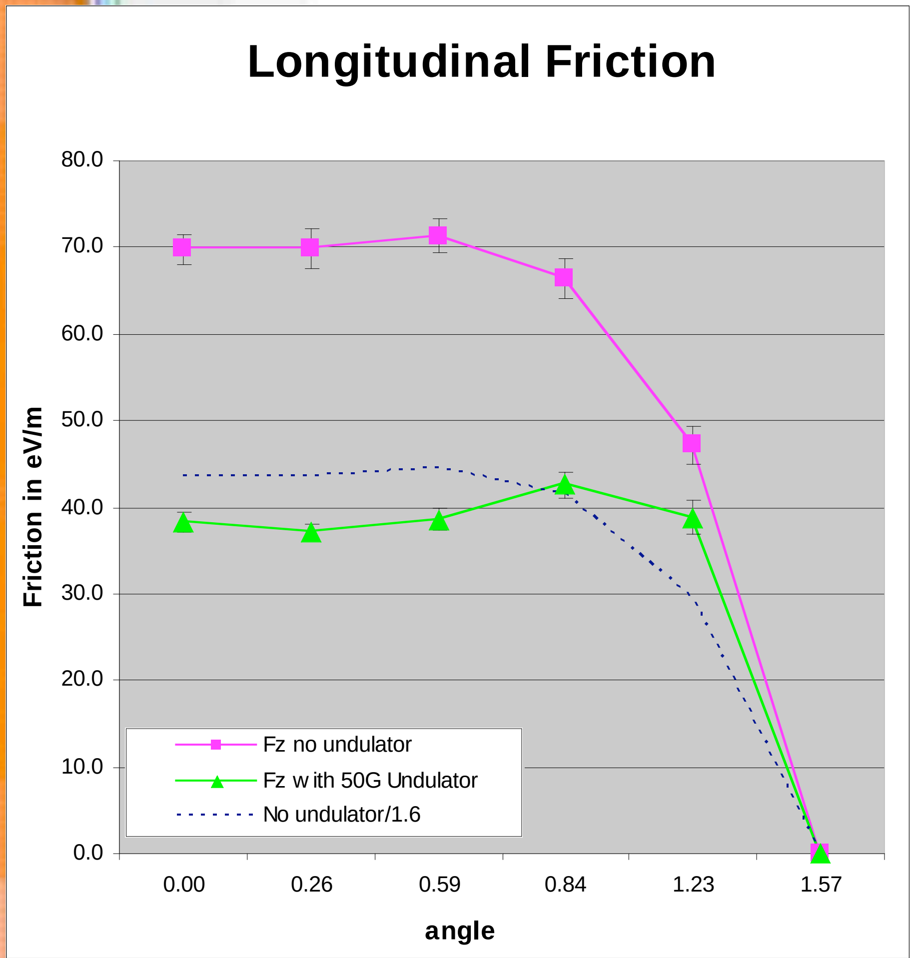
  – Primed variables represent beam frame variables
- If velocities in the beam frame are non-relativistic, we can ignore the magnetic field.
  – 10G field gives a transverse velocity in the beam frame of .006*c

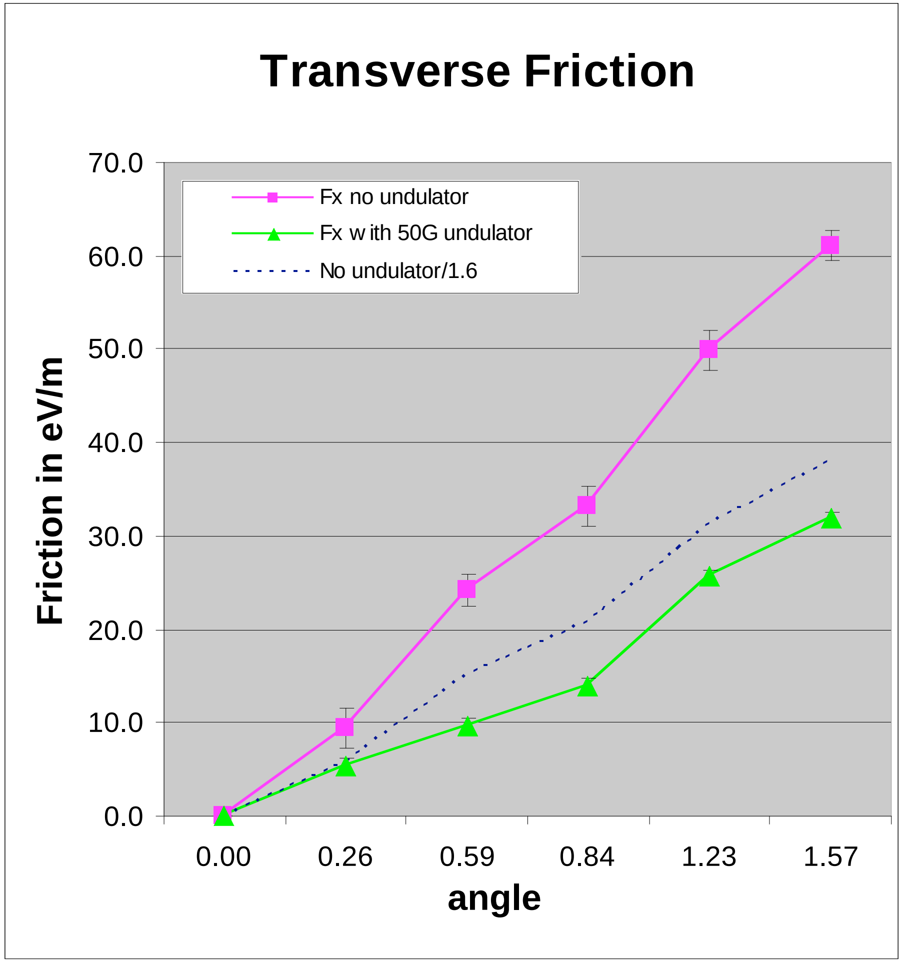
Wiggler results (10 Gauss)





Wiggler results (50 Gauss)





Conclusions

- Reliable first-principles simulation of dynamical friction is now routine with VORPAL
  - unmagnetized, wiggler, solenoids, errors
  - requires (can take advantage of) parallel computers
    - scales well up to 64 processors and probably higher
  - typically ignores e-/e- interactions
    - these are included via electrostatic PIC, when necessary
- VORPAL simulations confirmed that the effect of a wiggler is to increase ρ_{min}

Acknowledgements

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