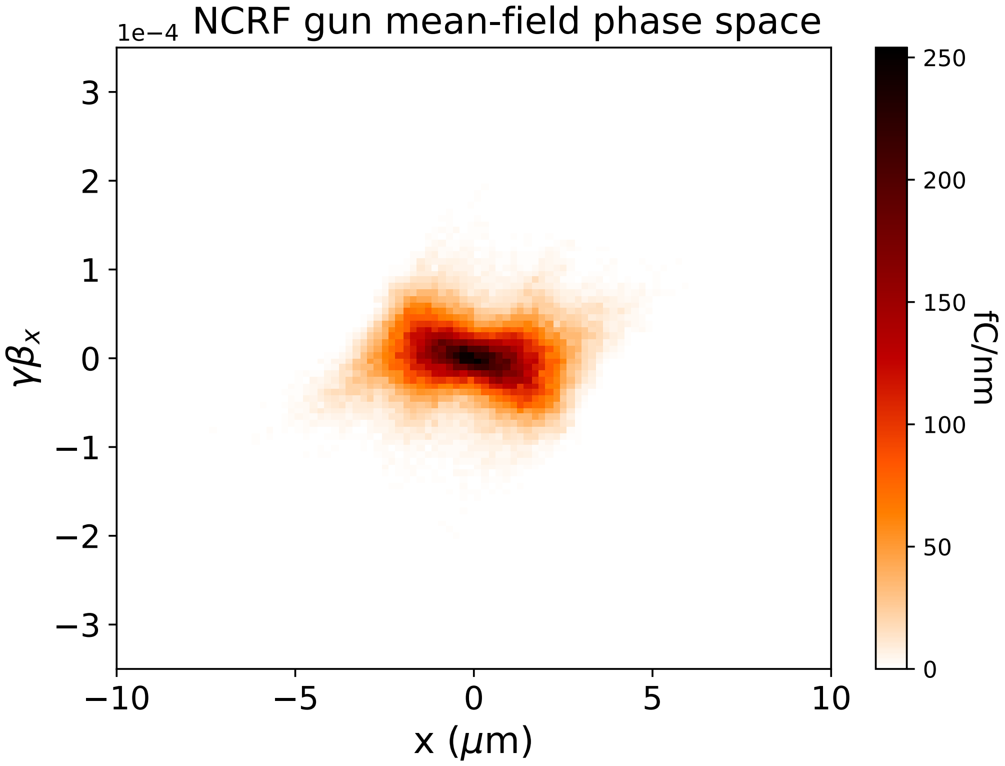
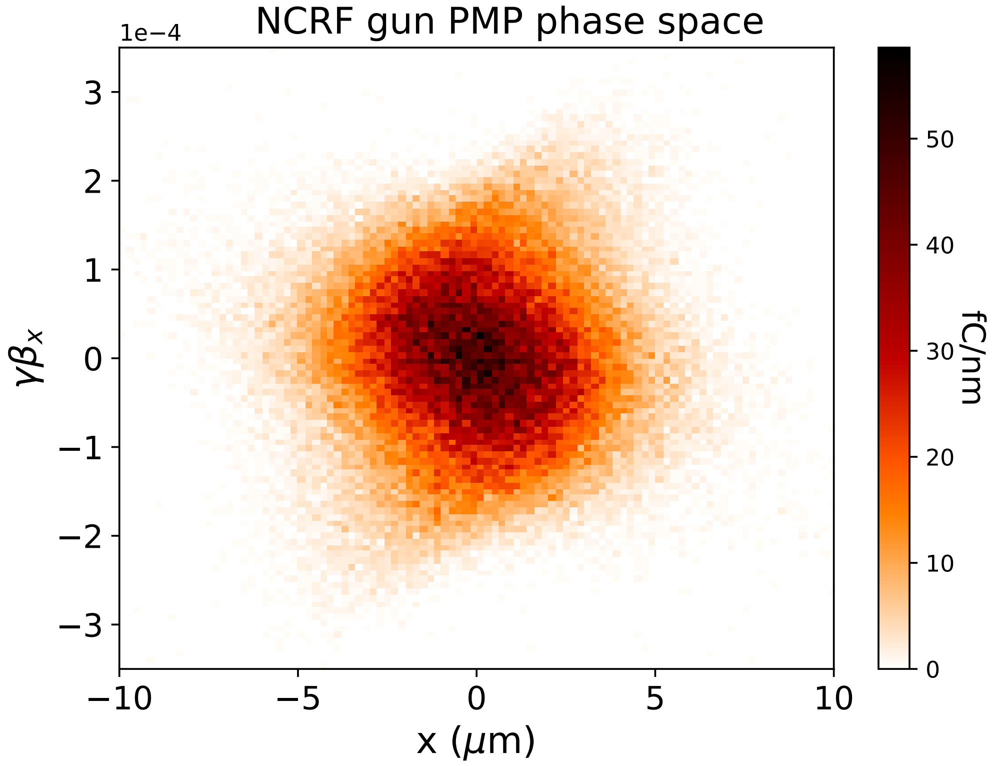
Beyond Space Charge: Simulating Ultracold Photoemission Beamlines

Matt Gordon

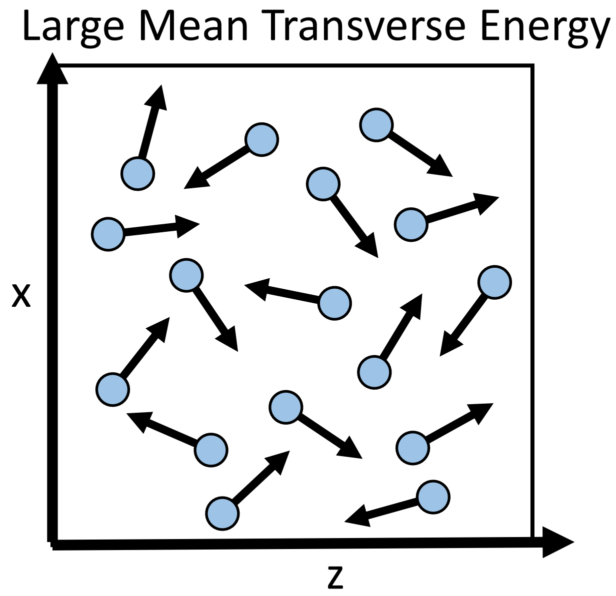


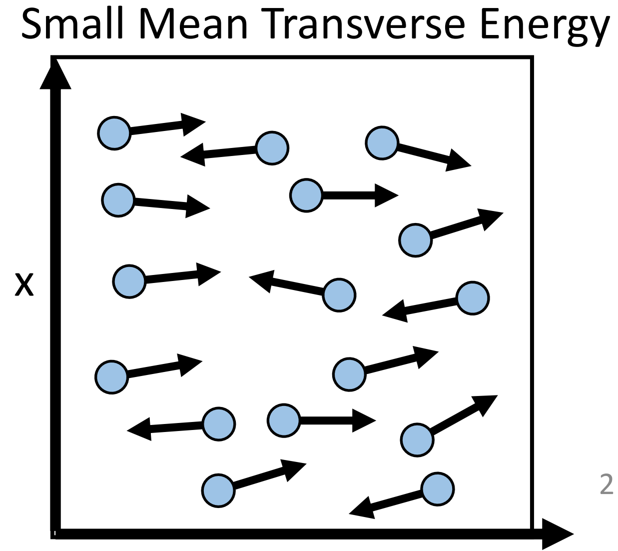
Add Reality



Motivation

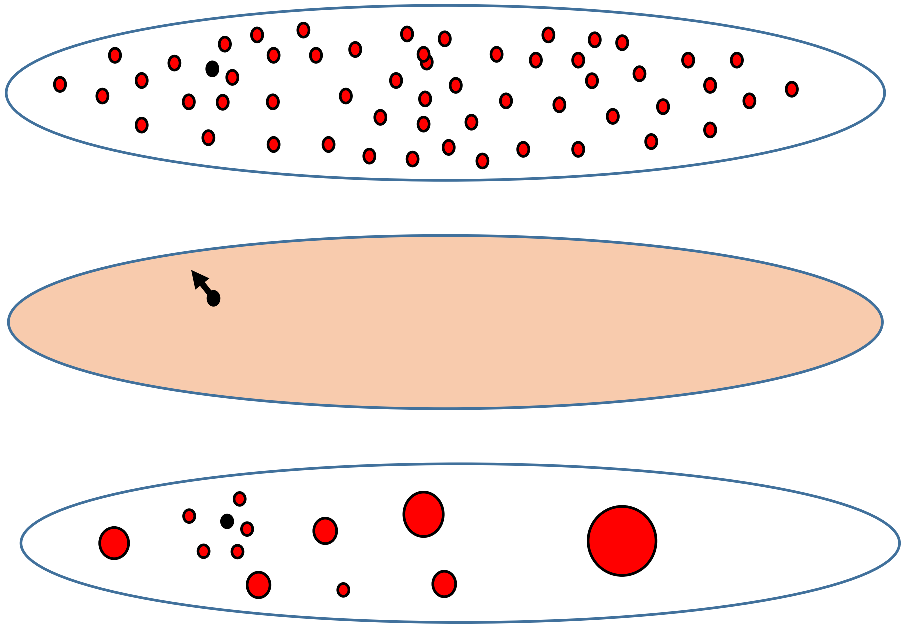
- Typical photocathodes have a mean transverse energy of hundreds of meV
- Want to reduce this to tens or even single digit meV
- At low temperatures, typical approximations used for electron interactions in simulation become less valid
- When will reducing MTE no longer improve beam quality?
- **Simulate the transport of cold electron beams**





How are Electron Interactions Simulated?

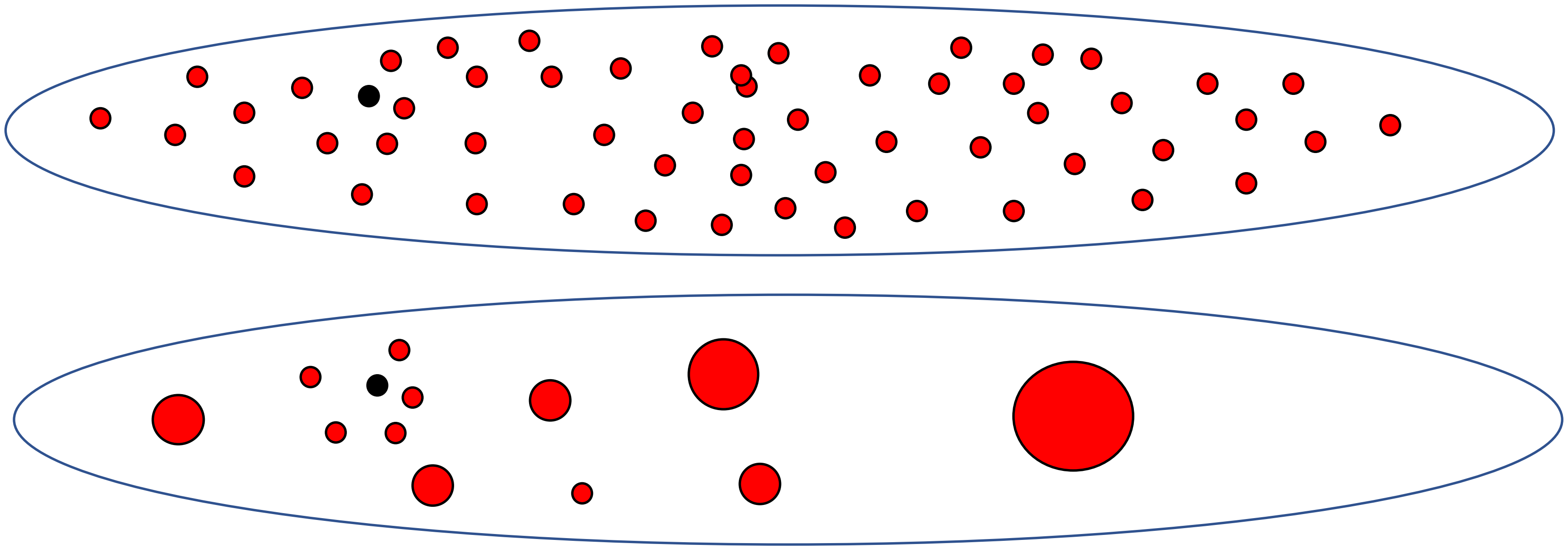
- An electron beam is a collection of point particles
- Exact interaction is computationally expensive
- Charge smoothed in a beam to approximate the interaction (space charge)
- Want to calculate short range interactions precisely and approximate long range interactions
- One method to do this is the Barnes-Hut Algorithm



From top to bottom:
Full Beam Brute Force Calculation
Mean-field Approximation
Barnes-Hut Approximation

Faster Simulation of Non-Mean-field Space Charge

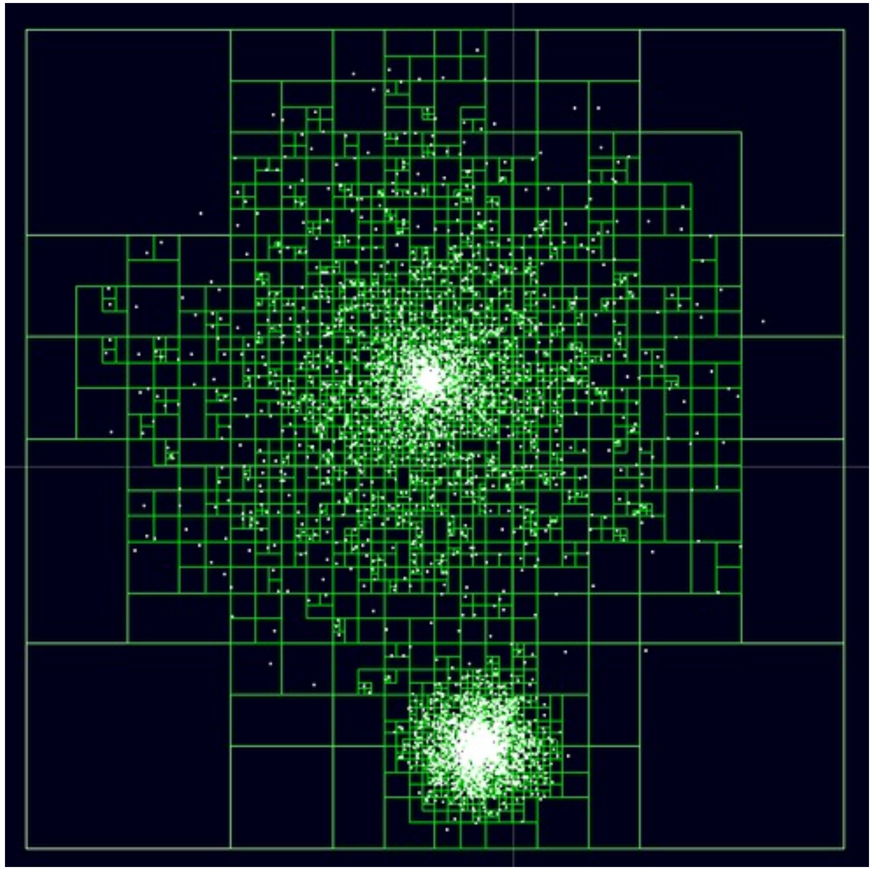
- To make simulating non-mean-field effects possible, rely on the multipole expansion
- E field of collection of charges approximated as series of static multipoles
- The Barnes Hut Tree Algorithm finds which groups of particles are far enough away, such that the monopole term is the only term which contributes to a desired accuracy
- Approximates long range forces, exactly calculates interactions from nearby particles



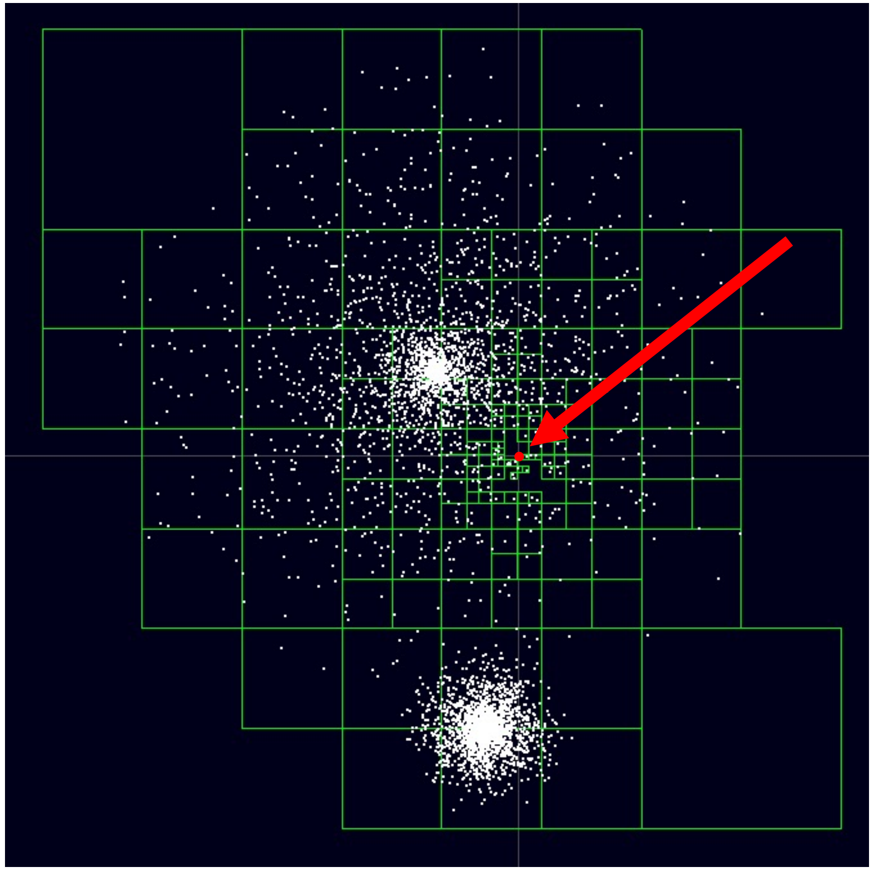
Barnes-Hut Algorithm

- Barnes-Hut tree algorithm for simulation of 2 nearby galaxies

Full Barnes-Hut Tree

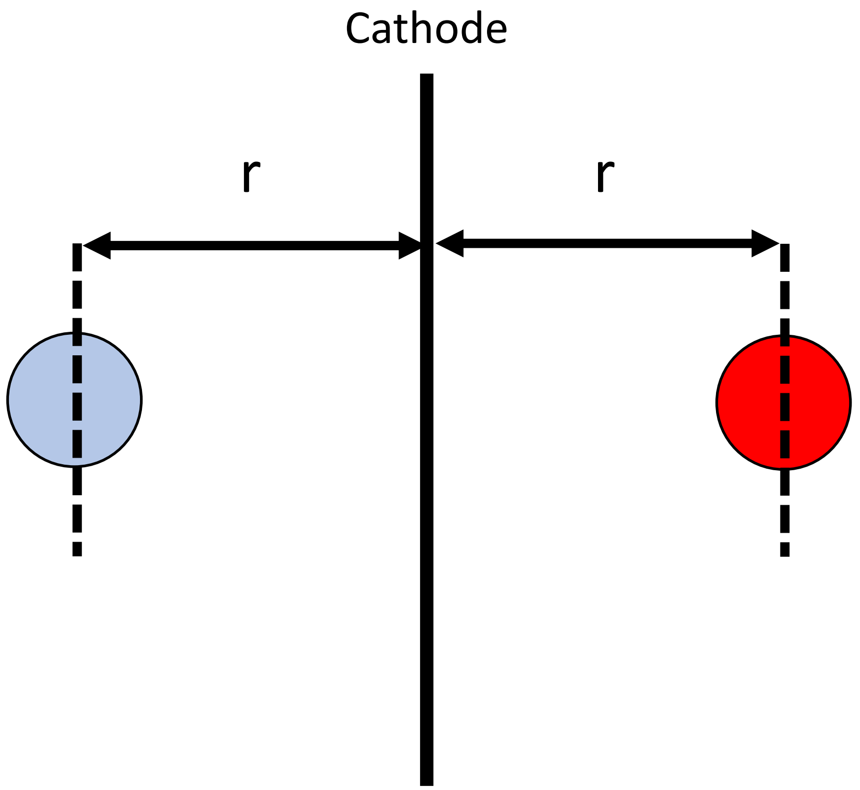


Grouped Nodes for force calculation of particle at origin (red)



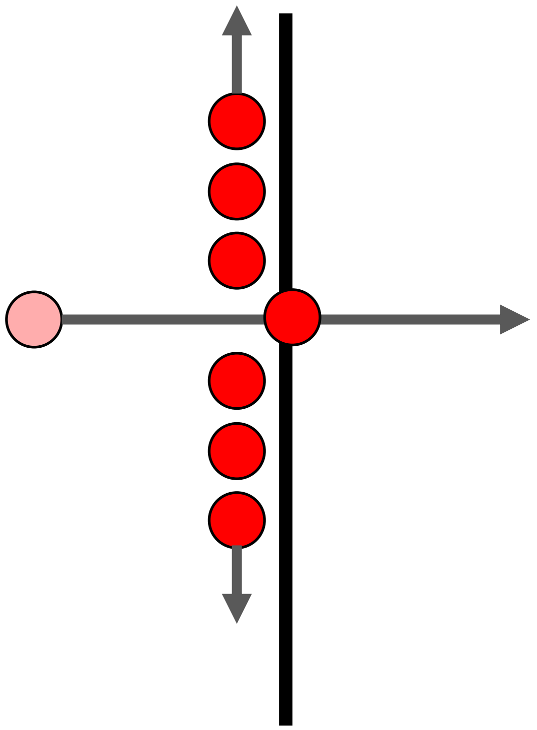
Cathode Divergence

- Model cathode interaction with image charge method
- Image potential diverges as distance from cathode goes to 0
- Not physical, we know electrons can escape
- Need to model the cathode in a different way



Dynamic Image Charge Method

- Semiclassical approximation of photoemission
- Image charge form on timescale set by the cathode material
- Image potential is velocity dependent and non-divergent
- Self-consistently solve for the image potential for different starting energies



The Plus-Minus-Plus(PMP) Method

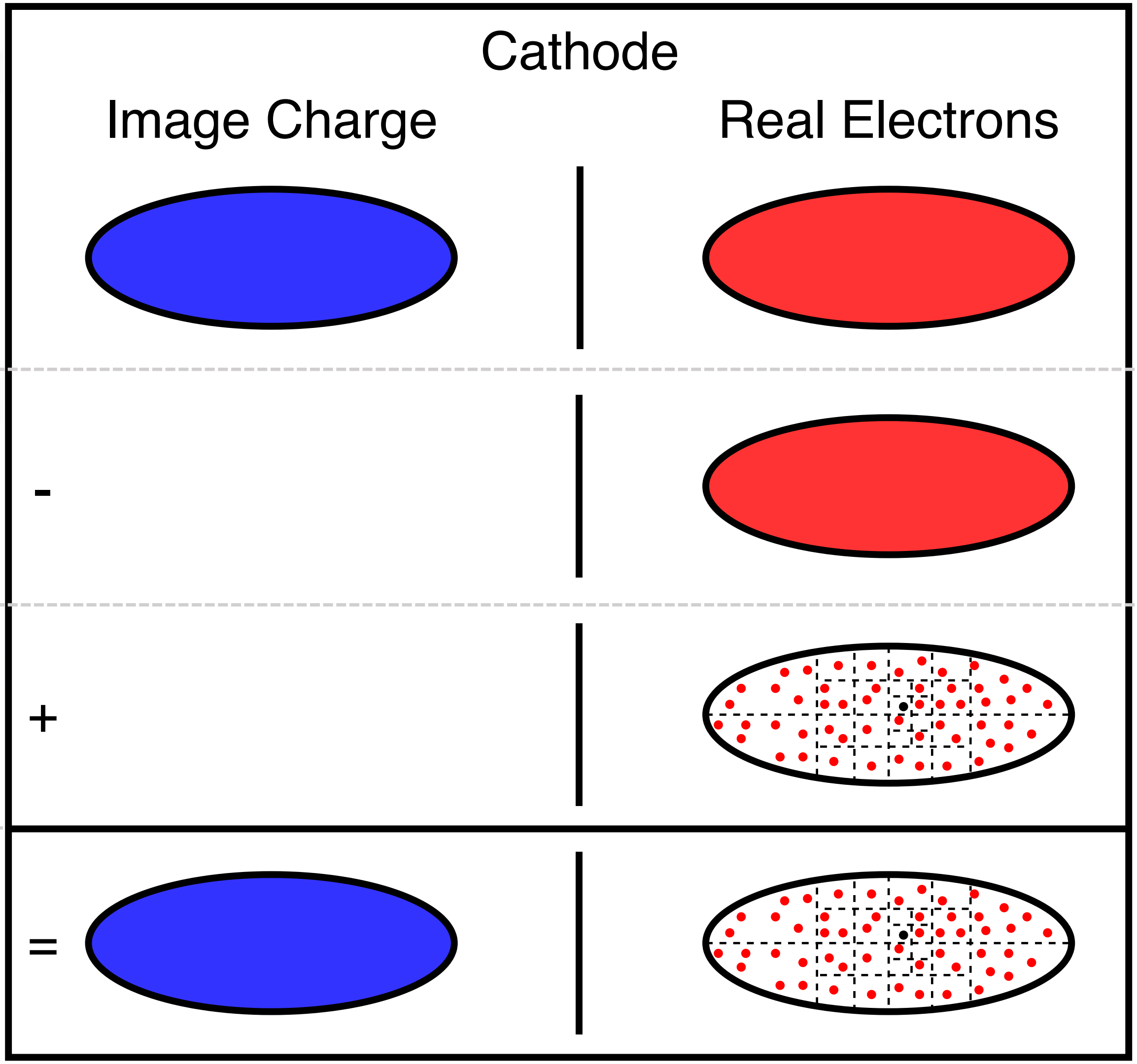
- Fields calculated in a 3 step process

- We will calculate the mean-field electric fields including cathode

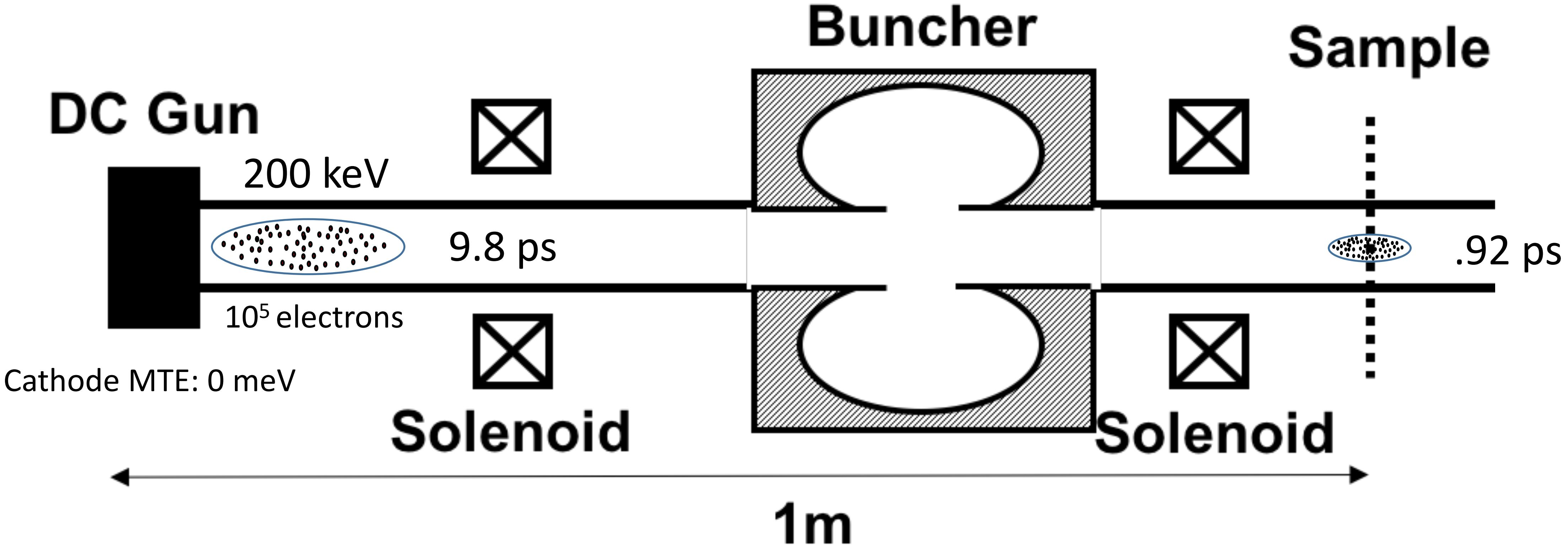
- Subtract out the mean field calculation without the cathode

- Add in the point-to-point interaction of the real particles

- Final Result

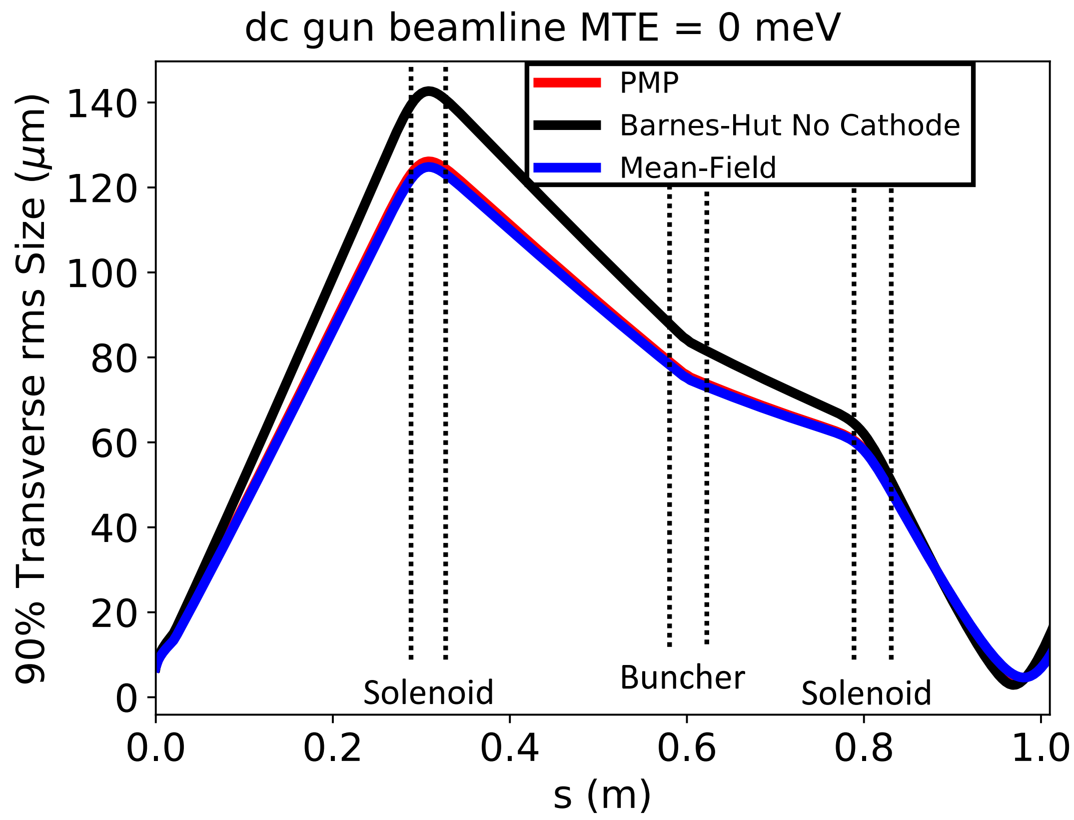


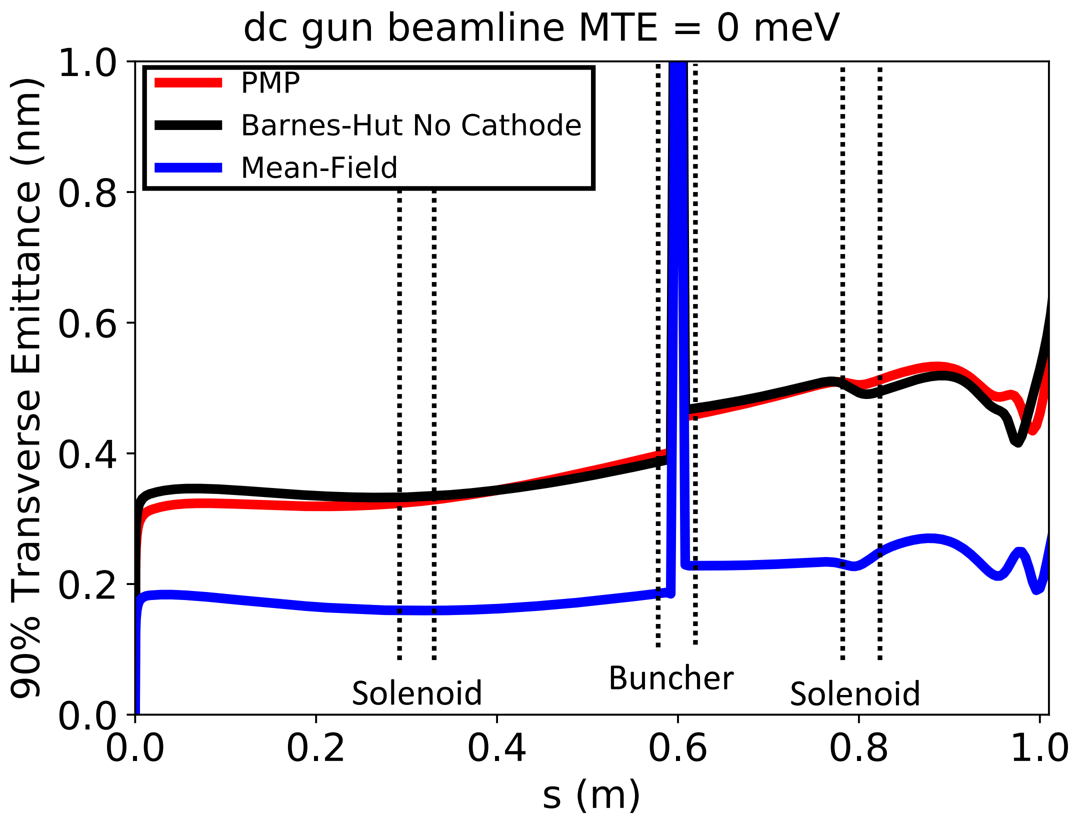
DC Ultrafast Electron Diffraction Beamline Details



DC Beamline Simulations

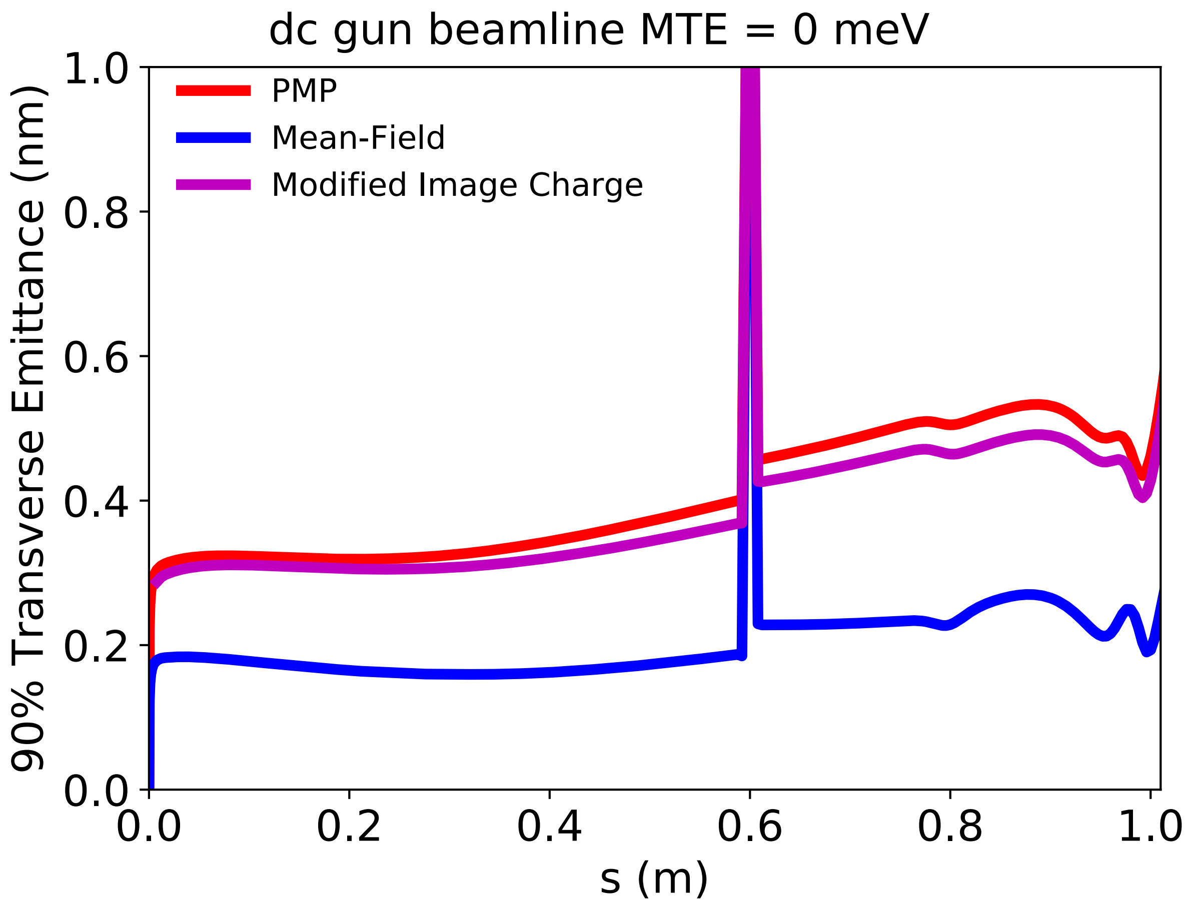
- Cathode effects needed to model beam correctly
- Point-to-point interactions increase emittance by a factor of 2



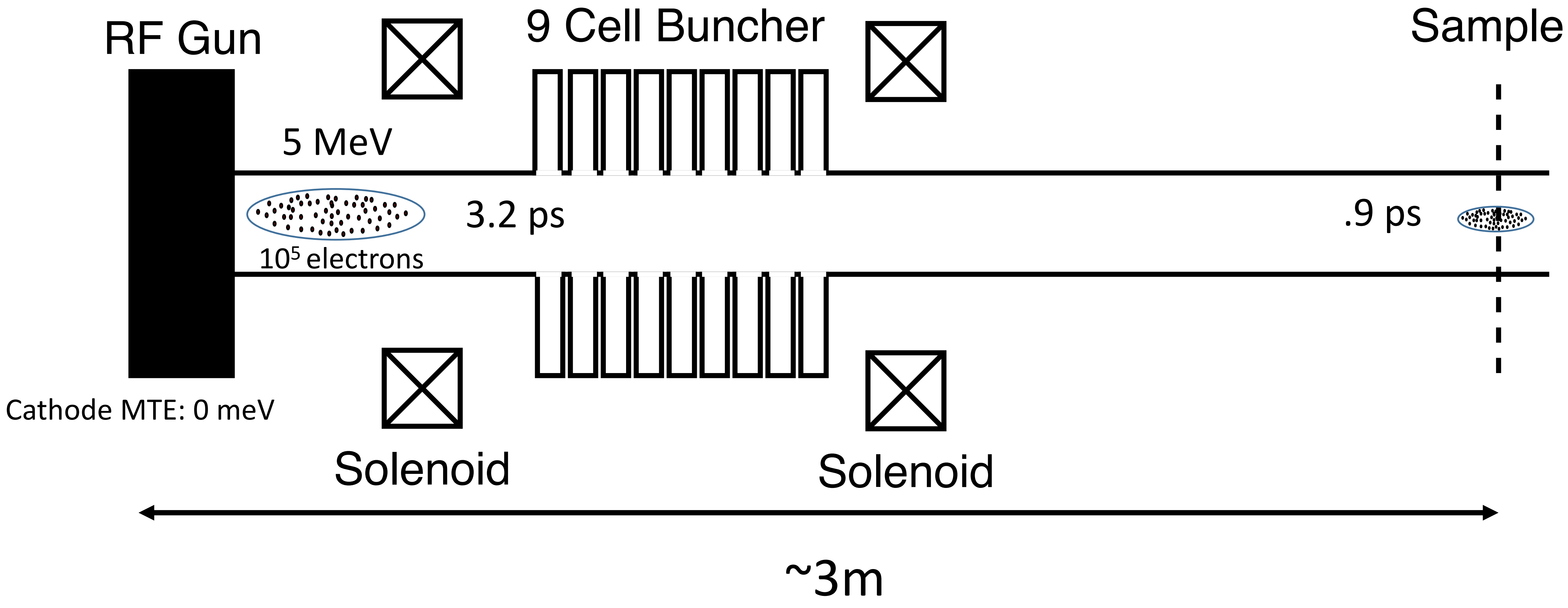


Dynamic Image Charge Comparison

- See how well the more exact calculation compares to the PMP method
- Qualitatively, the graph behave similarly
- Compares to PMP method quite well

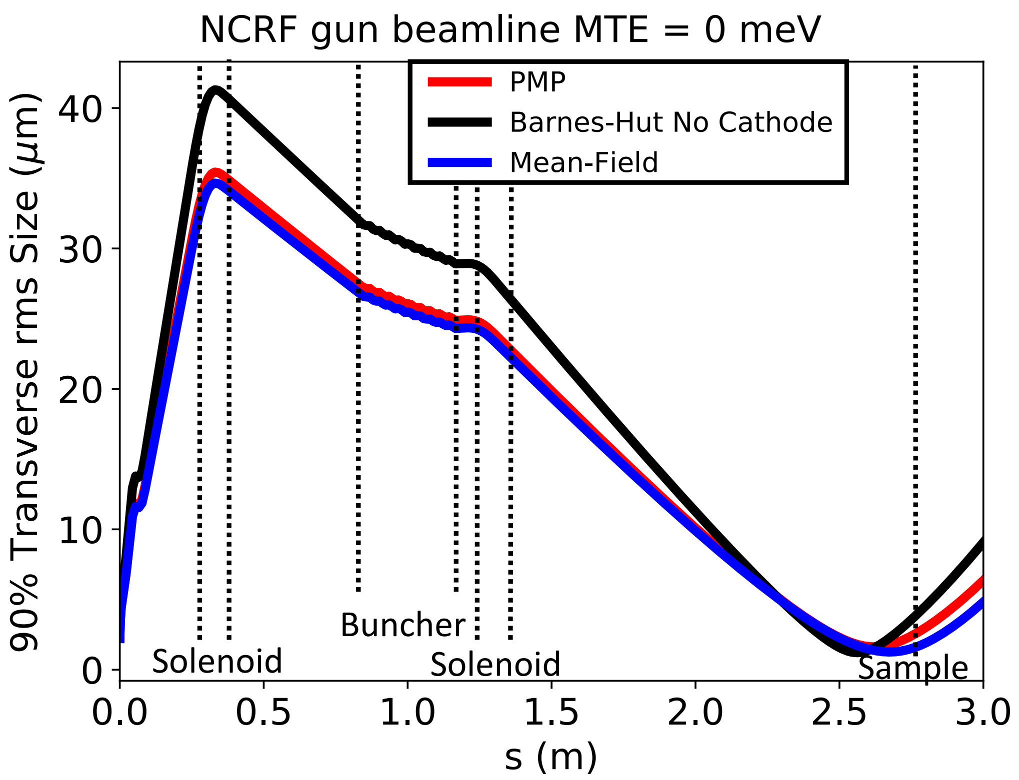


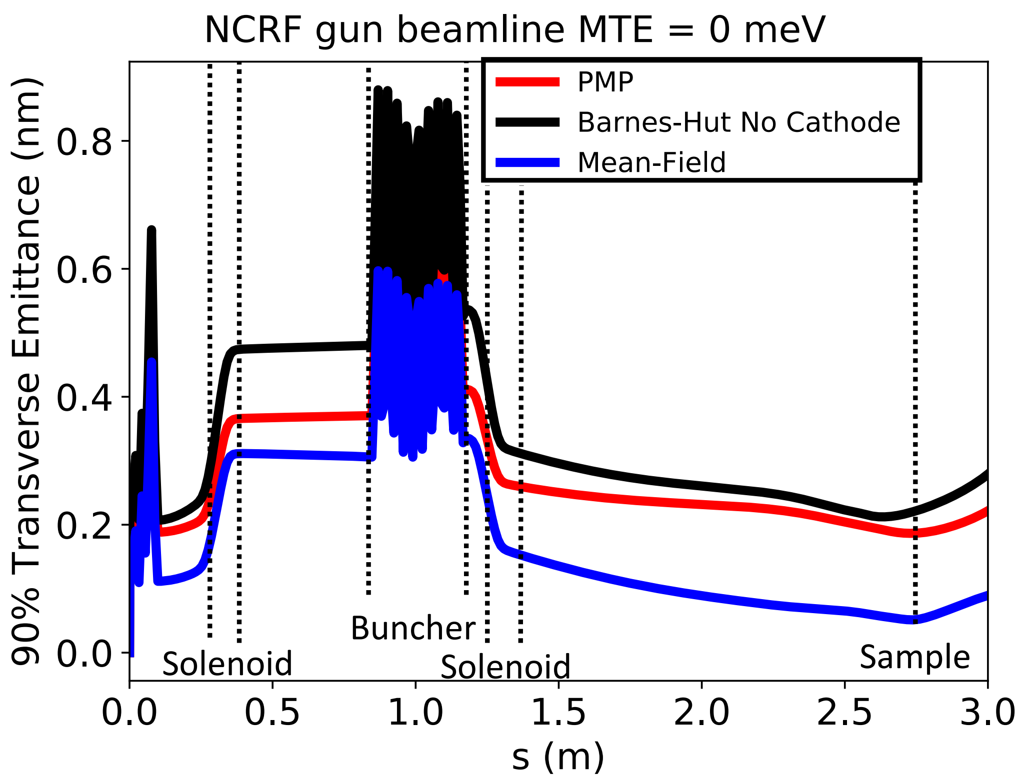
RF Ultrafast Electron Diffraction Beamline Details



RF Beamline Simulations

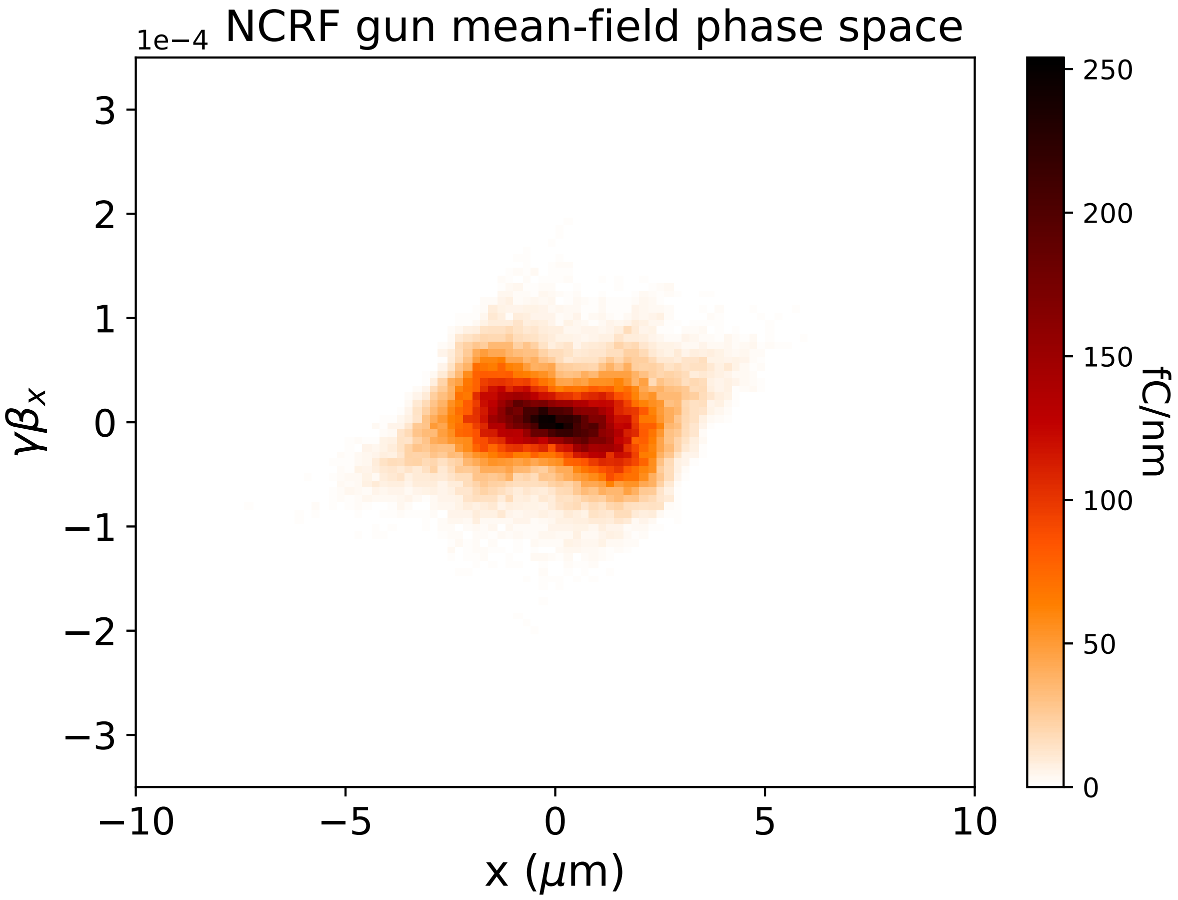
- At higher beam densities P2P effects matter more
- Point-to-point interactions increase emittance by a factor of 3.7

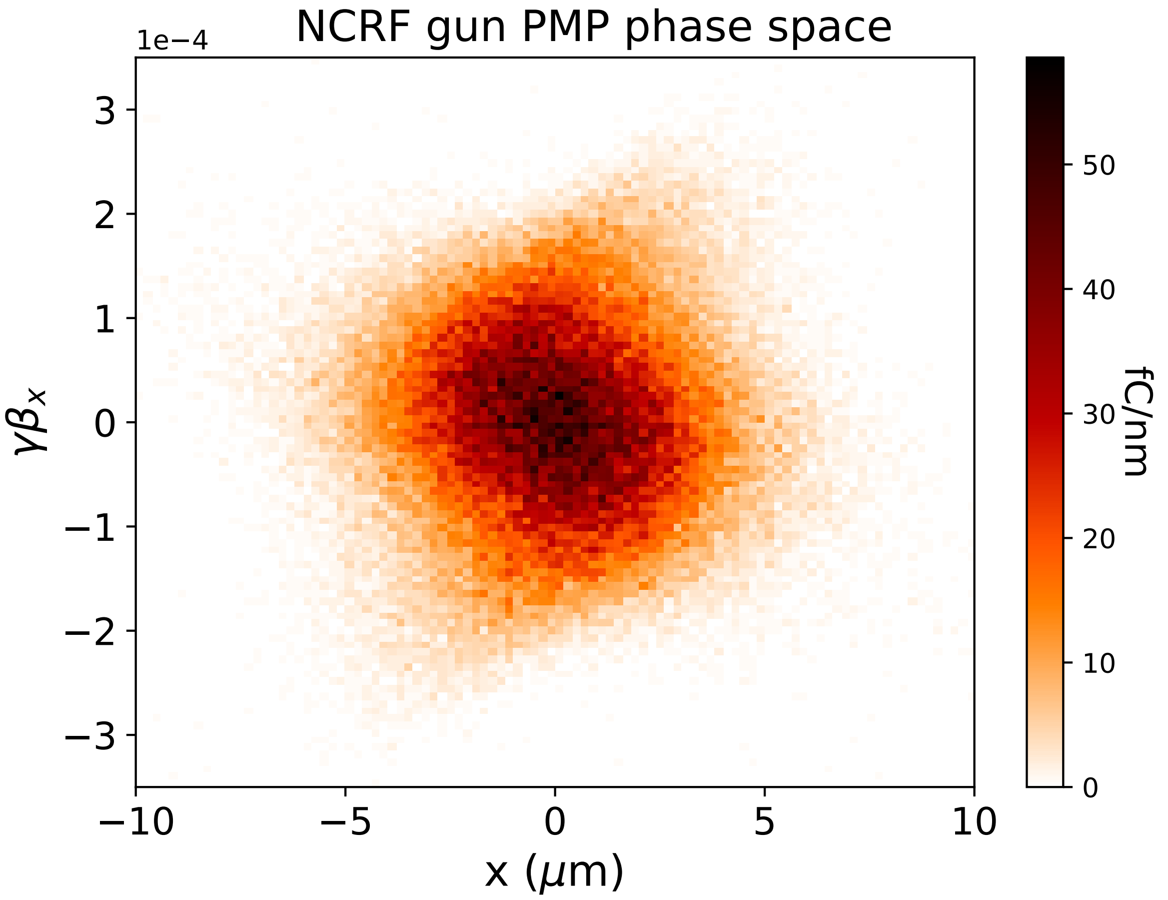




Phase Space Portraits

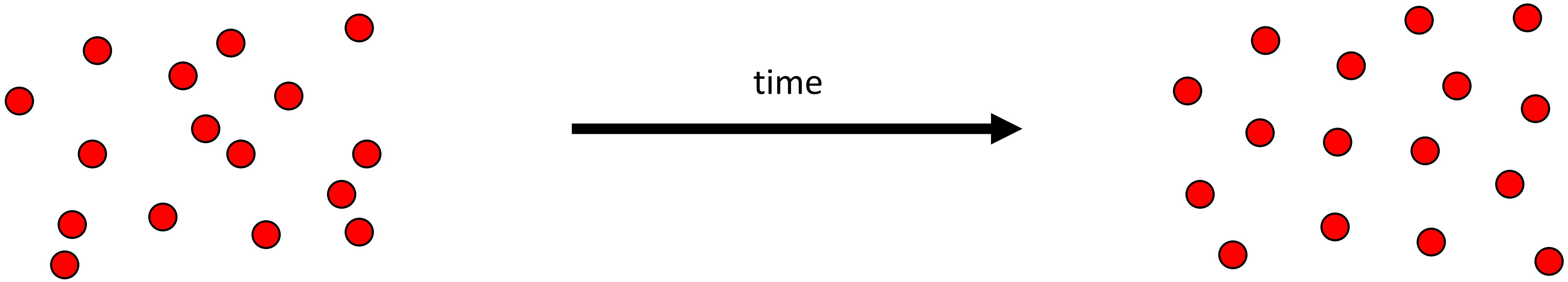
- Core density drops by a factor of 4
- Not just an effect in the tails
- What caused this?





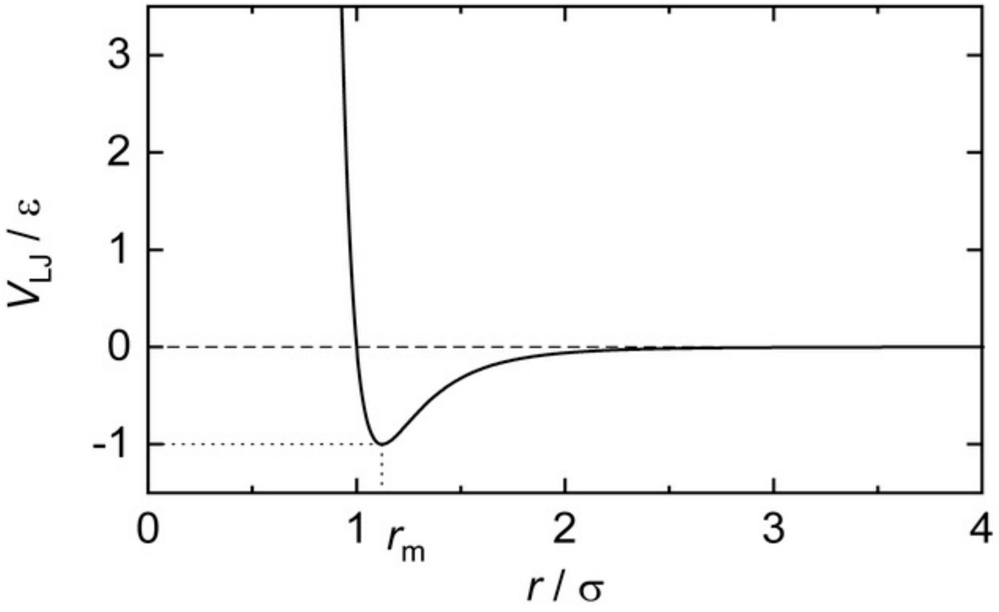
Disorder Induced Heating (The Coulomb Hole)

- The probability of finding an electron in a small region near another electron is near 0 due to Coulomb repulsion
- Charges with positions randomly chosen from a uniform distribution have a higher potential energy than if the charges were ordered
- If the kinetic energy of the particles is small enough, the charges will interact such that the charges become more evenly spaced and thus will warm up

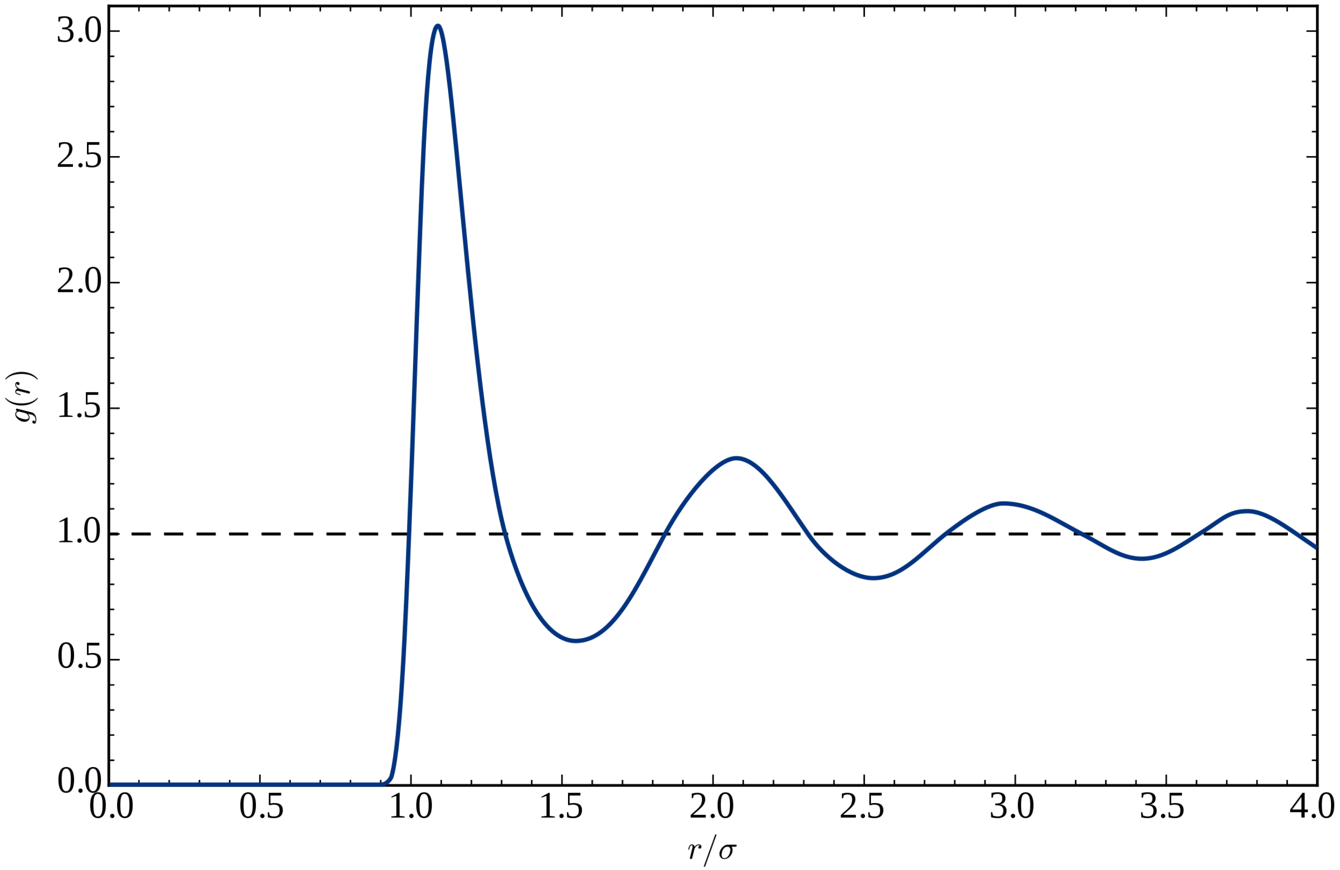


Radial Distribution Function g(r)

- How the density of particles varies as a function of distance form a reference particle
- ρ(r) = ρ g(r)



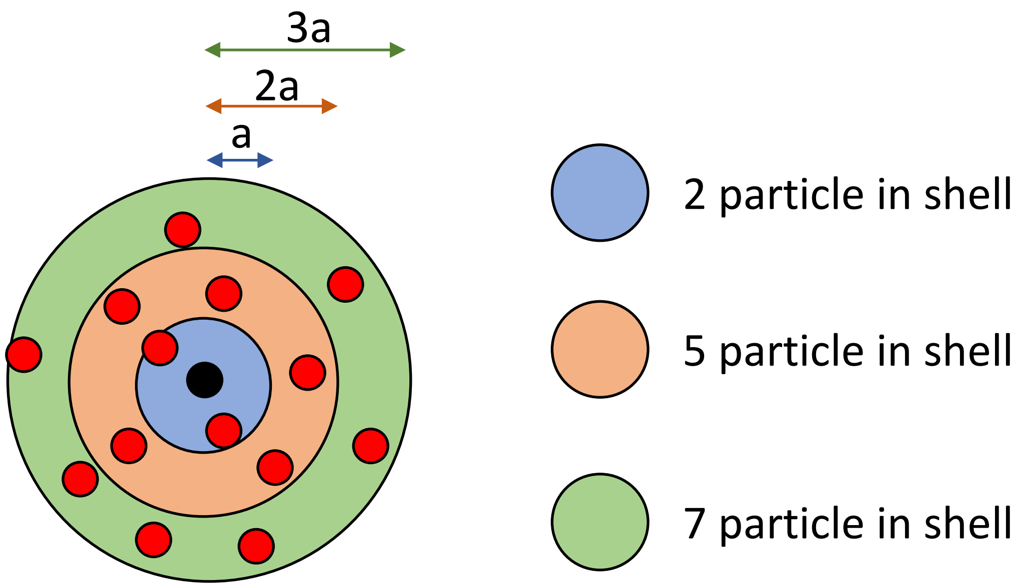
Lennard-Jones potential

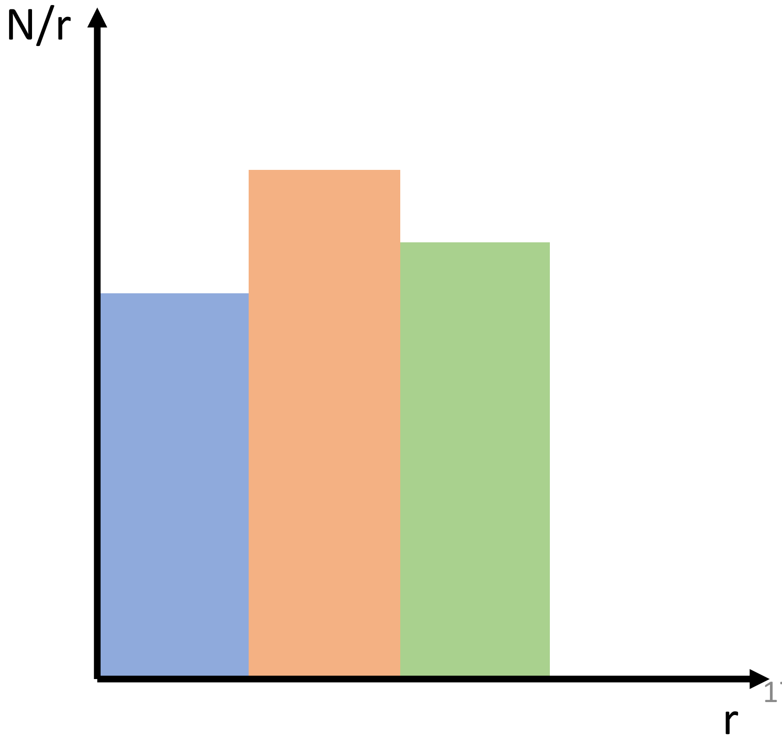


Radial distribution function of the Lennard-Jones potential

Calculating g(r)

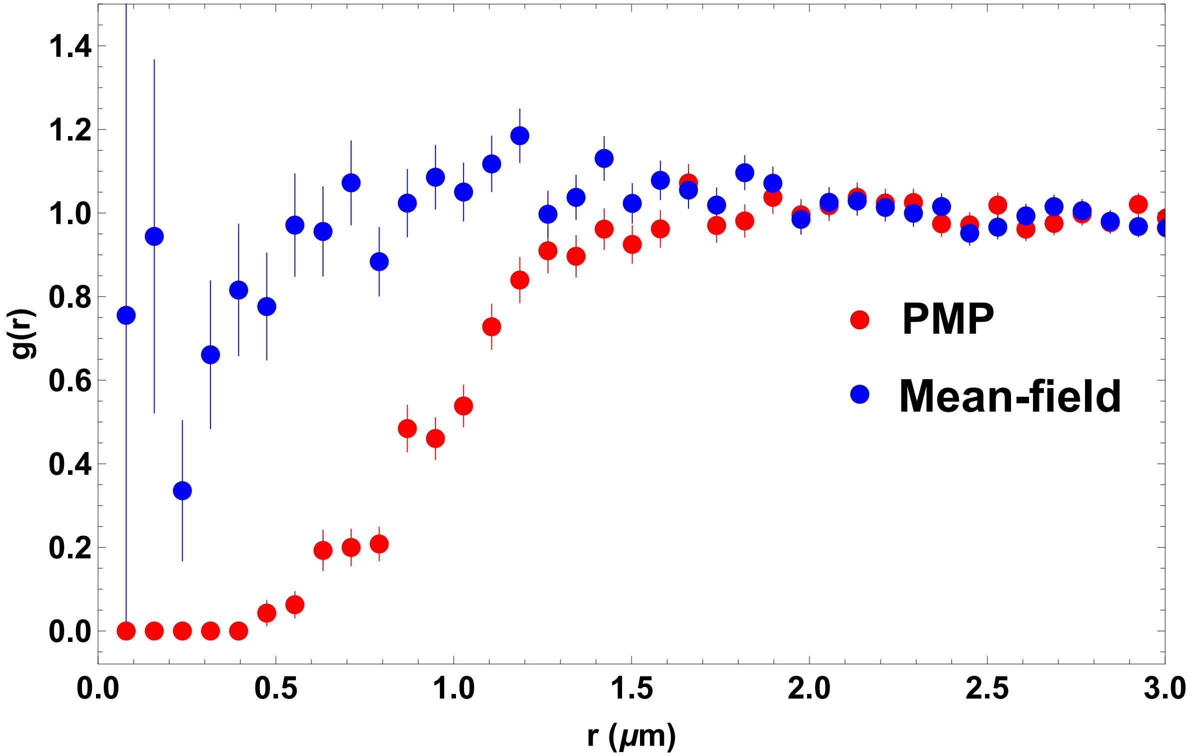
- Find distance between 1 particle and every other particle
- Bin the results and normalize the number of particles in the shell by the volume of the shell (for 3D $4\pi r^2\Delta r$)
- Repeat with all other particles and make an average
- This histogram plots ρ*g(r) vs r





The Coulomb Hole

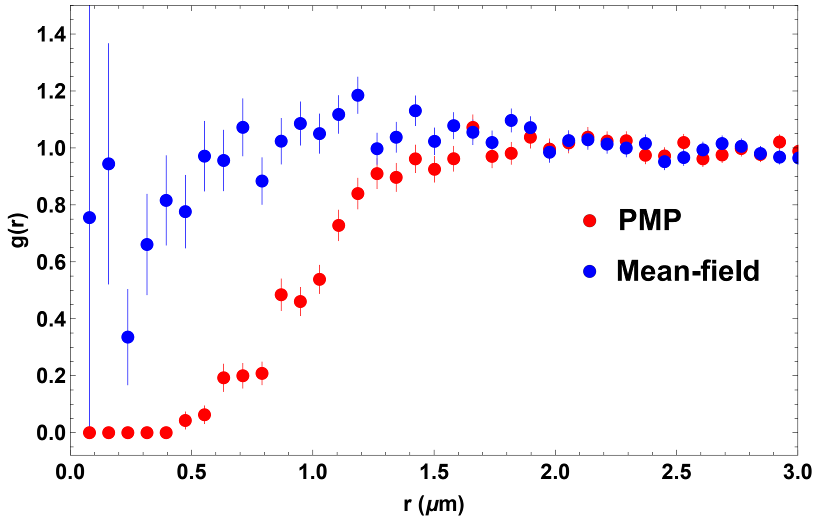
- g(r) 3 mm away from the cathode
- A perfectly uniform distribution would have a constant g(r)
- Both distributions started flat up to statistical noise
- PMP simulation g(r) becomes visibly non-flat for small r



Potential Energy From g(r)

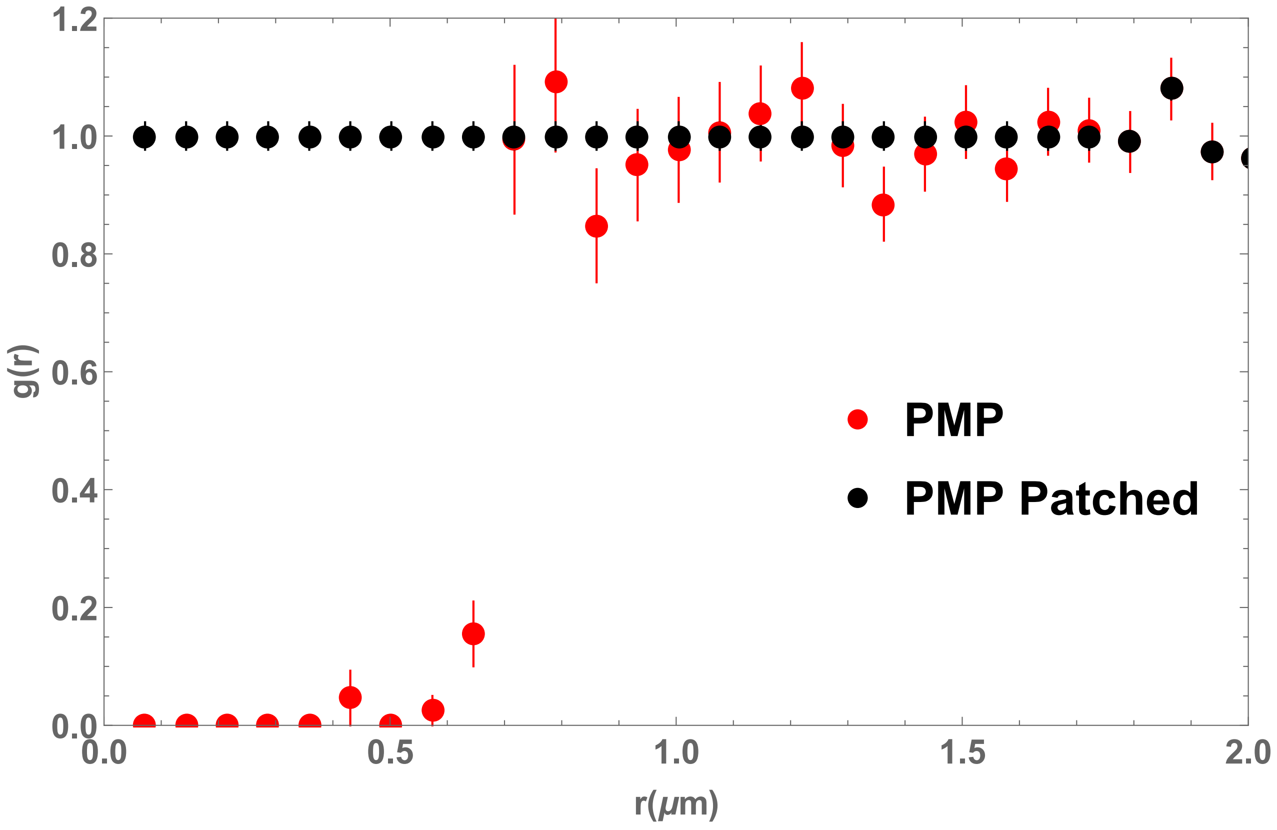
- To find the heating from this, we will find the change in potential energy
- Let u(r) be the interaction potential between particles in the system
- The potential energy of a single particle due to this interaction is:

$$E_{pot}(t) = \int_0^\infty dr\, 4\pi r^2 \rho g(r,t) u(r)$$



Energy of the Coulomb Hole

- “Patch up” the Coulomb hole
- Potential energy for these 2 different g(r) can be calculated
- Subtract to roughly calculate the energy from the Coulomb hole



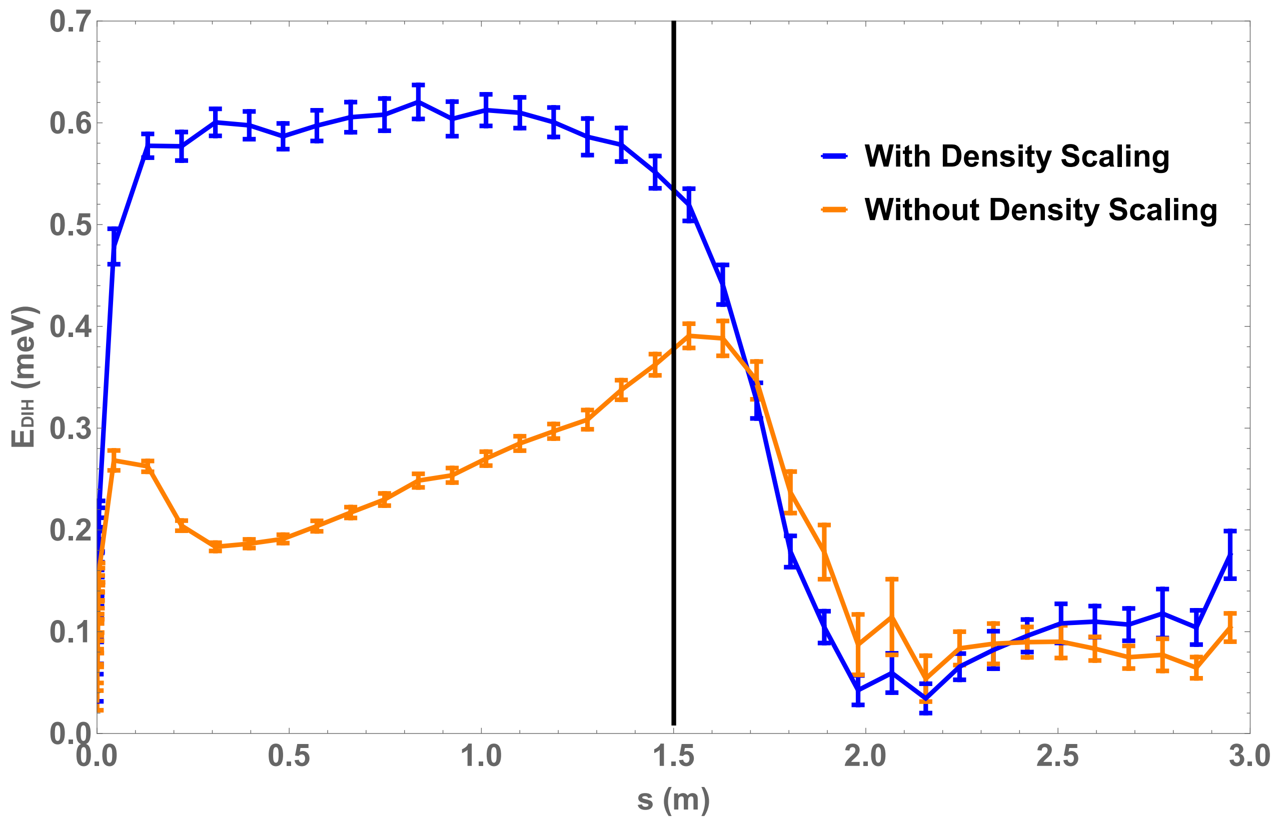
*This plot comes from a simulation at a lower particle density then the plots shown before

Energy of the Coulomb Hole

- Subtracting these energies gives us the energy of disorder induced heating, E_{DIH}

- When the beam travels further down the beamline, you can extract out E_{DIH} as long as the shape of g(r) doesn't change

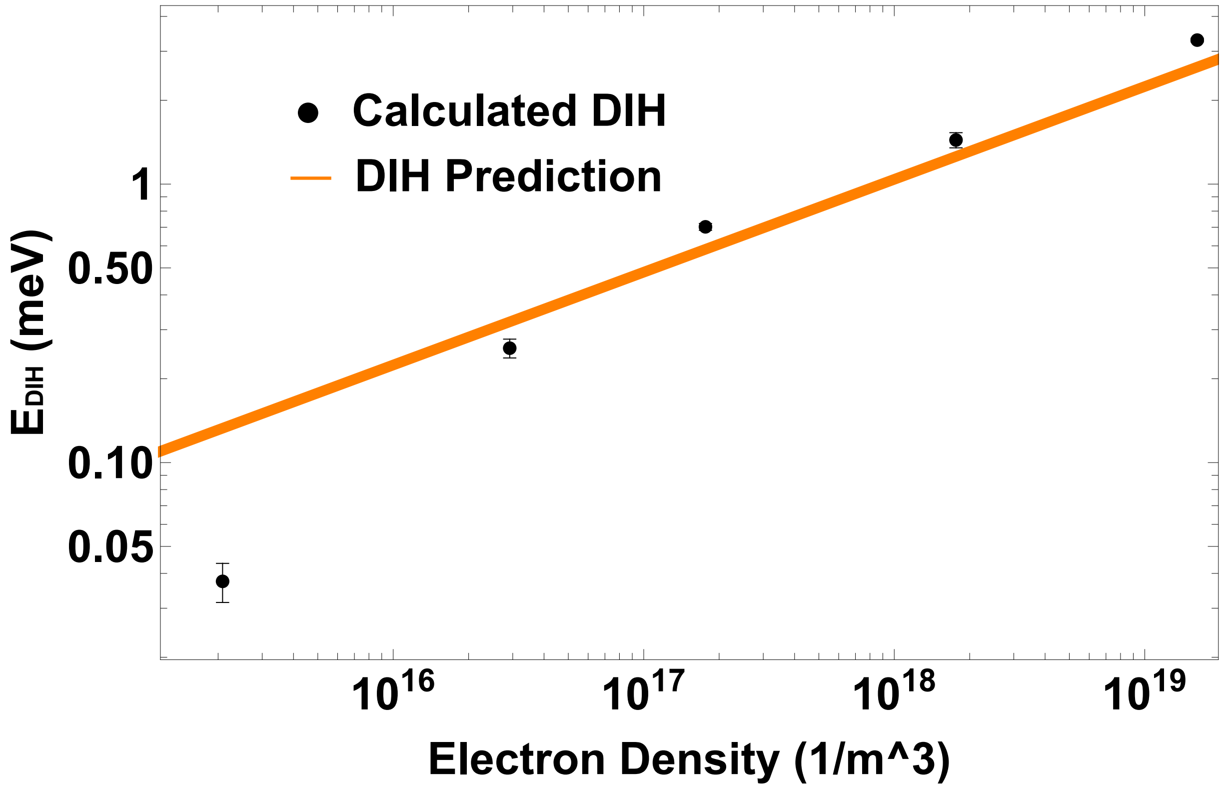
- One common way to lose the shape is to go through a focus



*This plot comes from a simulation at a lower particle density then the plots shown before

Disorder Induced Heating

- Found heating for several densities
- Disorder induced heating scales with density to the 1/3 power
- For large densities, heating scales with density with power of .39±.03
- At low densities, you can "outrun" the heating effect



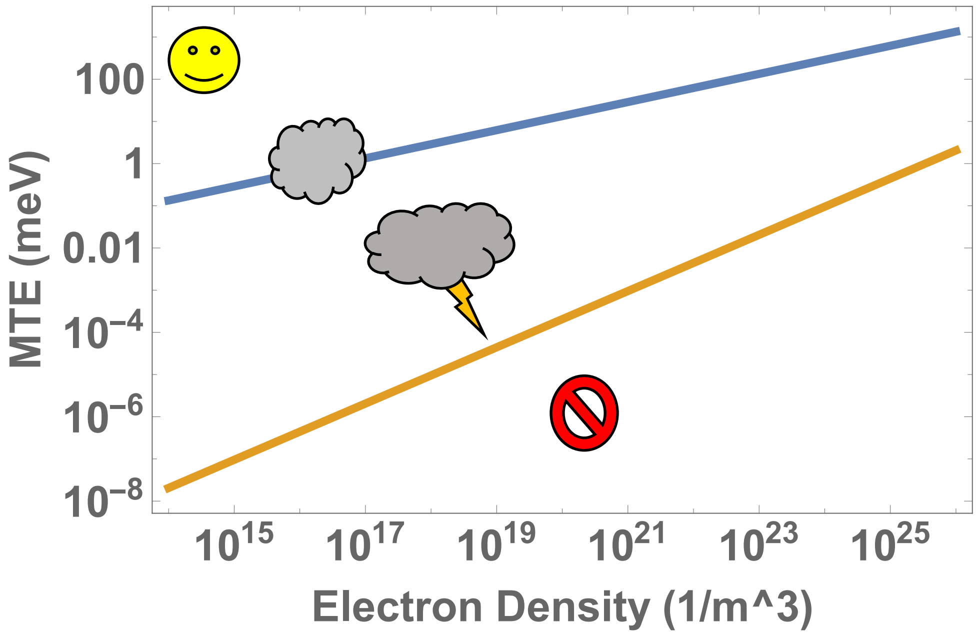
“What can I do with this?”

- Simulating these interactions is computational intensive and should be avoided when possible

- Calculate order of magnitude of effect

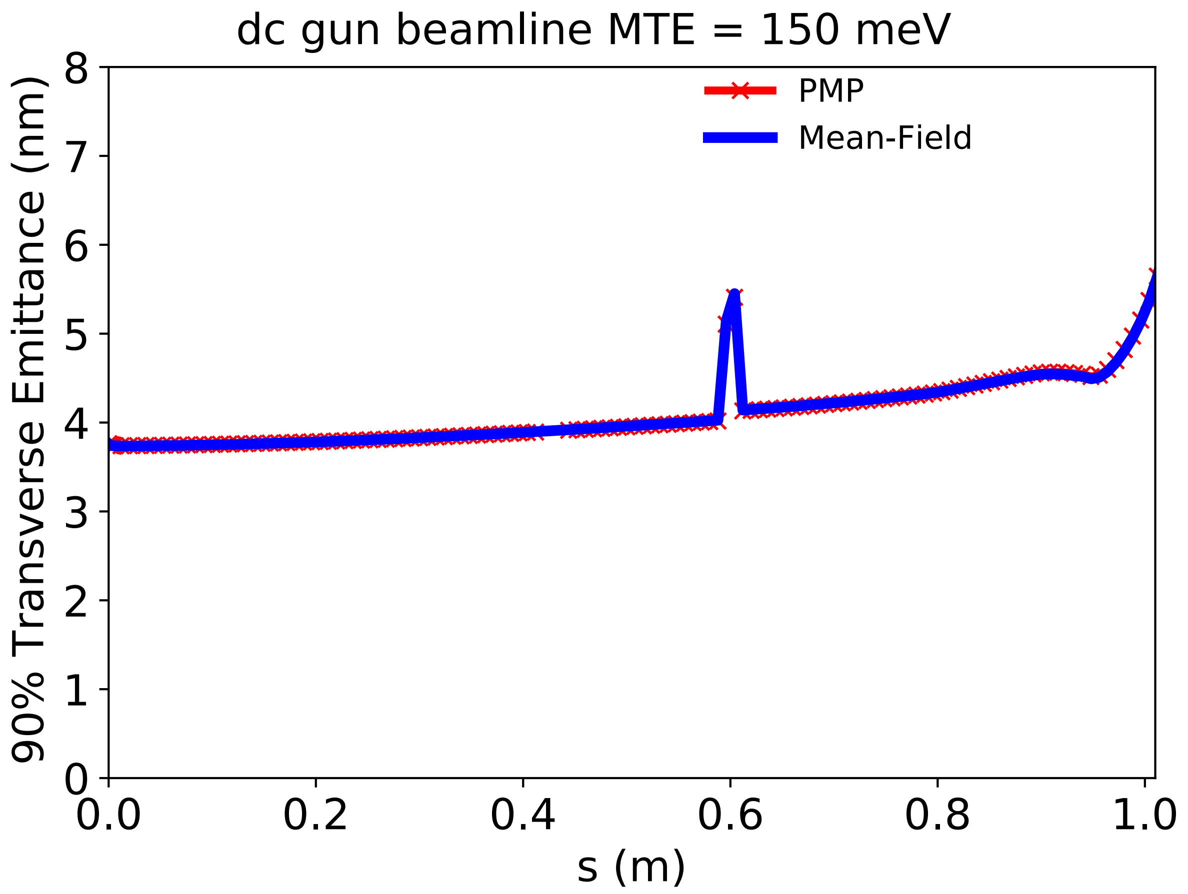
- If near the order of magnitude of MTE, consider instantaneous heating approximation

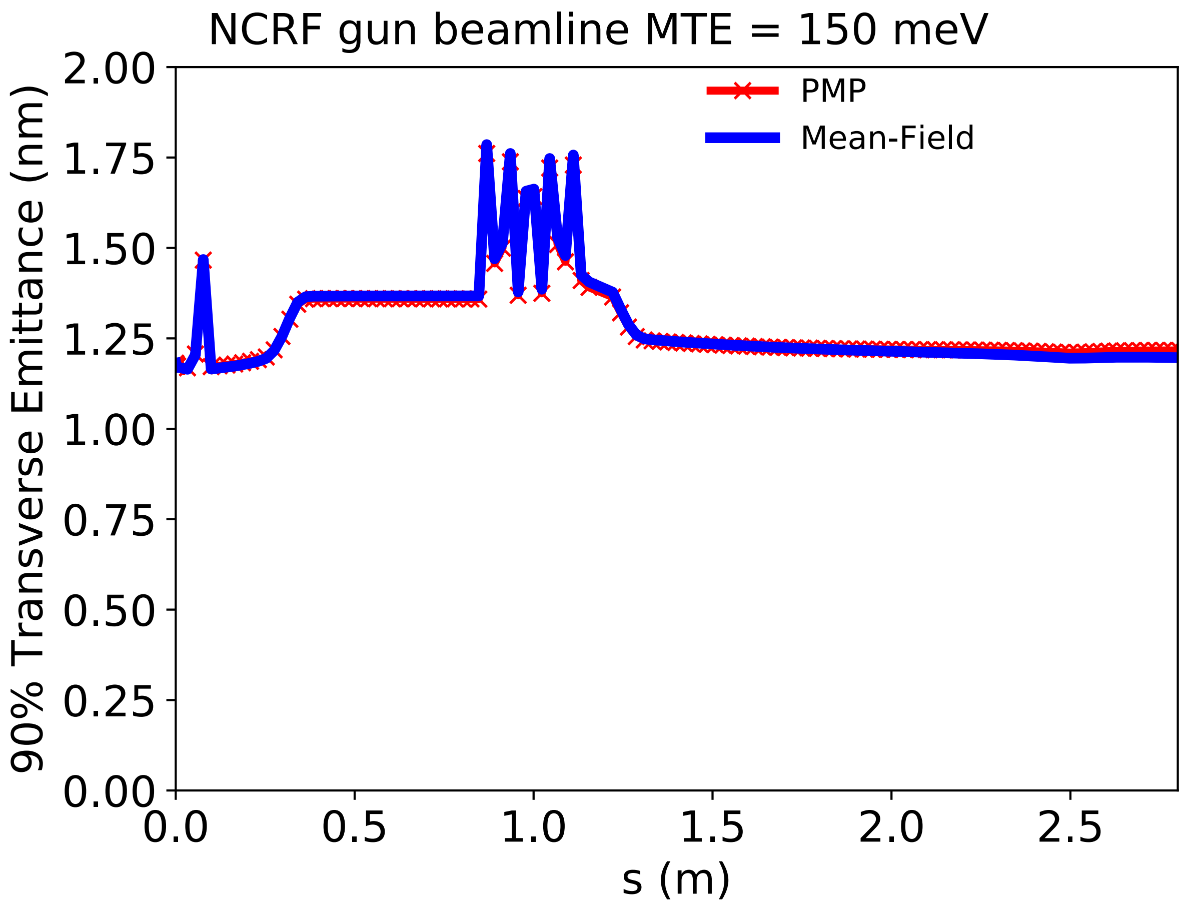
- Macroparticle extrapolation method(only for the brave)



Large MTE Comparison

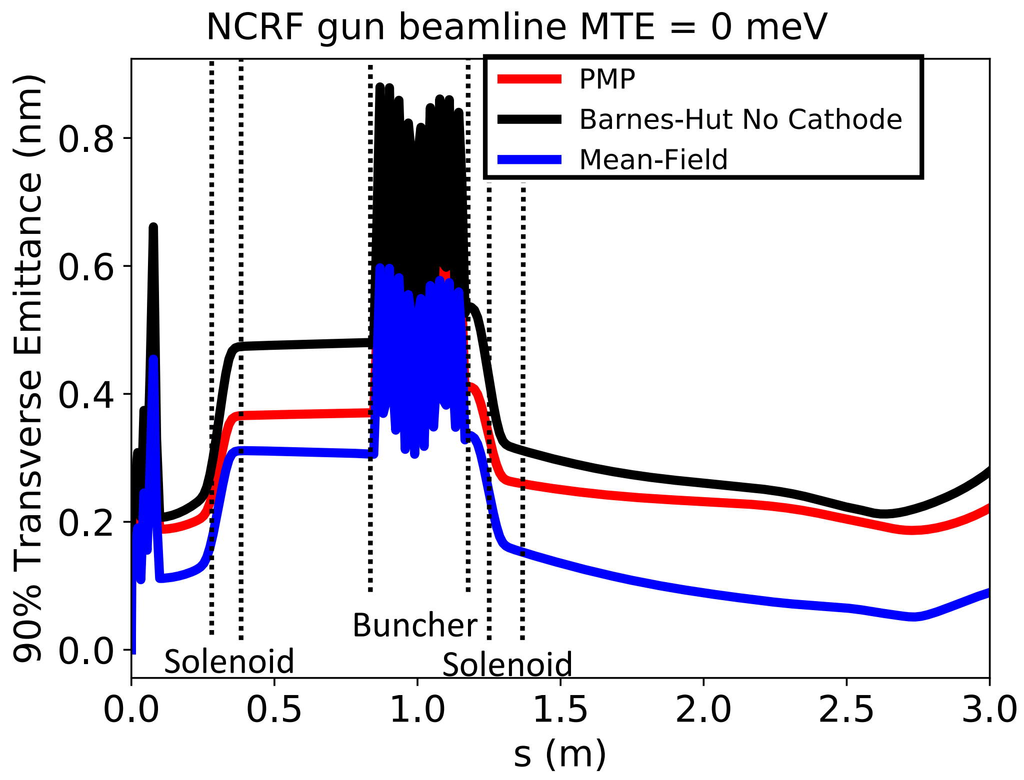
- With a 150 meV MTE the simulations are identical as expected
- Noticeable changes occur only below ~30 meV for these densities 10^{17}-10^{18}





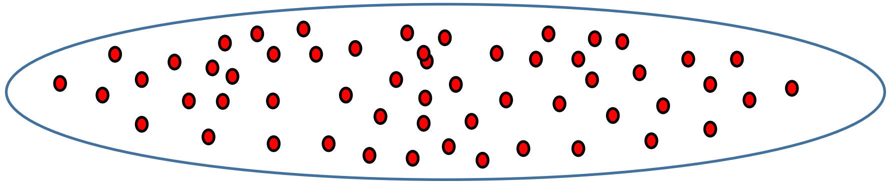
Instantaneous Heating Approximation

- Ignore finite size effects
- The heating is isotropic
- If the heating is "quick", 2/3 of E_{DIH} can be added as an effective MTE
- Approximations aren't great, but the results are good
- ~80% of the RMS emittance growth can be explained in this way

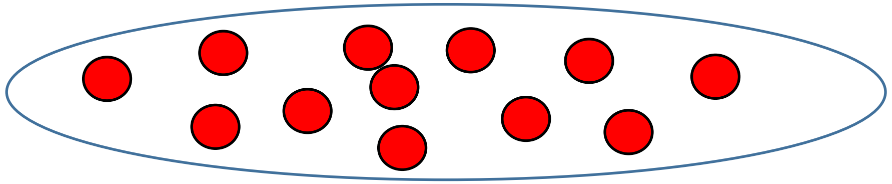


Simulating Systems with a lot more Particles

- What if you wanted to do the full P2P simulation anyway, but you have far too many particles to track them all
- People often use macroparticles to speed up simulations
- Point-to-point effects are number density dependent
- If you use macroparticles, you will **overestimate** DIH
- But it still can be useful



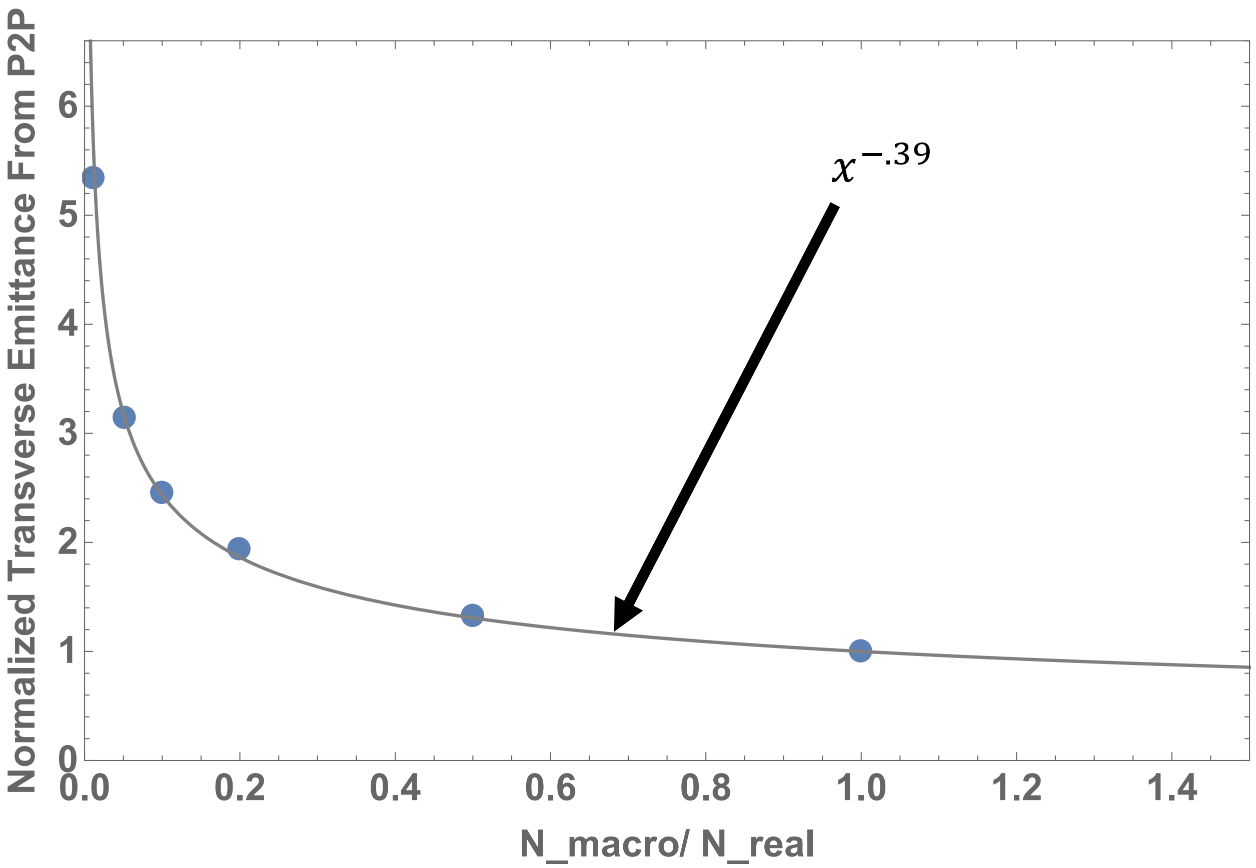
Full Simulation



Simulation With Macroparticles

Point-to-Point Macroparticle Extrapolation

- The effect of macroparticles is the inverse of increasing the actual charge density
- Run a few simulations with different macroparticle numbers
- Extract out the DIH density dependence and determine impact on emittance for full simulation



Summary

- Interactions between large numbers of particles cannot be computed exactly
- First results on simulating cold photoelectron beamlines with a non-mean-field electron interaction
- Beam quality decreases significantly, up to and including the core
- Heating effect consistent with disorder induced heating
- Ways to include point-to-point effects without full simulation

Questions?

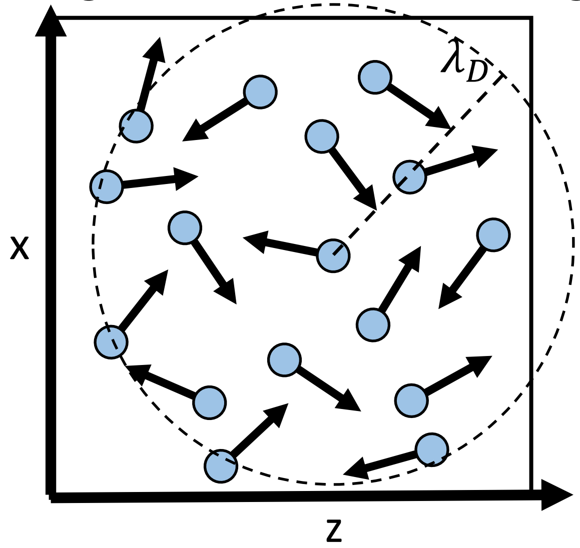
Low Mean Transverse Energy(MTE)

- MTE is the transverse momentum spread of a particle bunch
- When the momentum spread is large enough, the electron beam acts as a liquid, and the mobility of the charges screen the effect of local density fluctuations in the beam
- Screened electric potential: $\varphi(r) = \frac{q}{4\,\pi\,\epsilon_0 r} e^{-\frac{r}{\lambda_D}}$
- A low MTE leads to a small Debye screening length:

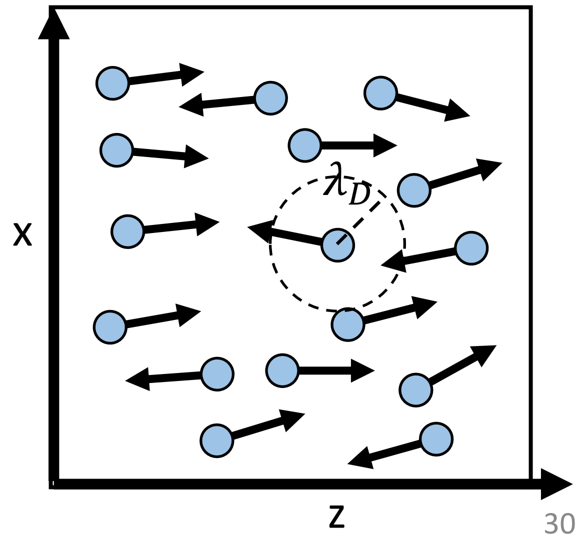
$$\lambda_D = \sqrt{\frac{\varepsilon_0 k_b T}{\rho e^2}}$$

- We are at a point where λ_D is less than the average inter particle spacing(IPS) (λ_D ~ .5 µm, IPS ~ 1µm)
- Thus we have reached the breaking point of this approximation

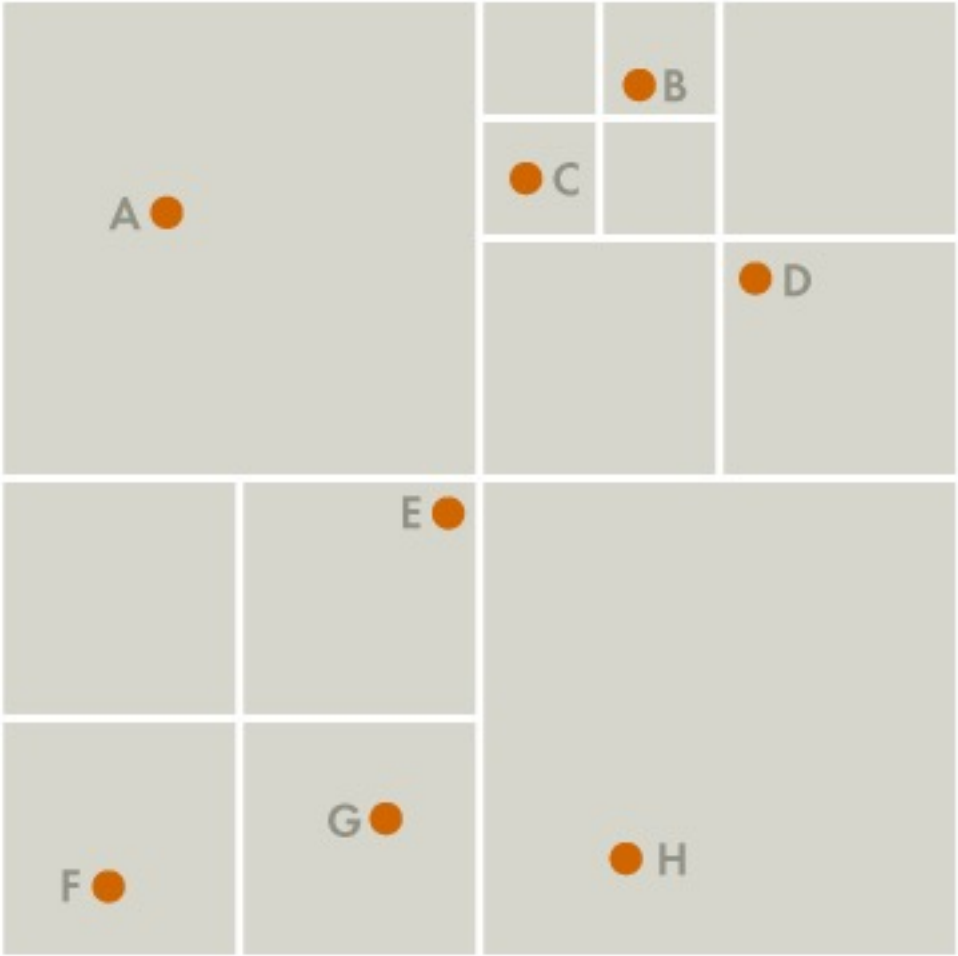
Large Mean Transverse Energy



Small Mean Transverse Energy



Barnes Hut Algorithm



Making a Barnes Hut Tree

1) Divide 3D Space into Octants
2) For Each Octant
   Store center of mass charge
   If(Octant contains < 2 particles) Stop
   Else Bring Octant to Step 1

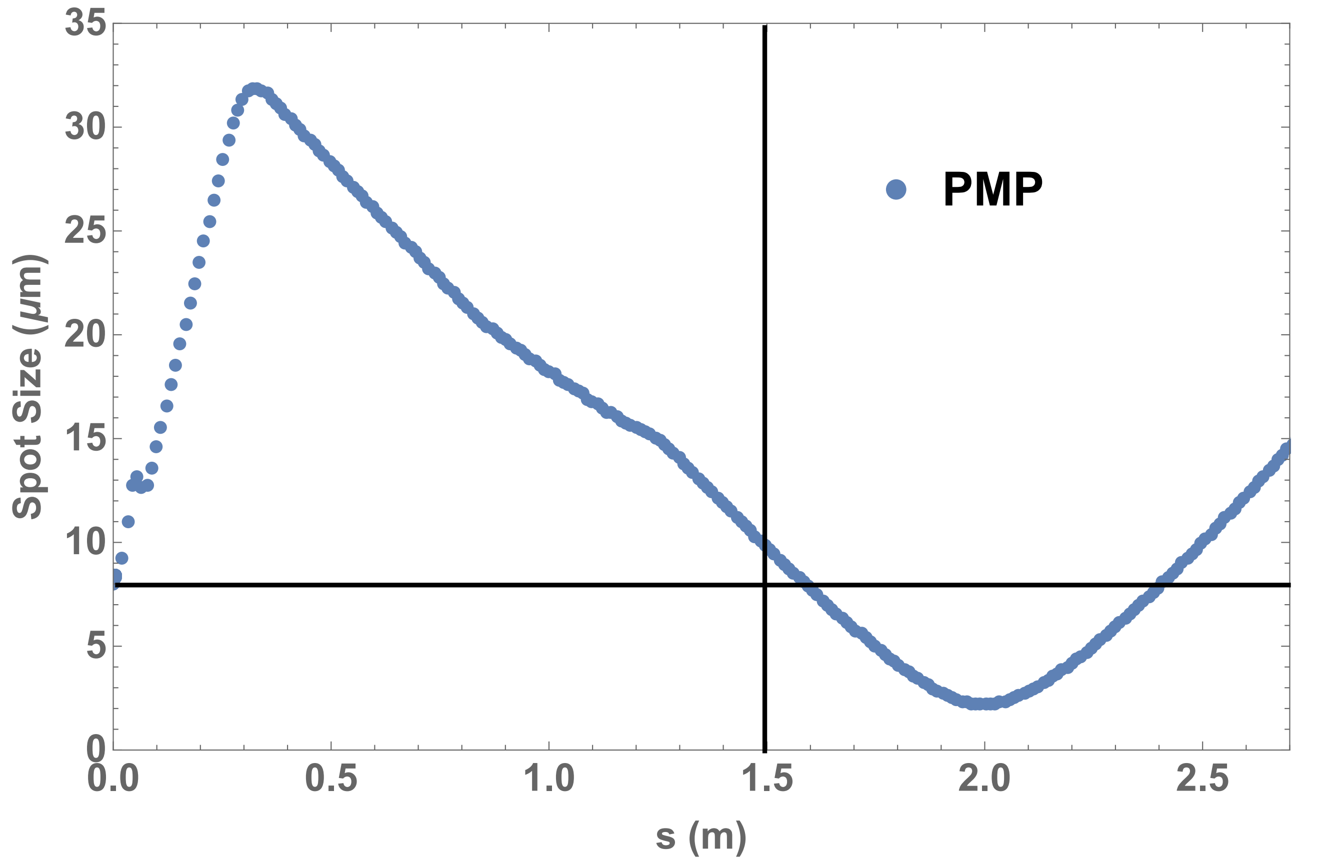
Calculating Forces

For Each Particle

1) Take ratio of distance from particle to center of mass charge to size of whole space
2) If larger than user specified value calculate force
   Else Repeat for 8 octants

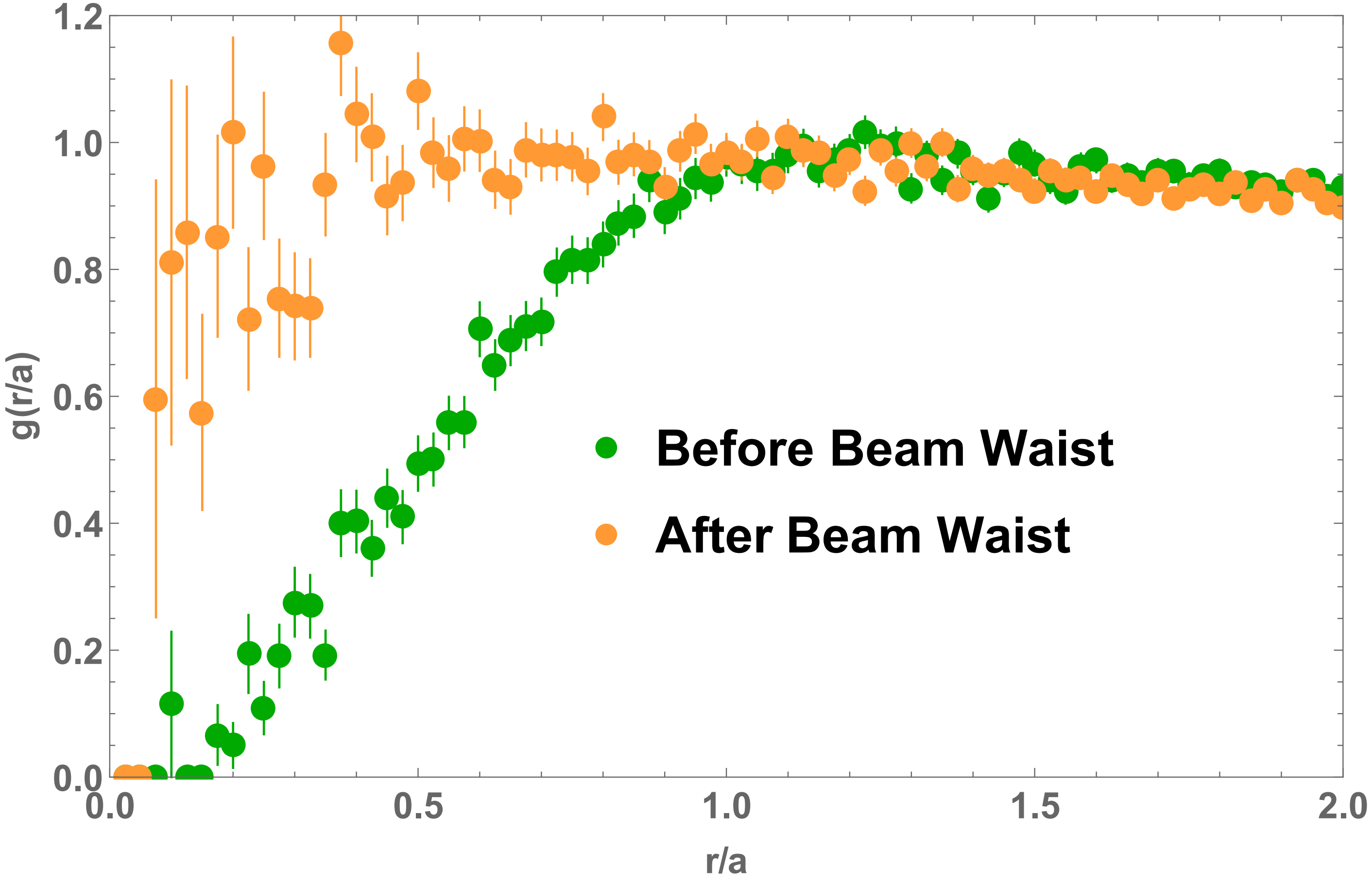
Going Through a Focus

- E_{DIH} decreases when the bunch becomes smaller than its original size
- The warm beam can fill in the original Coulomb hole
- g(r) can no longer be used this way to calculate E_{DIH}



*This plot comes from a simulation at a lower particle density then the plots shown before

g(r) through a Focus



DIH Scaling

- Plasma frequency: $\omega_p = \sqrt{\frac{n_e\, e^2}{m\, \varepsilon_0}}$
- Heating: $E_{DIH}[meV] = 1.04 * 10^{-6}(n_0[m^{-3}])^{1/3}$

Theoretical Scaling with Macroparticles

- DIH Kinetic energy per particle approx. potential
- $k_b T \;\propto\; \frac{e^2}{r}$
- For a fixed number of real particles N in a volume V and a varying number of macroparticles N_m:

  $e \propto N_m^{-1}\;, m \propto N_m^{-1}\;,\;\; r \propto N_m^{-\frac{1}{3}}$
- $k_b T \;\propto\; N_m^{-\frac{5}{3}}$
- $\epsilon \propto \sqrt{\frac{k_b T}{mc^2}}$
- $\epsilon \propto N_m^{-1/3}$