SAND2025-01203C

Sandia National Laboratories

Exceptional service in the national interest

3D PIC-DSMC Simulation of Vacuum Arc Initiation: A Cautionary Tale of Strongly Coupled Plasmas

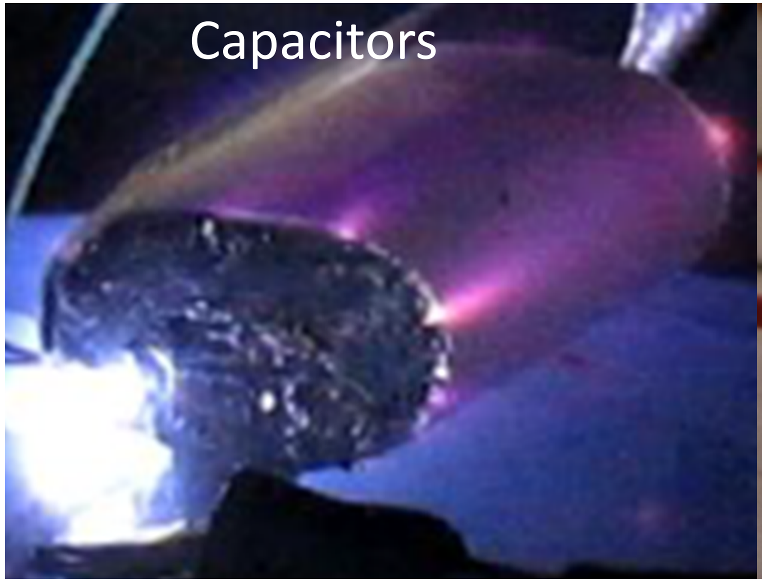
Christopher Moore, Marco Acciarri, Dejan Nikic, Scott Baalrud, Andy Fierro and Matthew Hopkins
Sandia National Laboratories, Albuquerque, NM USA

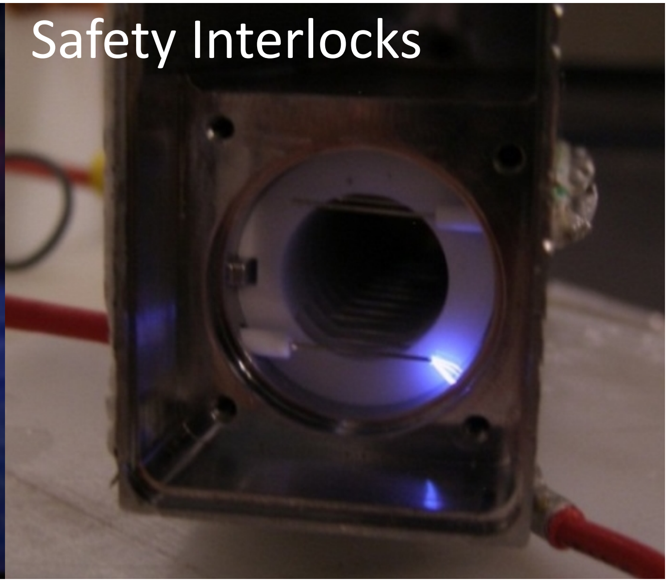
SAND2024-XXXX C

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Why do we care about vacuum arcs?

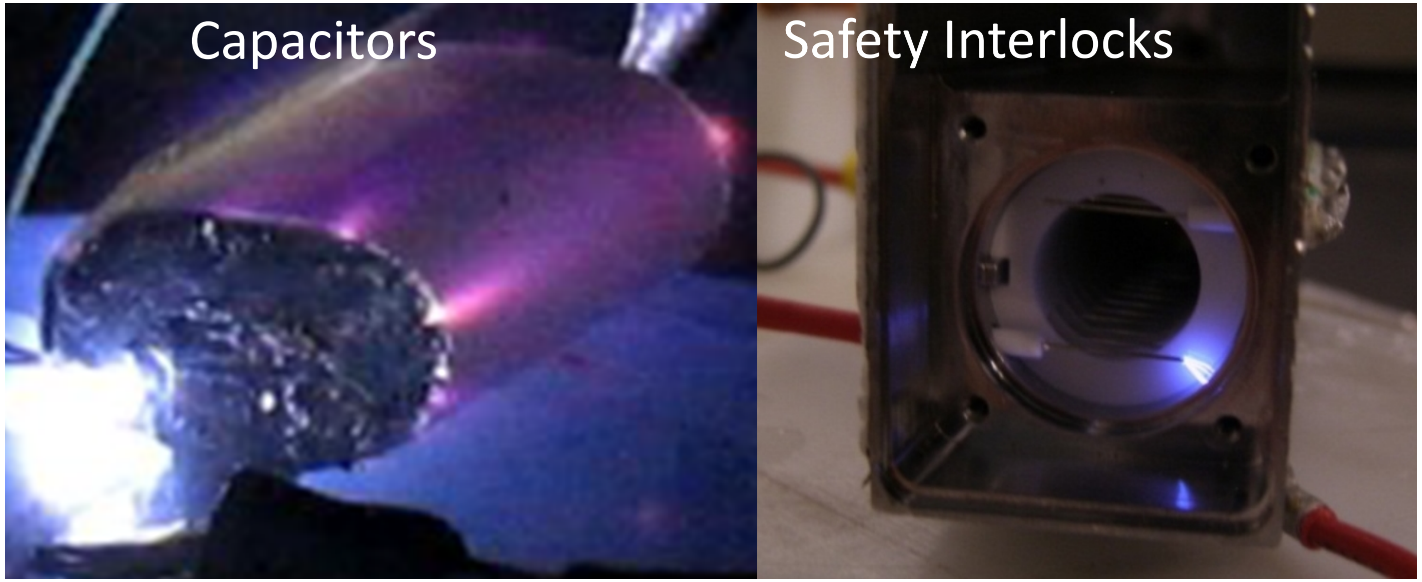
- Vacuum discharge is critical to many modern devices as a failure mechanism or mode of operation (e.g. trigger switches):





Why do we care about vacuum arcs?

- Vacuum discharge is critical to many modern devices as a failure mechanism or mode of operation (e.g. trigger switches):



- But we don't understand the dynamics of initiation:

How do neutrals expand away from the cathode at velocities ≫ thermal*?

* Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

Why care about modeling Strongly Coupled Plasmas

Cathode spot plasmas during vacuum arc initiation are a Strongly Coupled Plasma (SCP):

> When the cathode material takes the path of explosive transformation from solid to plasma, ... , there is a certain, short-lived, high-density state that is best described as *non-ideal* plasma.
>
> -- André Anders, Cathodic Arcs (pg. 159)

Why does this matter for PIC modeling?

- What is a Strongly Coupled, or non-ideal, plasma?
  - Very few particles in Debye sphere
  - N-body collisions dominate collective far-field interactions
  - A plasma is strongly coupled if the coupling parameter:

$$\Gamma = \frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} > 1$$

Why does this matter for PIC modeling?

- What is a Strongly Coupled, or non-ideal, plasma?
  - Very few particles in Debye sphere
  - N-body collisions dominate collective far-field interactions
  - A plasma is strongly coupled if the coupling parameter:

$$\Gamma = \frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} > 1$$

- Traditional PIC leverages the ***opposite*** characteristics:
  - Many particles in Debye sphere → Represent them statistically (fewer particles)
  - Collective far-field interactions → Handle by fields on mesh (neglect N-body)

Why does this matter for PIC modeling?

- What is a Strongly Coupled, or non-ideal, plasma?
  - Very few particles in Debye sphere
  - N-body collisions dominate collective far-field interactions
  - A plasma is strongly coupled if the coupling parameter:

$$\Gamma = \frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} > 1$$

- Traditional PIC leverages the ***opposite*** characteristics:
  - Many particles in Debye sphere → Represent them statistically (fewer particles)
  - Collective far-field interactions → Handle by fields on mesh (neglect N-body)

This talk will explore the limitations of PIC in the strongly coupled regime as applied to vacuum arc initiation

Are vacuum arc conditions strongly coupled?

- Let’s assume our cathode spot plasma has the following conditions:

Are vacuum arc conditions strongly coupled?

- Let's assume our cathode spot plasma has the following conditions:

- Copper thermally vaporizing off the surface:
  - T_{Cu} = 2000K
  - $n_{Cu} = 10^{27}$ #/m^3 (solid copper density ~ 10^{29} #/m^3)

Are vacuum arc conditions strongly coupled?

- Let's assume our cathode spot plasma has the following conditions:

- Copper thermally vaporizing off the surface:
  - T_{Cu} = 2000K
  - $n_{Cu} = 10^{27}$ #/m^3 (solid copper density ~ 10^{29} #/m^3)

- It is reasonable to assume based on prior observations (and theory):
  - $x_{Cu+,\,Cu++} > 0.01$
  - Mean charge state, <*Z*> = 2*

* Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

Are vacuum arc conditions strongly coupled?

- Let's assume our cathode spot plasma has the following conditions:

- Copper thermally vaporizing off the surface:
  - T_{Cu} = 2000K
  - $n_{Cu} = 10^{27}$ #/m^3 (solid copper density ~ 10^{29} #/m^3)

- It is reasonable to assume based on prior observations (and theory):
  - $x_{Cu+,\,Cu++} > 0.01$
  - Mean charge state, <Z> = 2*

For these parameters, $\Gamma_i(x_i = 0.1) \cong 25$

* Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

How Strongly Coupled Plasmas affect dynamics

- Pressure ionization*:
  - Overlapping potential surfaces effects ionization cross sections

* Anders, et al., PSST **1**, 263-270 (1992)

How Strongly Coupled Plasmas affect dynamics

- Pressure ionization*
  - Overlapping potential surfaces effects ionization cross sections

- Disorder-Induced Heating (DIH)

Plasma Sources Sci. Technol. **33** (2024) 02LT02 (6pp) https://doi.org/10.1088/1361-6595/ad257e

Letter

Disorder-induced heating as a mechanism for fast neutral gas heating in atmospheric pressure plasmas

M D Acciarri[1,*], C Moore[2] and S D Baalrud[1]

[1] Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI 48109, United States of America
[2] Sandia National Laboratories, Albuquerque, NM 87185, United States of America

E-mail: acciarri@umich.edu

Received 27 November 2023, revised 18 January 2024
Accepted for publication 1 February 2024
Published 8 February 2024

DIH results in significant heating on ω_p^{-1} timescales

What about for cathode spot plasma?

* Anders, et al., PSST **1**, 263-270 (1992)

How Strongly Coupled Plasmas affect dynamics

- Pressure ionization*
  - Overlapping potential surfaces effects ionization cross sections

- Disorder-Induced Heating (DIH)

- PIC-DSMC's ability to accurately simulate the vacuum arc!

Plasma Sources Sci. Technol. **33** (2024) 035009 (14pp) https://doi.org/10.1088/1361-6595/ad35e6

When should PIC simulations be applied to atmospheric pressure plasmas? Impact of correlation heating

M D Acciarri[1,*], C Moore[2], L P Beving[2] and S D Baalrud[1]

[1] Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI 48109, United States of America
[2] Sandia National Laboratories Albuquerque, NM 87185, United States of America

E-mail: acciarri@umich.edu

Received 5 October 2023, revised 1 March 2024
Accepted for publication 20 March 2024
Published 2 April 2024

PIC is not ideal for resolving DIH and avoiding Artificial Correlation Heating (ACH) in atmospheric pressure plasmas.

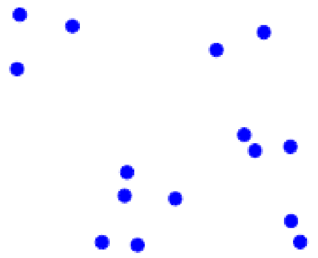
What about for cathode spot plasma?

* Anders, et al., PSST **1**, 263-270 (1992)

SCP Effects: Disorder Induced Heating

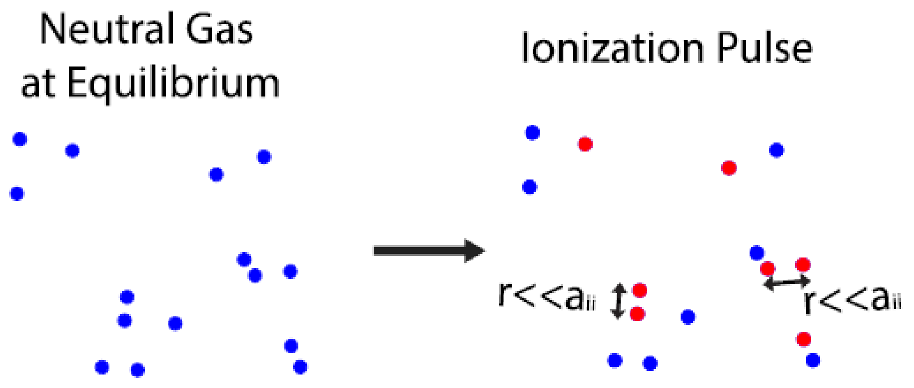
- Start with an uncorrelated state: The neutral atoms are randomly distributed and are, on average, $a_{NN} = \left(\frac{4\pi n_N}{3}\right)^{-1/3}$ apart

Neutral Gas
at Equilibrium



SCP Effects: Disorder Induced Heating

- Start with an uncorrelated state: The neutral atoms are randomly distributed and are, on average, $a_{NN} = \left(\frac{4\pi n_N}{3}\right)^{-1/3}$ apart



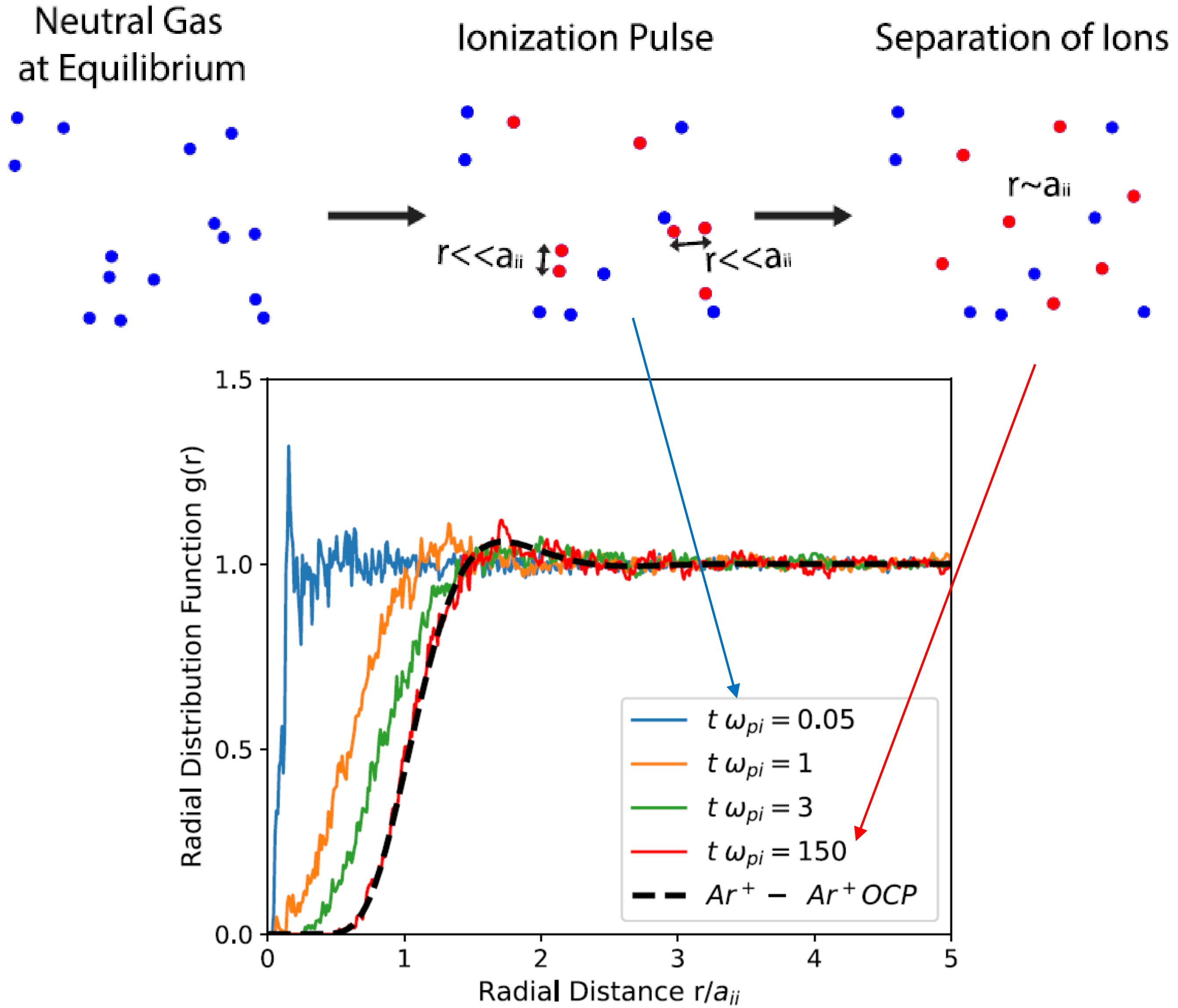
- Ionization occurs and now ions are too close together: Their initial positions are based on the neutral state

SCP Effects: Disorder Induced Heating

- Start with an uncorrelated state: The neutral atoms are randomly distributed and are, on average, $a_{NN} = \left(\frac{4\pi n_N}{3}\right)^{-1/3}$ apart

- Ionization occurs and now ions are too close together: Their initial positions are based on the neutral state

- The ions fly apart due to Coulomb repulsion on the ion plasma period timescale



*These figures & results from MD simulations in M.D. Acciarri *et al*, PSST **31**, 125005 (2022)

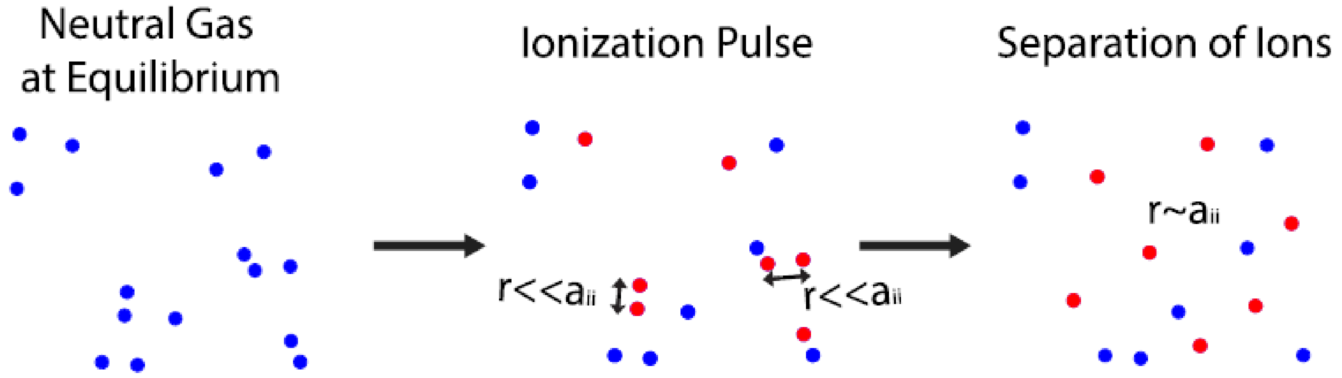
SCP Effects: Disorder Induced Heating

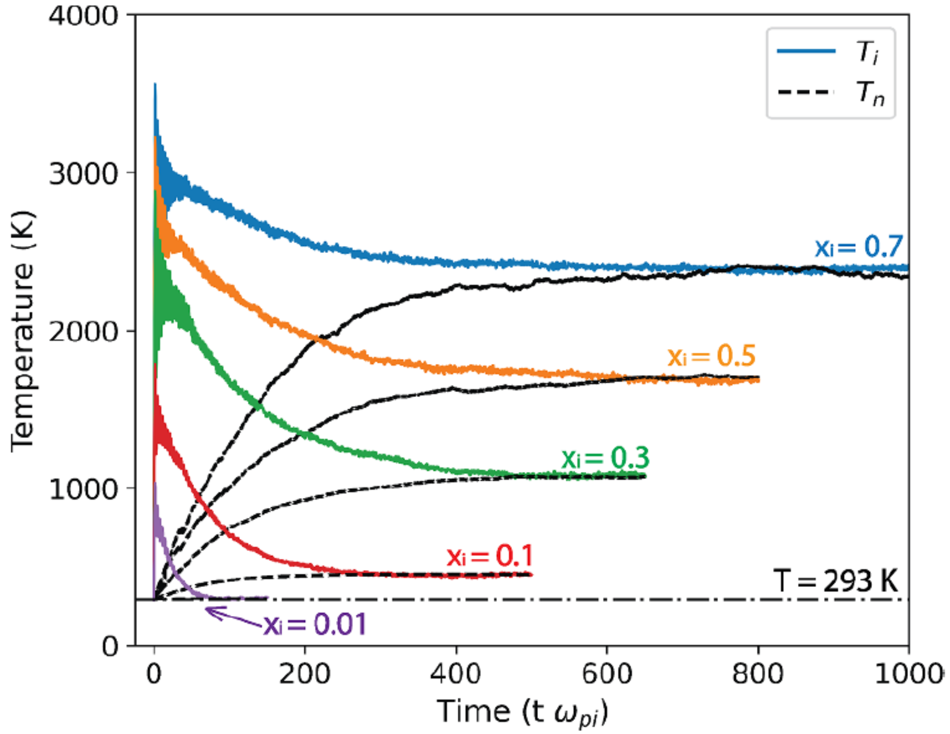
- Start with an uncorrelated state: The neutral atoms are randomly distributed and are, on average, $a_{NN} = \left(\frac{4\pi n_N}{3}\right)^{-1/3}$ apart

- Ionization occurs and now ions are too close together: Their initial positions are based on the neutral state

- The ions fly apart due to Coulomb repulsion on the ion plasma period timescale:

  → The ions and neutrals gain substantial thermal energy!





*These figures & results from MD simulations in M.D. Acciarri *et al*, PSST **31**, 125005 (2022)

SCP Effects: Disorder Induced Heating

- Will heating still be significant if the ionization happens gradually?

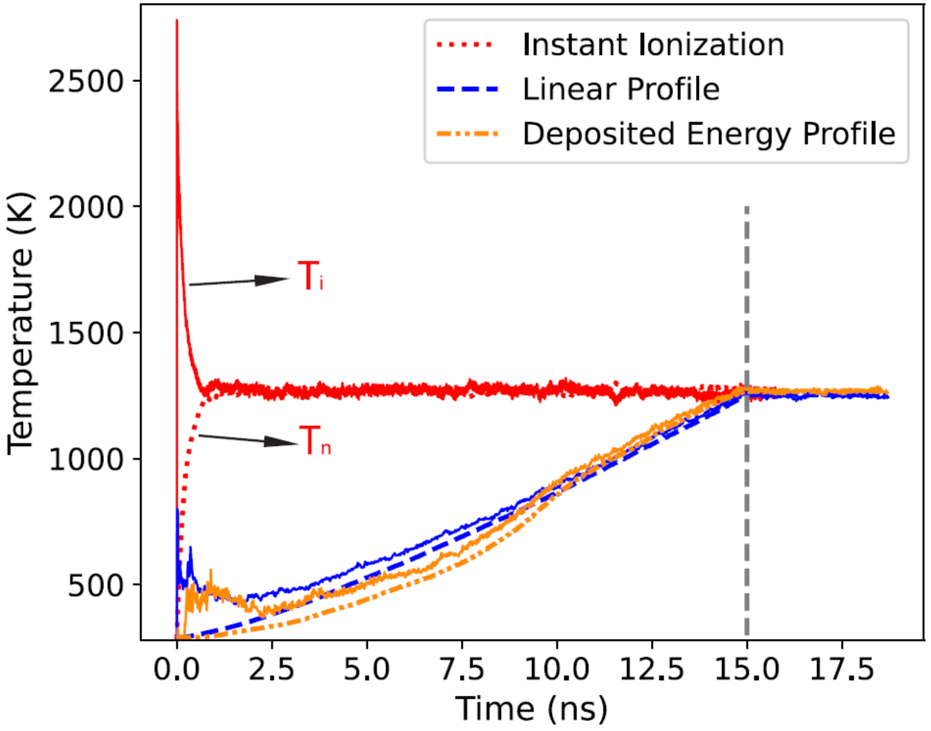
SCP Effects: Disorder Induced Heating

- Will heating still be significant if the ionization happens gradually?

- Yes! The total energy released by DIH depends only on the end ionization fraction and coupling parameter:

$$x_i = \frac{n_i}{n_N + n_i} \qquad \frac{T_i^{max}}{T_0} = \frac{\Gamma_i}{1.91}$$

$$\frac{T_{eq}}{T_0} = x_i \frac{T_i^{max}}{T_0} + (1 - x_i)$$



*These figures & results from M.D. Acciarri *et al*, PSST **33**, O2LT02 (2024)

SCP Effects: Disorder Induced Heating

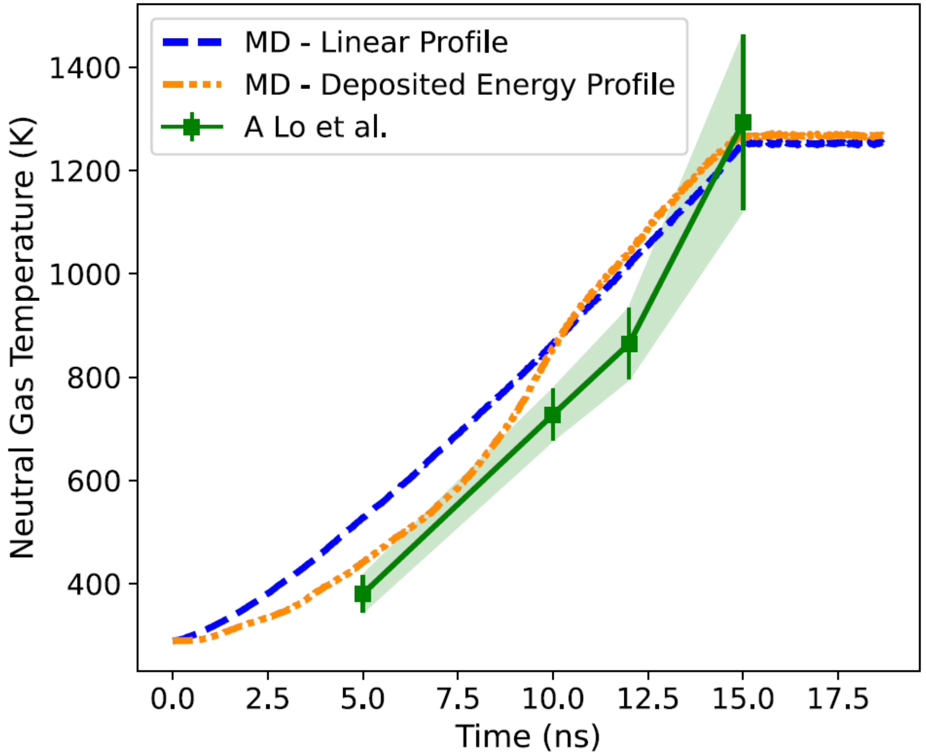
- Will heating still be significant if the ionization happens gradually?

- Yes! The total energy released by DIH depends only on the end ionization fraction and coupling parameter:

$$x_i = \frac{n_i}{n_N + n_i} \qquad \frac{T_i^{max}}{T_0} = \frac{\Gamma_i}{1.91}$$

$$\frac{T_{eq}}{T_0} = x_i \frac{T_i^{max}}{T_0} + (1 - x_i)$$

- Possibly the main ns-timescale heating mechanism for atmospheric pressure sparks



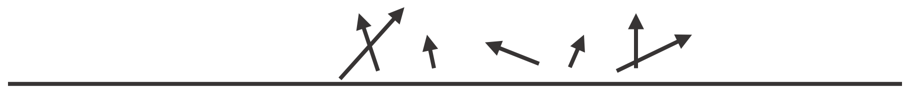
*These figures & results from M.D. Acciarri *et al*, PSST **33**, O2LT02 (2024)

SCP Effects: PIC-DSMC Challenges

- Typical cathode spot:

  Radius < 100nm

  $n_n \sim 10^{27}$ m^{-3} (vaporization of electrode)



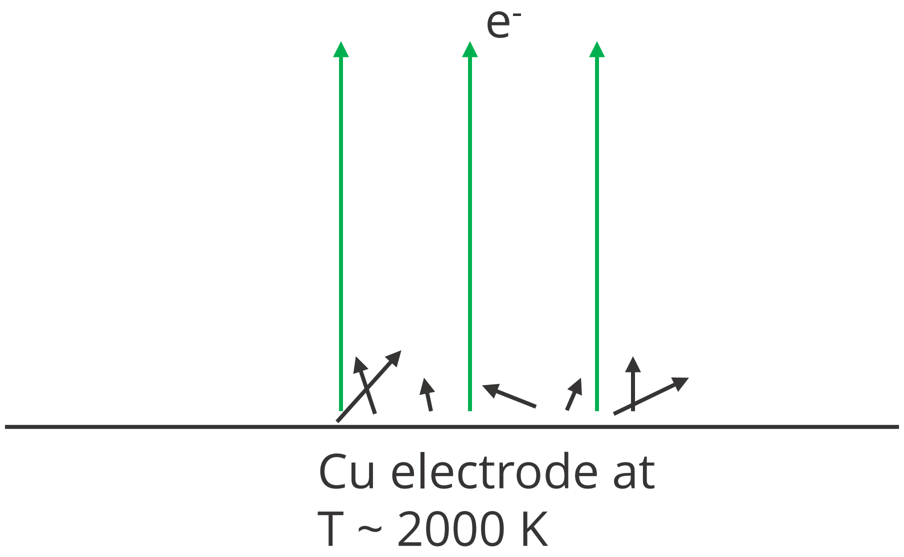
SCP Effects: PIC-DSMC Challenges

- Typical cathode spot:

  Radius < 100nm

  $n_n \sim 10^{27}\ m^{-3}$ (vaporization of electrode)

  $n_e \sim 10^{24}\ m^{-3}$ (field emission)



SCP Effects: PIC-DSMC Challenges

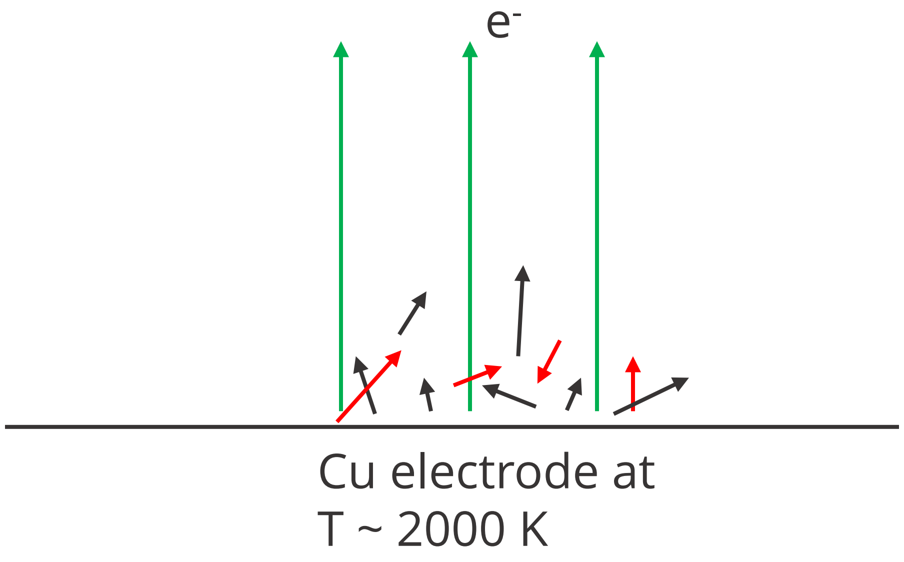
- Typical cathode spot:

  Radius < 100nm

  $n_n \sim 10^{27}$ m^{-3} (vaporization of electrode)

  $n_e \sim 10^{24}$ m^{-3} (field emission)

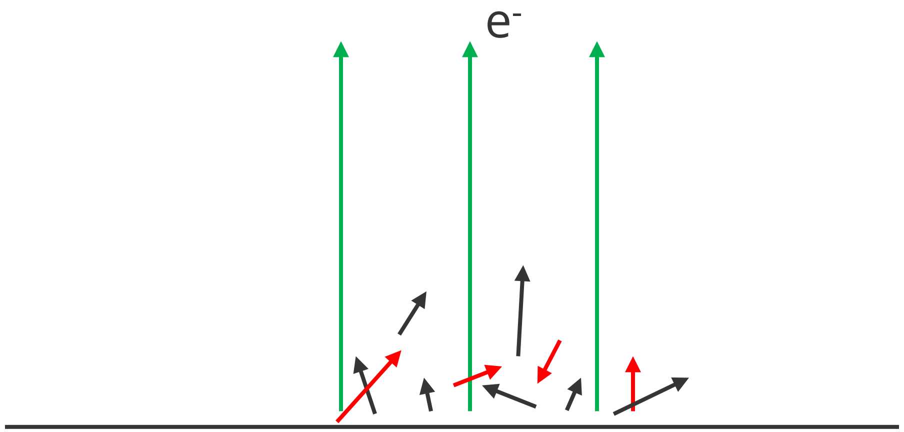
  $n_i \sim 5\times10^{25}$ m^{-3} (ionization, $\langle Z \rangle > 1$)



SCP Effects: PIC-DSMC Challenges

- Typical cathode spot:
  - Radius < 100nm
  - $n_n \sim 10^{27}$ m^{-3} (vaporization of electrode)
  - $n_e \sim 10^{24}$ m^{-3} (field emission)
  - $n_i \sim 5\times10^{25}$ m^{-3} (ionization, $\langle Z \rangle > 1$)

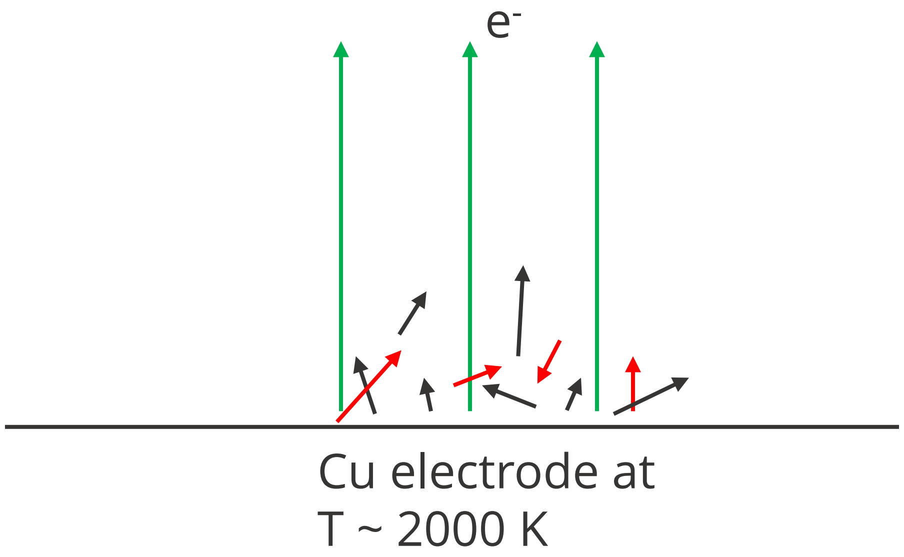
- Coupling parameter: $$\Gamma = \frac{(\langle Z \rangle e)^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} \gtrsim 5$$



Cu electrode at
T ~ 2000 K

SCP Effects: PIC-DSMC Challenges

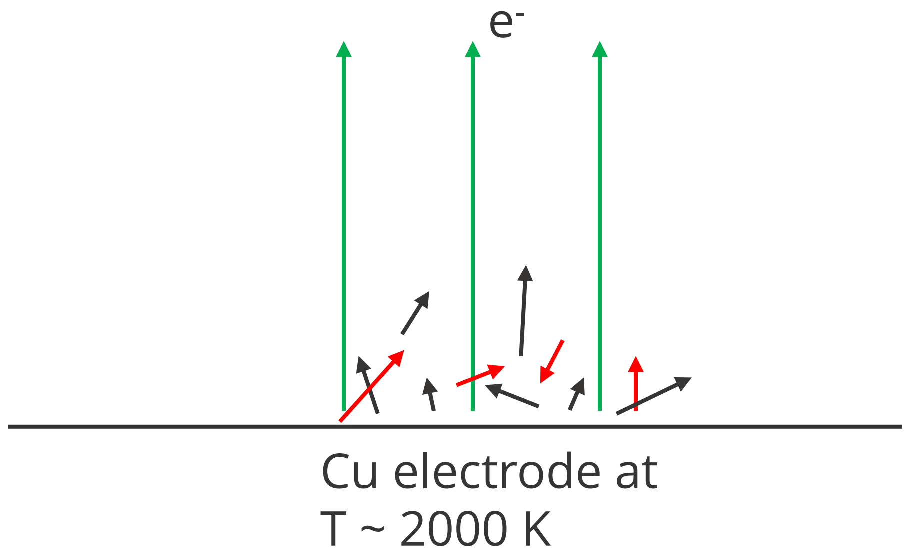
- Typical cathode spot:
  - Radius < 100nm
  - $n_n \sim 10^{27}\ m^{-3}$ (vaporization of electrode)
  - $n_e \sim 10^{24}\ m^{-3}$ (field emission)
  - $n_i \sim 5\times10^{25}\ m^{-3}$ (ionization, $\langle Z \rangle > 1$)
- Coupling parameter: $\Gamma = \frac{(\langle Z \rangle e)^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} \gtrsim 5$
- To resolve DIH: $\Delta x < a_{ii} \approx 1.7nm$



SCP Effects: PIC-DSMC Challenges

- Typical cathode spot:
  - Radius < 100nm
  - $n_n \sim 10^{27}$ m^{-3} (vaporization of electrode)
  - $n_e \sim 10^{24}$ m^{-3} (field emission)
  - $n_i \sim 5\times10^{25}$ m^{-3} (ionization, $\langle Z \rangle > 1$)
- Coupling parameter: $\Gamma = \frac{(\langle Z \rangle e)^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} \gtrsim 5$
- To resolve DIH: $\Delta x < a_{ii} \approx 1.7nm$
- To resolve PIC mesh-heating at initial ion temperature (2000 K):

$$\Delta x < \lambda_D \cong \sqrt{\frac{\varepsilon_0 k_B T_i}{(Ze)^2 n_i}} \approx 0.4nm$$

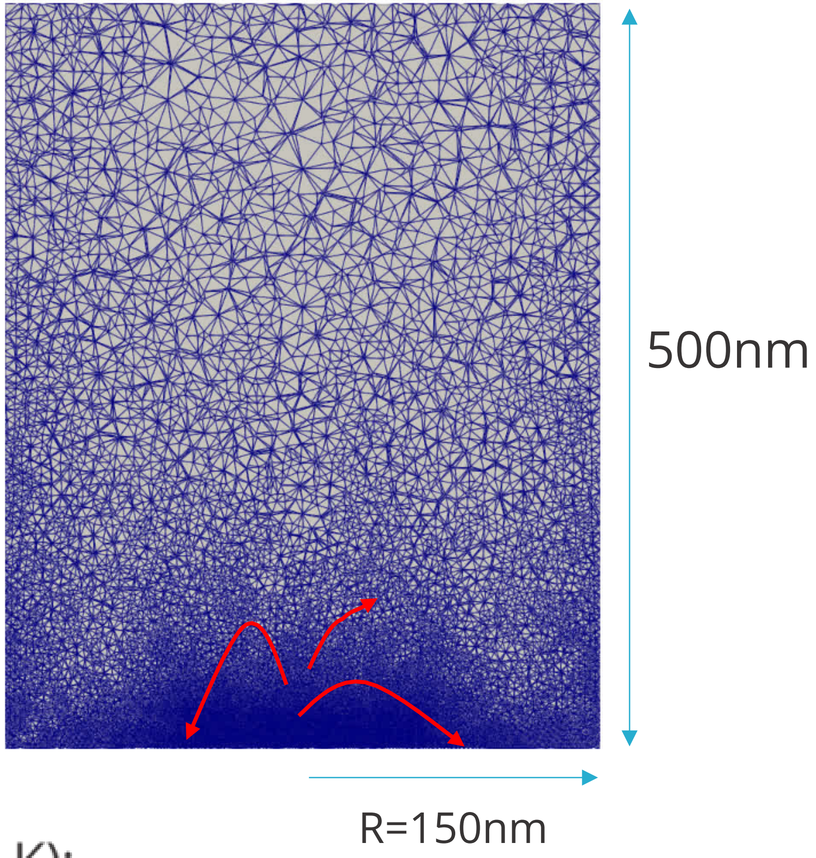


SCP Effects: PIC-DSMC Challenges

- Typical cathode spot:
  - Radius < 100nm
  - $n_n \sim 10^{27}\ m^{-3}$ (vaporization of electrode)
  - $n_e \sim 10^{24}\ m^{-3}$ (field emission)
  - $n_i \sim 5\times10^{25}\ m^{-3}$ (ionization, $\langle Z \rangle > 1$)
- Coupling parameter: $\Gamma = \frac{(\langle Z \rangle e)^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} \gtrsim 5$
- To resolve DIH: $\Delta x < a_{ii} \approx 1.7nm$
- To resolve PIC mesh-heating at initial ion temperature (2000 K):

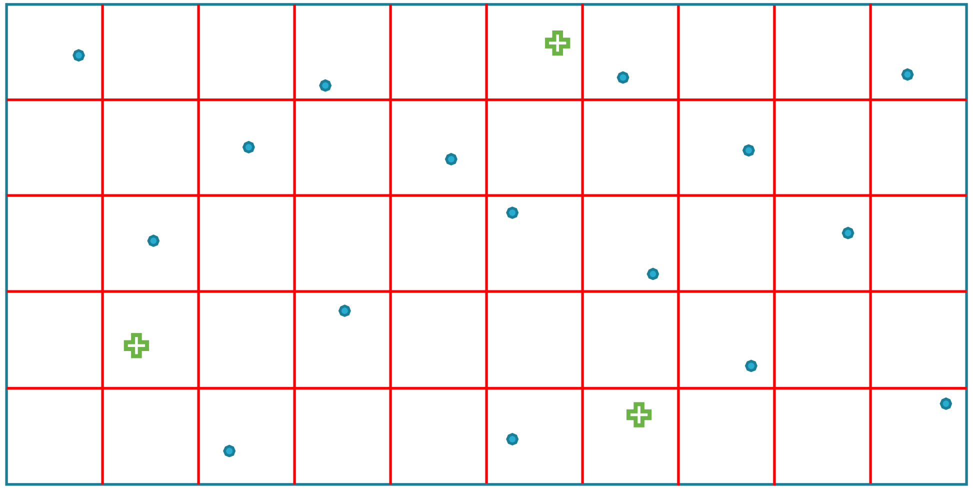
$$\Delta x < \lambda_D \cong \sqrt{\frac{\varepsilon_0 k_B T_i}{(Ze)^2 n_i}} \approx 0.4nm$$

Mesh has ~5×10^7 elements



SCP Effects: PIC-DSMC Challenges

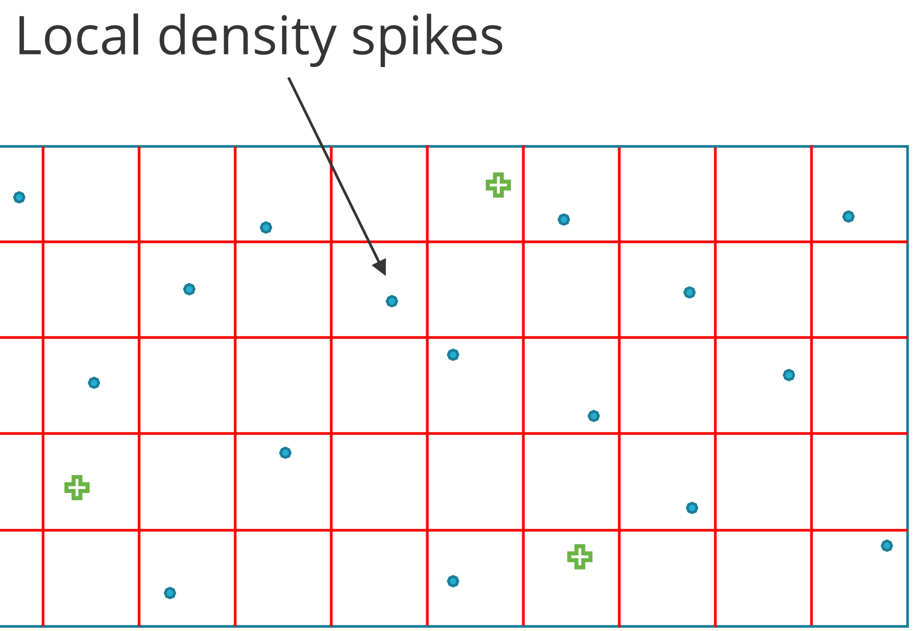
- Mean spacing between physical neutrals: $a_{nn} \sim 0.6nm$
- $\Delta x < \lambda_D \approx 0.4nm$ means there are less than one physical neutral particle per element volume and many fewer than one physical ion or electron per element!



- With this few particles/element, we will get numerical heating over 100's ω_p^{-1}

The PIC-DSMC Modeling Challenge

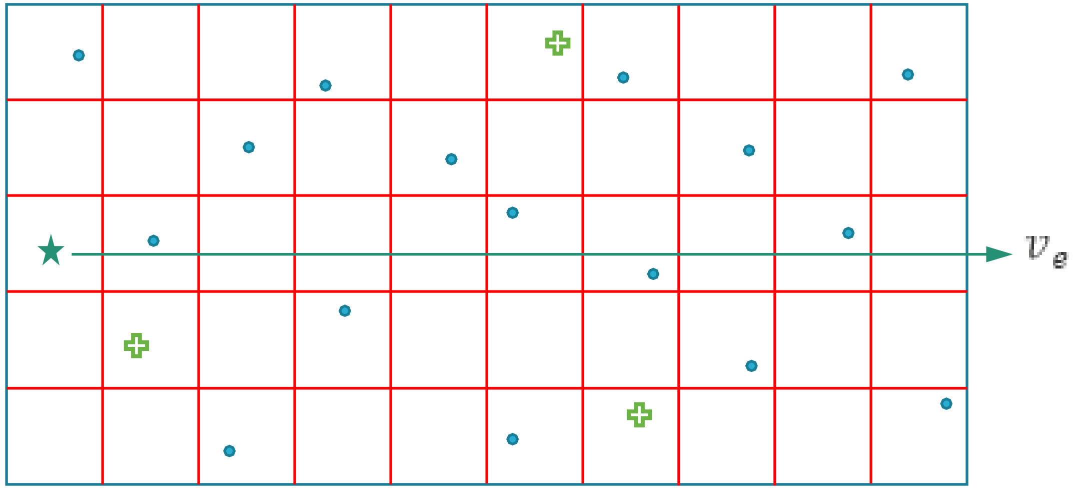
- Perhaps more fundamentally, the minimum density that can be represented by a single, weight=1 particle is 1/cell volume: $O(0.4^{-3}) \sim 6\times10^{29}\ m^{-3}$



The PIC-DSMC Modeling Challenge

- Perhaps more fundamentally, the minimum density that can be represented by a single, weight=1 particle is 1/cell volume: $O(0.4^{-3}) \sim 6\times10^{29}$ m^{-3}

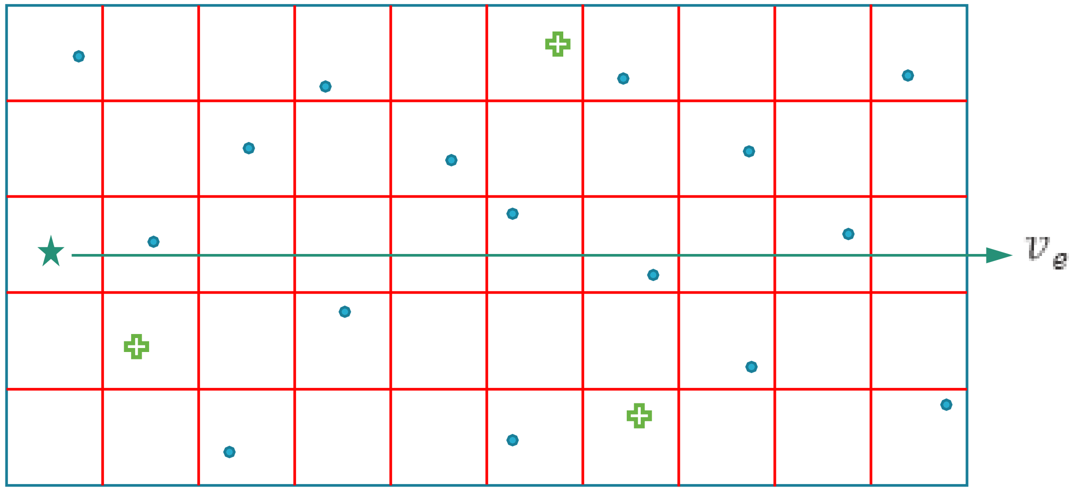
- Integrated ionization along the electron path will be wrong



The PIC-DSMC Modeling Challenge

- Perhaps more fundamentally, the minimum density that can be represented by a single, weight=1 particle is 1/cell volume: $O(0.4^{-3}) \sim 6\times10^{29}\ m^{-3}$

- Integrated ionization along the electron path will be wrong
  - Ionization rate is non-linear* with E/n:



Smooth E/n

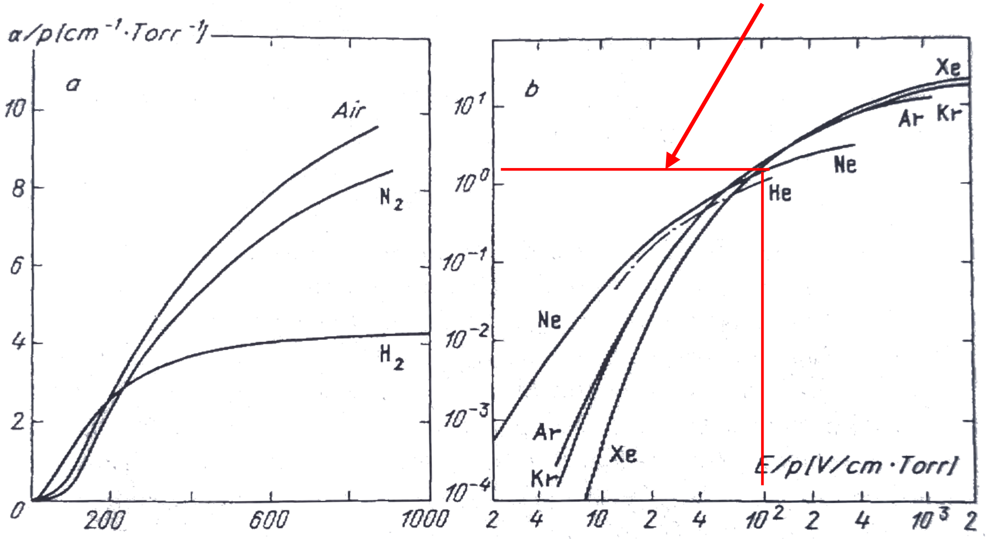


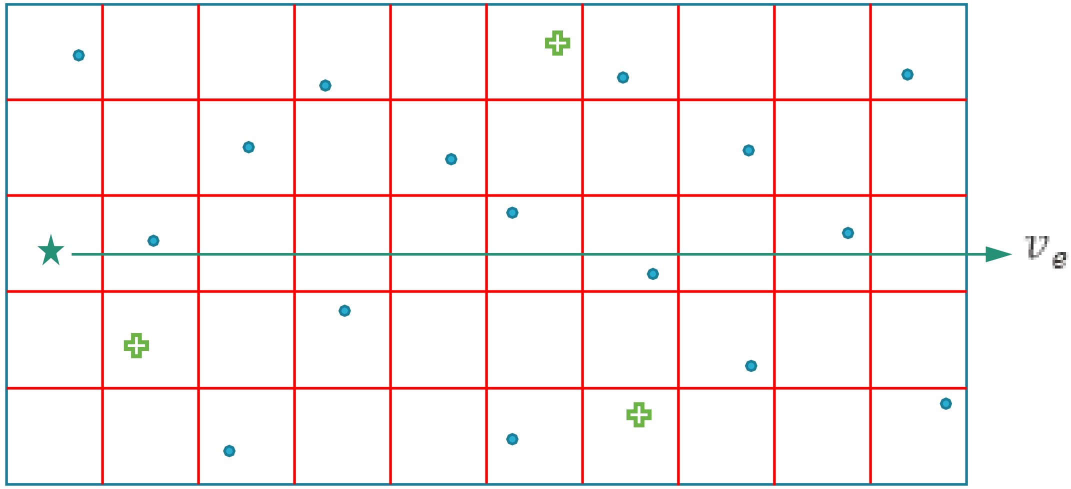
Fig. 4.3. Ionization coefficients for a wide range of E/p values (a) in molecular gases, (b) in inert gases. From [4.3]

*Raizer, *Gas Discharge Physics*, 1991

The PIC-DSMC Modeling Challenge

- Perhaps more fundamentally, the minimum density that can be represented by a single, weight=1 particle is 1/cell volume: $O(0.4^{-3}) \sim 6\times10^{29}\ m^{-3}$

- Integrated ionization along the electron path will be wrong
  - Ionization rate is non-linear* with E/n:



Density spikes E/n

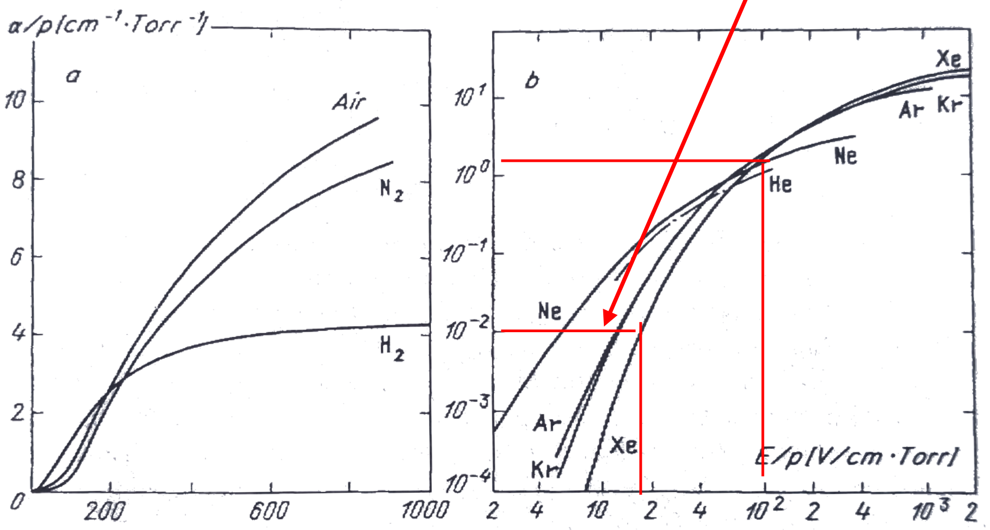


Fig. 4.3. Ionization coefficients for a wide range of E/p values (a) in molecular gases, (b) in inert gases. From [4.3]

*Raizer, *Gas Discharge Physics*, 1991

The PIC-DSMC Modeling Challenge

- We could solve the collision rate issue several ways:

The PIC-DSMC Modeling Challenge

- We could solve the collision rate issue several ways:
  - Use larger elements, don’t resolve Debye length

The PIC-DSMC Modeling Challenge

- We could solve the collision rate issue several ways:
  - Use larger elements, don't resolve Debye length
  - Use rates based on the nominal densities & velocities

The PIC-DSMC Modeling Challenge

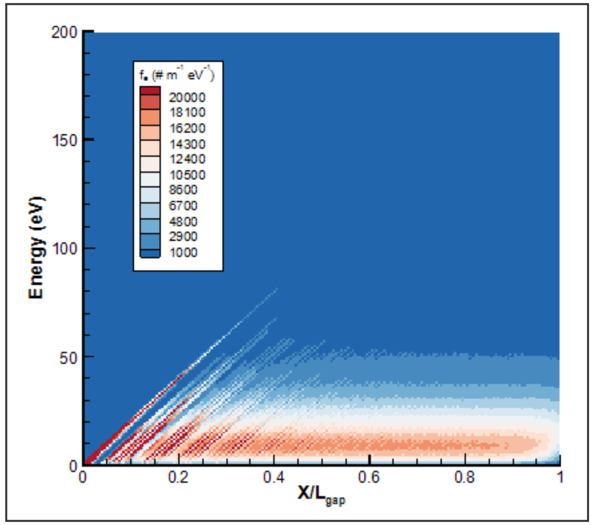
- We could solve the collision rate issue several ways:
  - Use larger elements, don't resolve Debye length
  - Use rates based on the nominal densities & velocities
  - Use a separate collision mesh and field solve mesh

The PIC-DSMC Modeling Challenge

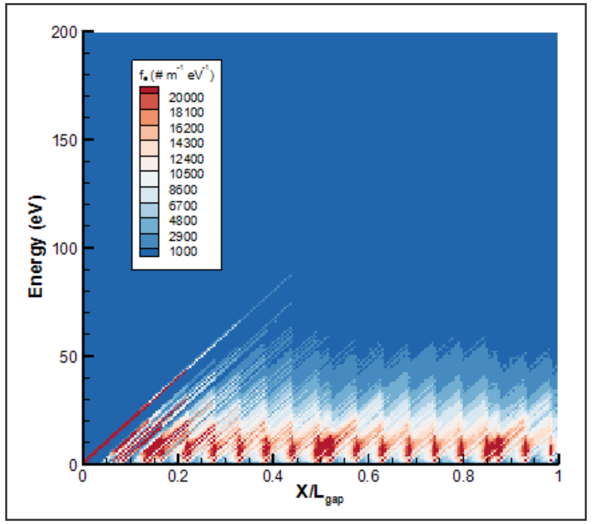
- We could solve the collision rate issue several ways:
  - Use larger elements, don’t resolve Debye length
  - Use rates based on the nominal densities & velocities
  - Use a separate collision mesh and field solve mesh

- Separate collision and field meshes does improve the accuracy for avalanche calculations:

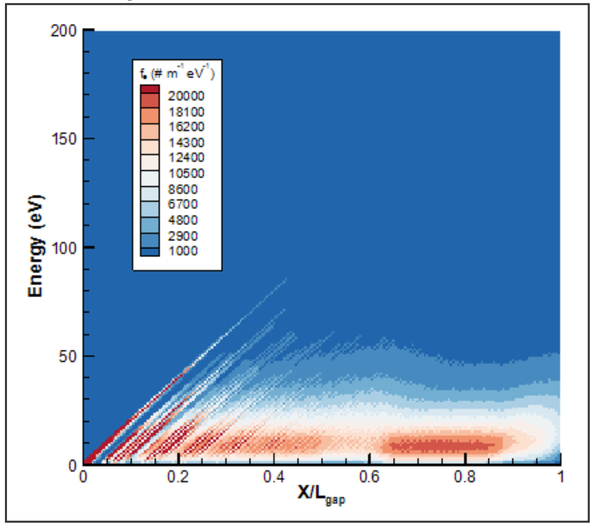
10 particles/cell



0.1 particles/cell



0.1 particles/field cell
10 particles/collision cell



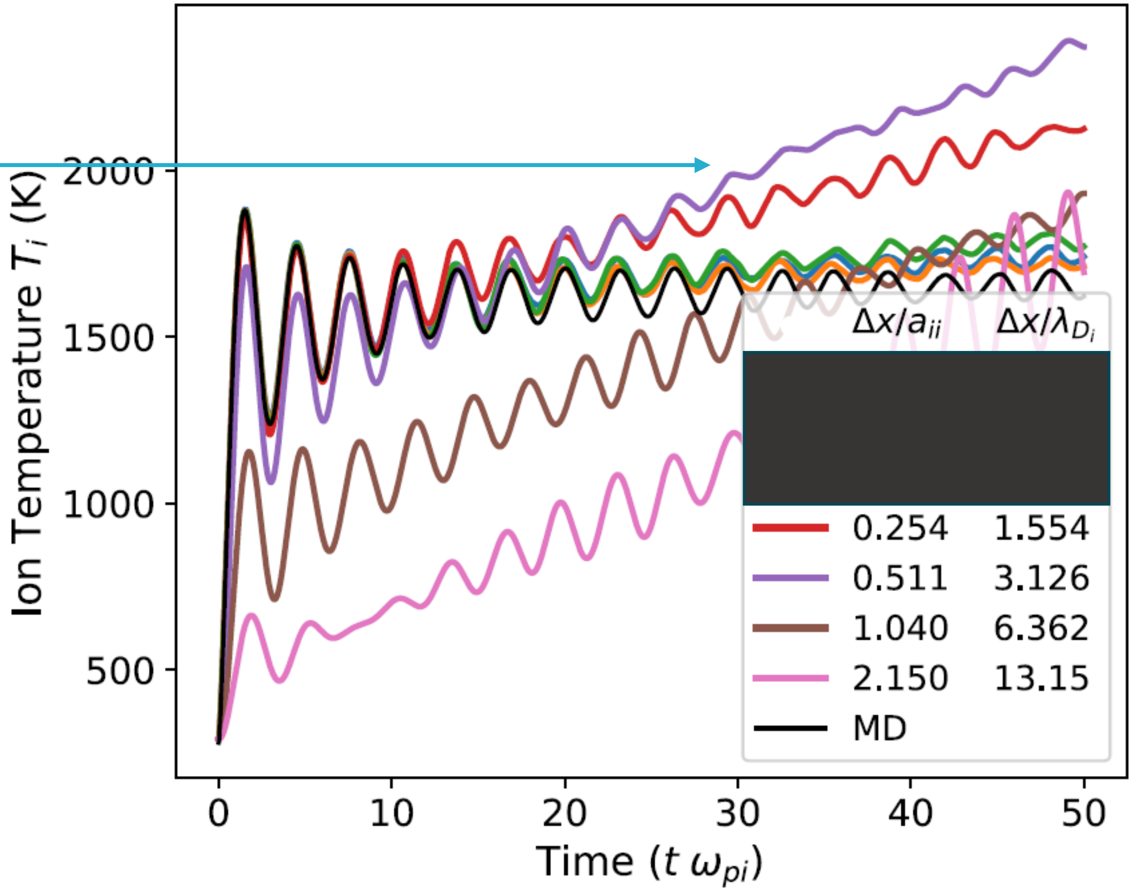
* S. Moore, P. Crozier, C. Moore, M. Bettencourt, and M. Hopkins, “Automatic Coarsening of the Particle Interaction Mesh in a Hybrid PIC-DSMC Simulation”, DSMC workshop, 2013

The PIC-DSMC Modeling Challenge

- Can we use $\Delta x > \lambda_D$?

The PIC-DSMC Modeling Challenge

- Can we use $\Delta x > \lambda_D$?
- Numerical mesh heating over 10's ω_p^{-1}

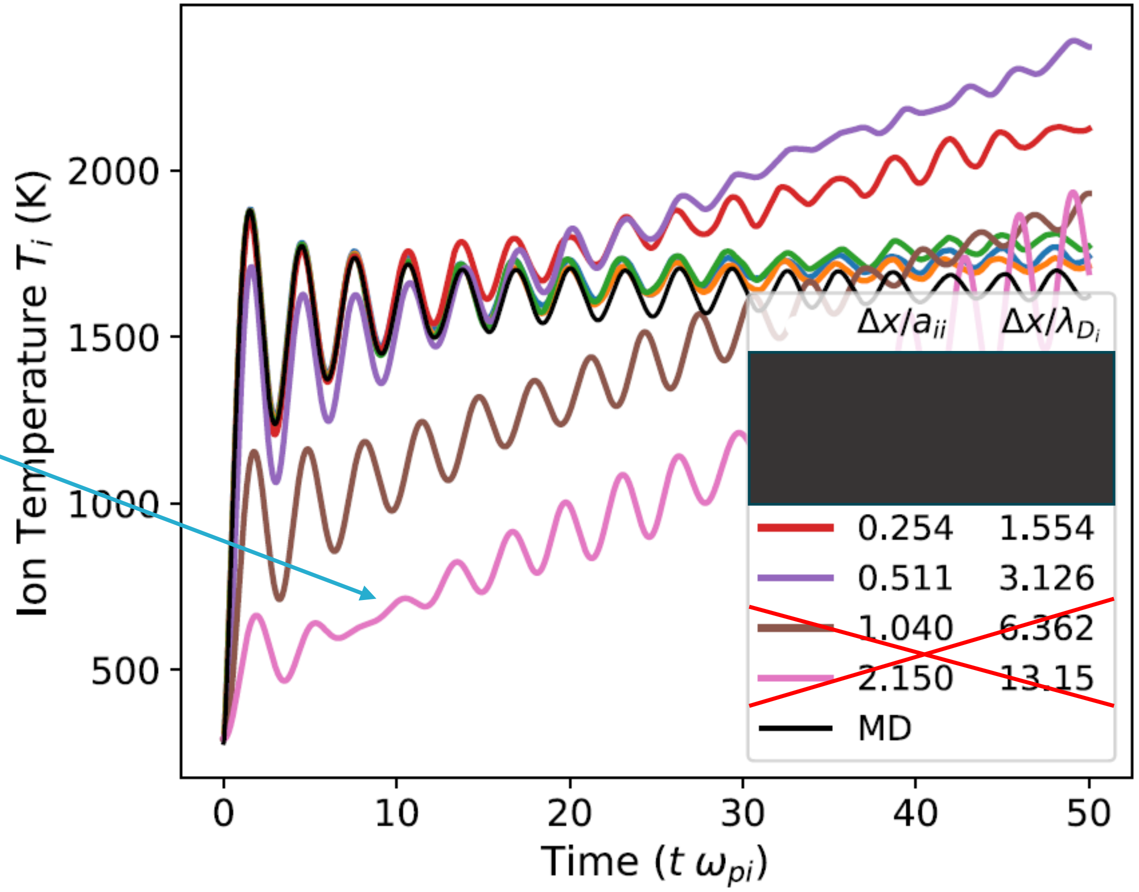


PIC simulation of periodic box with neutrals ionized at t=0

*Figure from M.D. Acciarri *et al*, PSST, **33** 035009 (2024)

The PIC-DSMC Modeling Challenge

- Can we use $\Delta x > \lambda_D$?
- Numerical mesh heating over 10's ω_p^{-1}
- Must still resolve the mean ion spacing to capture physical Disorder Induced Heating



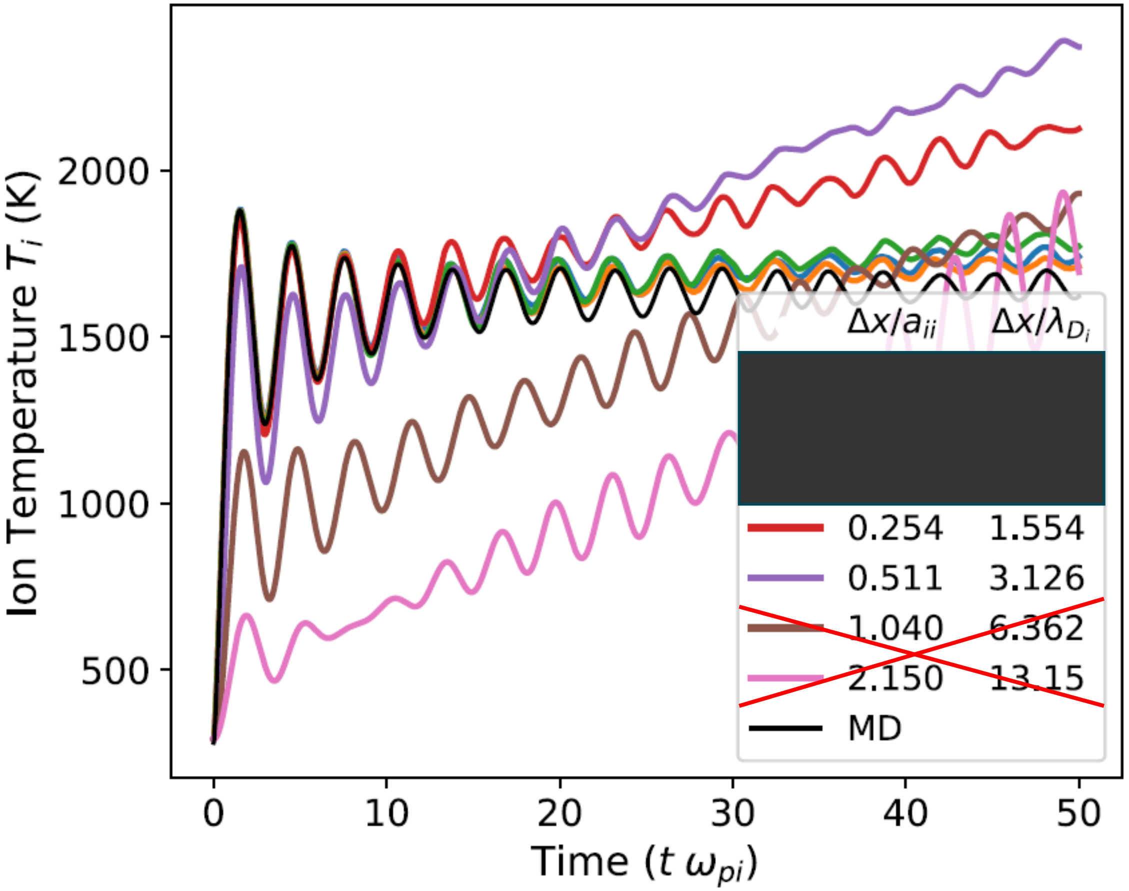
PIC simulation of periodic box with neutrals ionized at t=0

*Figure from M.D. Acciarri *et al*, PSST, **33** 035009 (2024)

The PIC-DSMC Modeling Challenge

- Can we use $\Delta x > \lambda_D$?
- Numerical mesh heating over 10's ω_p^{-1}
- Must still resolve the mean ion spacing to capture physical Disorder Induced Heating

We can't increase the mesh size enough with traditional PIC. There will be unphysically large fluctuations in the densities.



PIC simulation of periodic box with neutrals ionized at t=0

*Figure from M.D. Acciarri *et al*, PSST, **33** 035009 (2024)

The PIC-DSMC Modeling Challenge

- Do particle weights < 1 solve grid heating?

The PIC-DSMC Modeling Challenge

- Do particle weights < 1 solve grid heating?
  - Have more than 1 ion per cell
  - Avoid numerical heating over 100s ω_p^{-1}?

The PIC-DSMC Modeling Challenge

- Do particle weights < 1 solve grid heating?
  - Have more than 1 ion per cell
  - Avoid numerical heating over 100s ω_p^{-1}

- No. This changes the radial distribution function, g(r), and thus the amount of DIH.

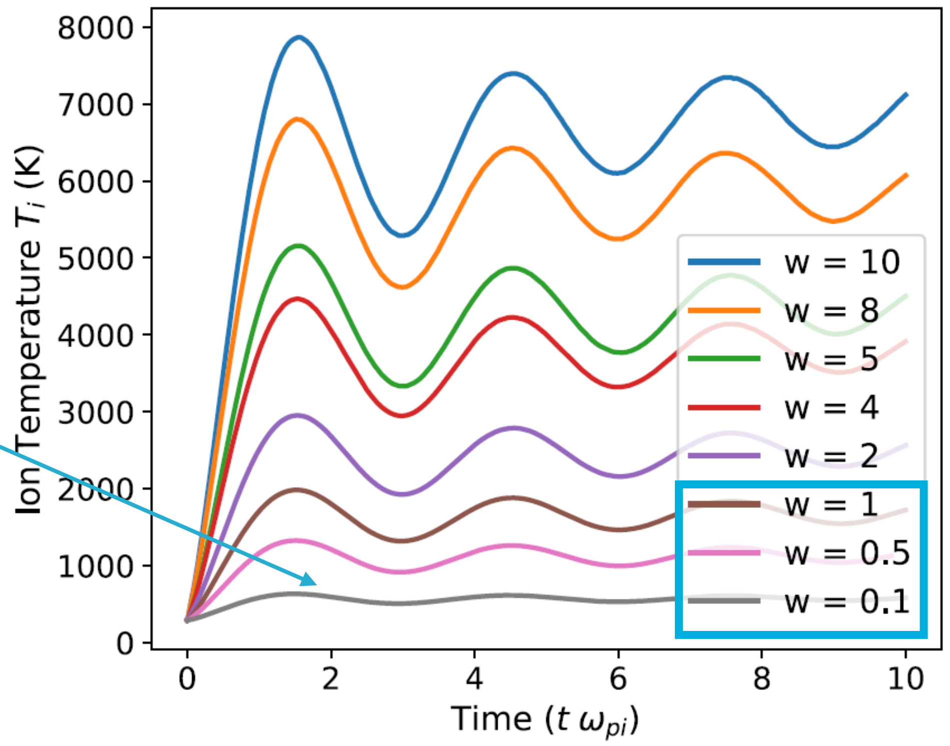


FIG. 4. Evolution of the ion temperature using a grid spacing of $\Delta x/a_{ii} \approx 0.042$ for different macroparticle weights w.

* Figure from M.D. Acciarri *et al*, PSST, **33** 035009 (2024)

The PIC-DSMC Modeling Challenge

- Do particle weights < 1 solve grid heating?
  - Have more than 1 ion per cell
  - Avoid numerical heating over 100s ω_p^{-1}

- No. This changes the radial distribution function, g(r), and thus the amount of DIH.

- Furthermore, it's possible when using weights>1 to introduce Artificial Correlation Heating (ACH)!

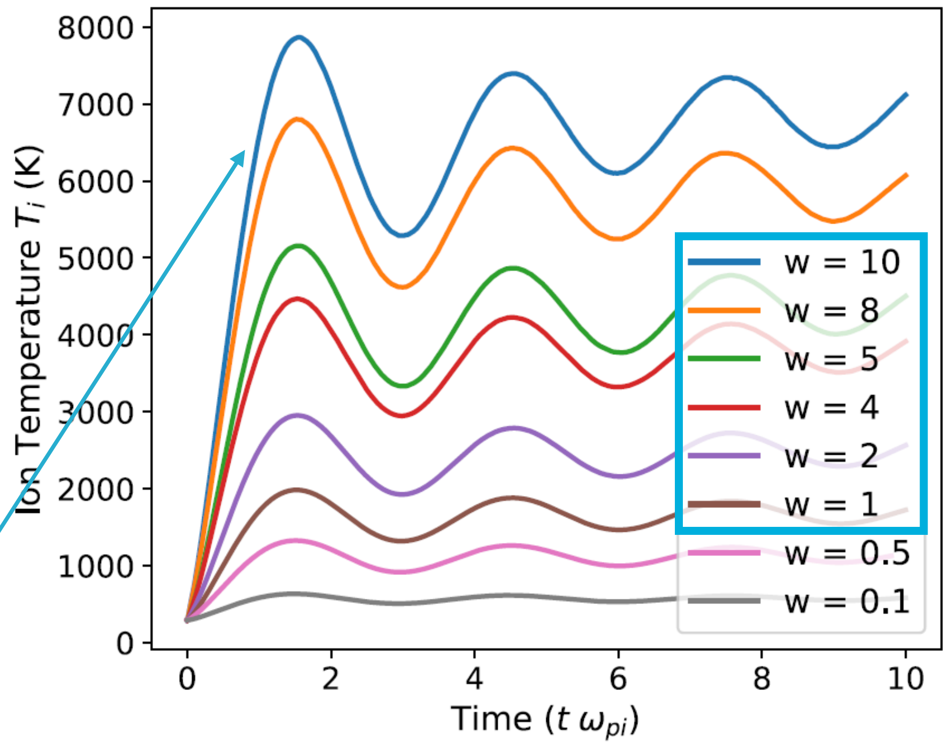


FIG. 4. Evolution of the ion temperature using a grid spacing of $\Delta x/a_{ii} \approx 0.042$ for different macroparticle weights w.

* Figure from M.D. Acciarri *et al*, PSST, **33** 035009 (2024)

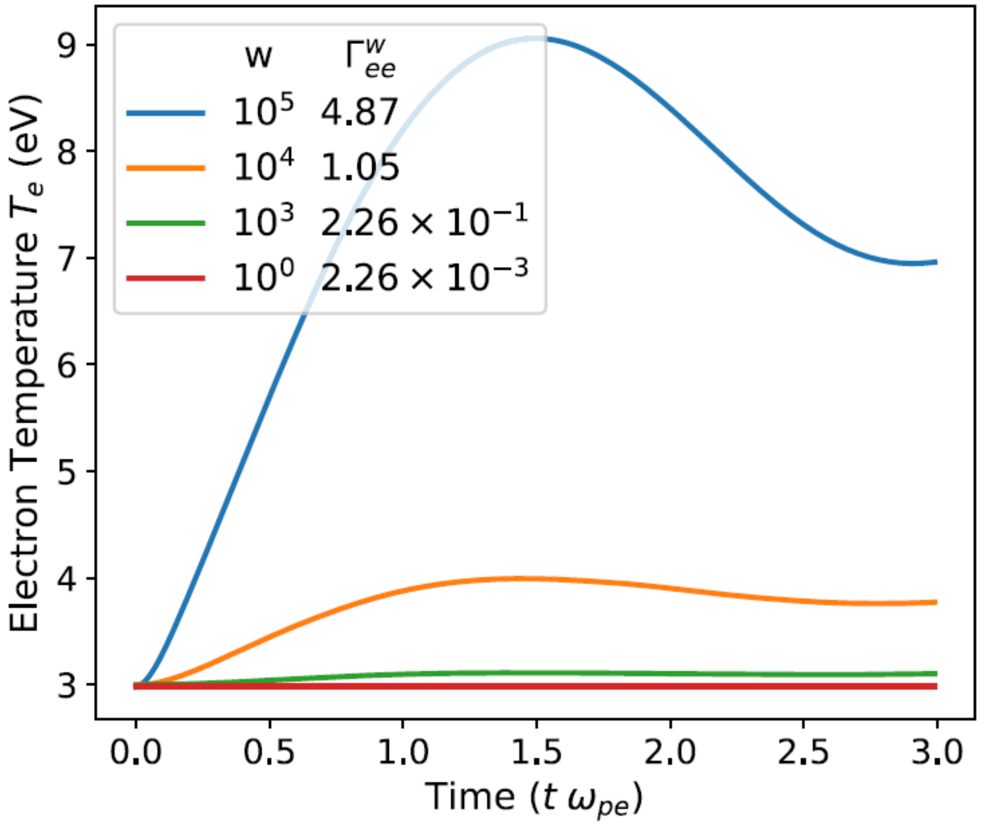
The PIC-DSMC Modeling Challenge

- Can Artificial Correlation Heating (ACH) occur for PIC simulation of ideal plasmas?

The PIC-DSMC Modeling Challenge

- Can Artificial Correlation Heating (ACH) occur for PIC simulation of ideal plasmas?

- Yes*!



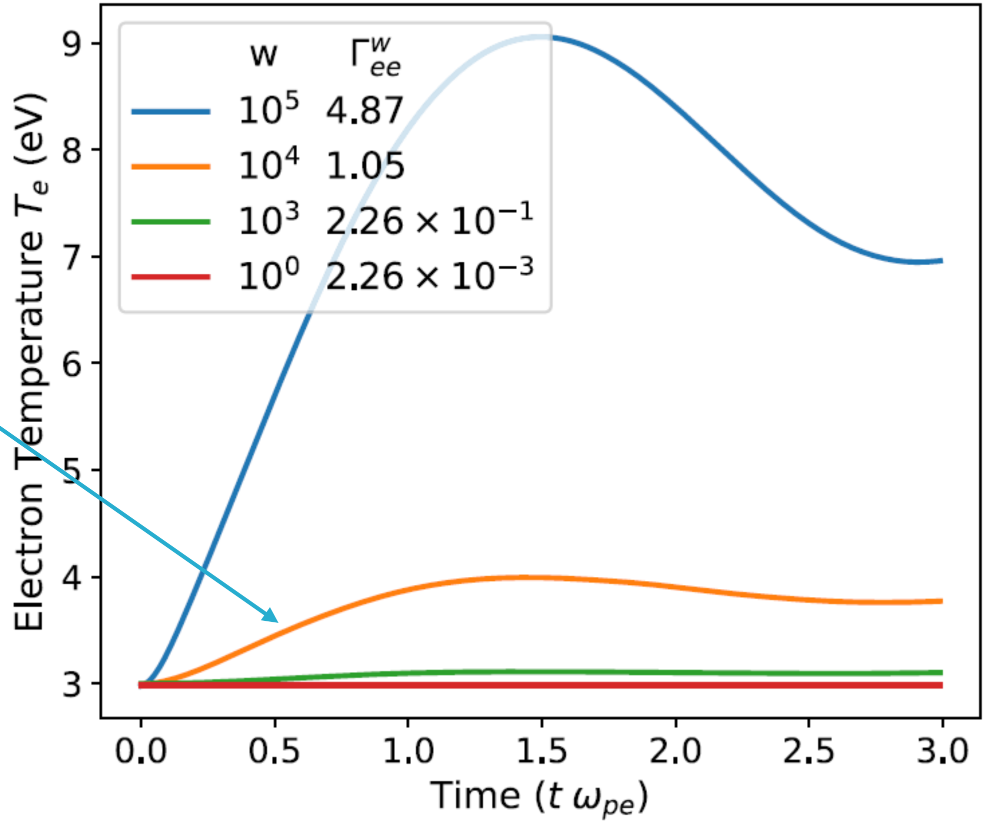
Temperature evolution for $n_e = 2.5\times10^{19}$ m^{-3} and $\Delta x/\lambda_D = 0.5$

* Figure from M.D. Acciarri *et al*, Phys. Plasmas, **31** 093903 (2024)

The PIC-DSMC Modeling Challenge

- Can Artificial Correlation Heating (ACH) occur for PIC simulation of ideal plasmas?
- Yes*!
- Significant ACH occurs when $\Gamma^w > 1$:

$$\Gamma^w = w^{2/3}\frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} = w^{2/3}\Gamma$$



Temperature evolution for $n_e = 2.5\times10^{19}$ m^{-3} and $\Delta x/\lambda_D = 0.5$

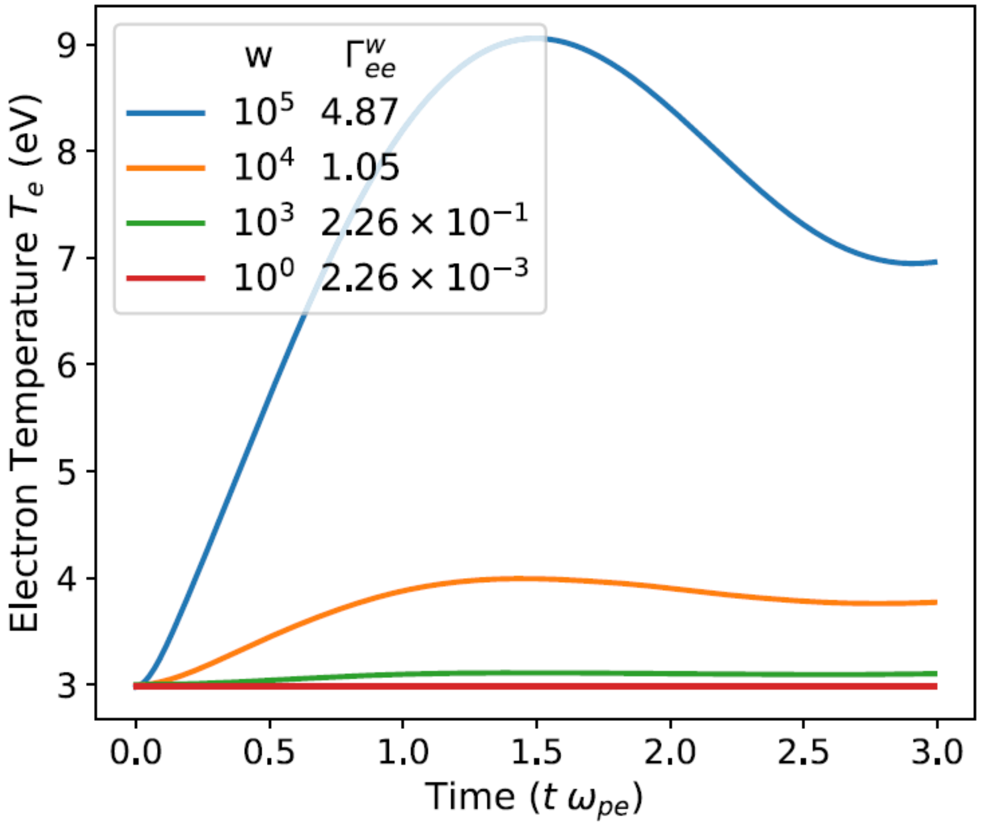
* Figure from M.D. Acciarri *et al*, Phys. Plasmas, **31** 093903 (2024)

The PIC-DSMC Modeling Challenge

- Can Artificial Correlation Heating (ACH) occur for PIC simulation of ideal plasmas?
- Yes*!
- Significant ACH occurs when $\Gamma^w > 1$:

$$\Gamma^w = w^{2/3} \frac{q^2}{4\pi\varepsilon_0 k_B T}\left(\frac{4\pi n}{3}\right)^{1/3} = w^{2/3}\Gamma$$

Acceptable particle weights are limited



Temperature evolution for $n_e = 2.5\times10^{19}$ m^{-3} and $\Delta x/\lambda_D = 0.5$

* Figure from M.D. Acciarri *et al*, Phys. Plasmas, **31** 093903 (2024)

PIC Challenges and Possible Solutions

- Challenges to resolving DIH:
  - Numerical heating due to small N_C
  - Numerical heating due to $\Delta x > \lambda_D$
  - Collision rate errors due to incorrect “local” density for W=1 particles
  - ACH due to particle weights other than unity

- Solutions??
  - Use a Particle-Particle-Particle-Mesh scheme**
    - MD inside the element and far-field charges via the fields on the mesh
    - Allows for $\Delta x > \lambda_D$ while still capturing DIH
    - However, one must still use W=1 and it’s expensive
  - Use $\Delta x > a_{ii}$ and “thermostat” estimated DIH into the ions

Bettencourt, IEEE Transactions on Plasma Science, **42, 5, 1189-1194 (2014).

EMPIRE Simulation Model

- We choose to use W=1 particles and resolve (or very nearly resolve) the Debye length such that numerical mesh heating is small and accept late time particle count heating with the goal of gaining insight about DIH on shorter timescales.

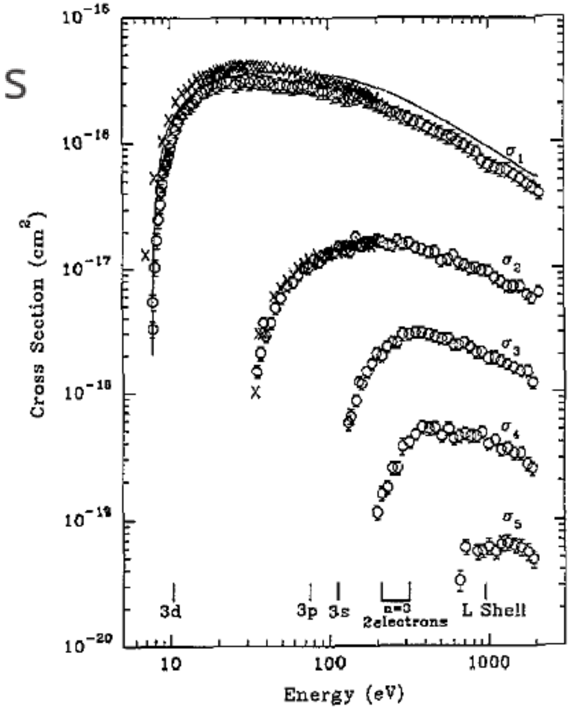
- Using standard DSMC collisions would give wrong ionization rates thus as an approximation we use a constant ionization rate where the neutral has a probability of ionizing ($Cu \rightarrow Cu^{+} + e^{-}$):

$$P_{iz} = 1 - exp^{-\Delta t n_e \langle \sigma v_e \rangle}$$

- Where we let $\langle \sigma v_e \rangle \sim \sigma_{max} v_e \approx 3 \times 10^{-20}(4 \times 10^{6}) = 1.2 \times 10^{-14}$ [m³/s]

- We include double ionization at 5% of the single ionization rate

- Note, we have neglected field and pressure ionization and are not accounting for ionization rate changes as the neutrals get further from the cathode. We also do not include e+Cu elastic or excitation collisions.



Bolorizadeh et al, J. Phys. B: At. Mol. Opt. Phys. **27**, 175

EMPIRE Simulation Model

- Inject neutrals on a regular lattice inside cathode spot to approximate starting from a solid Cu lattice

- Charge-Charge collisions are directly computed via the fields on the mesh since $N_{elem} \ll 1$

- Ion collisions:
  - Elastic collisions → Use approximate VHS parameters for Cu+Cu collisions*

    $$d_{ref} = 0.57 \text{ nm and } \omega = 0.92$$

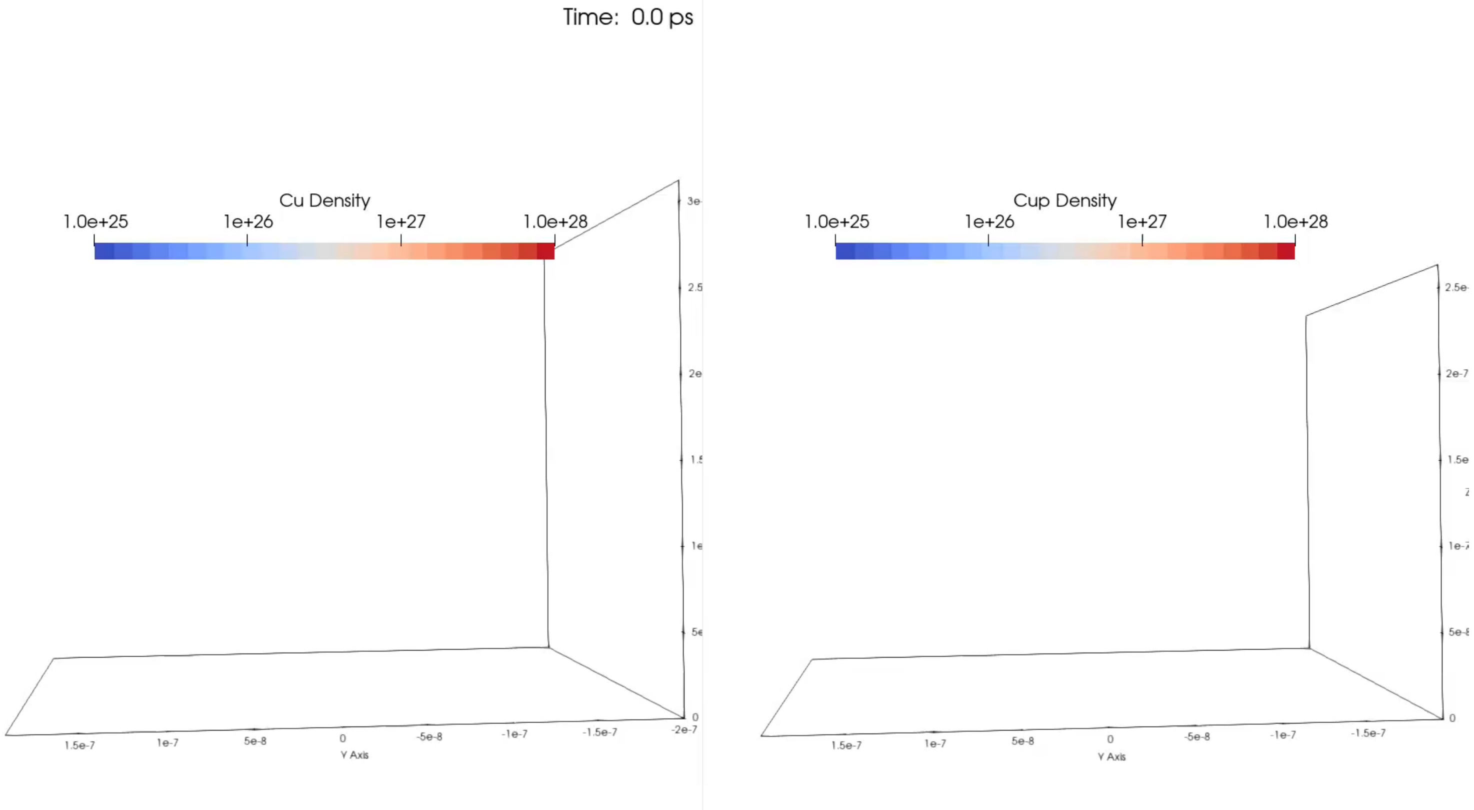
  - Charge exchange* → $\sigma_{CEX} \sim \frac{1}{I_B}\left(C_1 - C_2 ln(v)\right)^2, C_1 = 6.5\times10^{-7}, C_2 = 3\times10^{-8}$

  - However, note that charge exchange is a tunneling process and thus extremely short ranged (~Å) but DSMC allows collisions to occur across the element (which is ~8Å). This results in unphysically large ion “transport” across the element.

  - We neglect $Cu^{+} + e^{-} \rightarrow Cu^{++} + 2e^{-}$ and all ion-cathode feedback BCs (sputtering, SEE, heating, etc.)

*Venkattraman, “Direct Simulation Monte Carlo modeling of e-beam metal deposition”, 2010. http://dx.doi.org/10.1116/1.3386592
*Fridman and Kennedy, “Plasma Physics and Engineering”, 2004.

Results: Without Charge Exchange



- Neutrals expand out from the cathode spot and are gradually ionized
- Note that, until the mesh coarsens after ~18nm, the mesh is so small that we don't accurately capture the ion or neutral densities in a given element

→ The rest of our results will show quantities computed using all the particles in the domain (or a subset of it) in order to reduce noise since we typically have <1 particle/cell

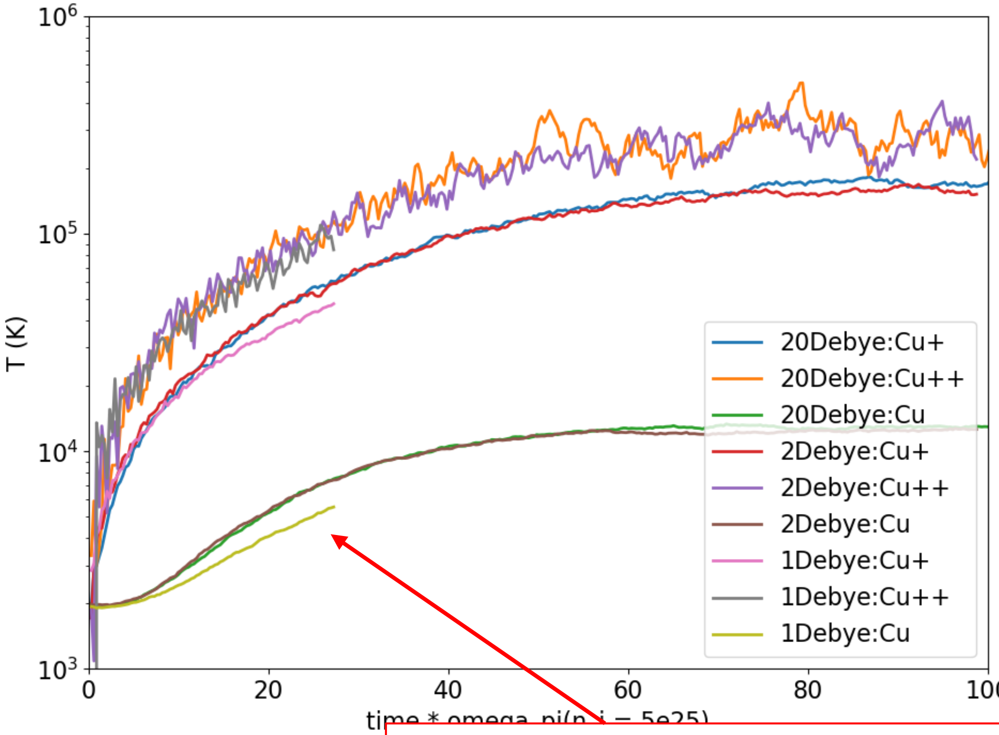
Results: Without Charge Excl

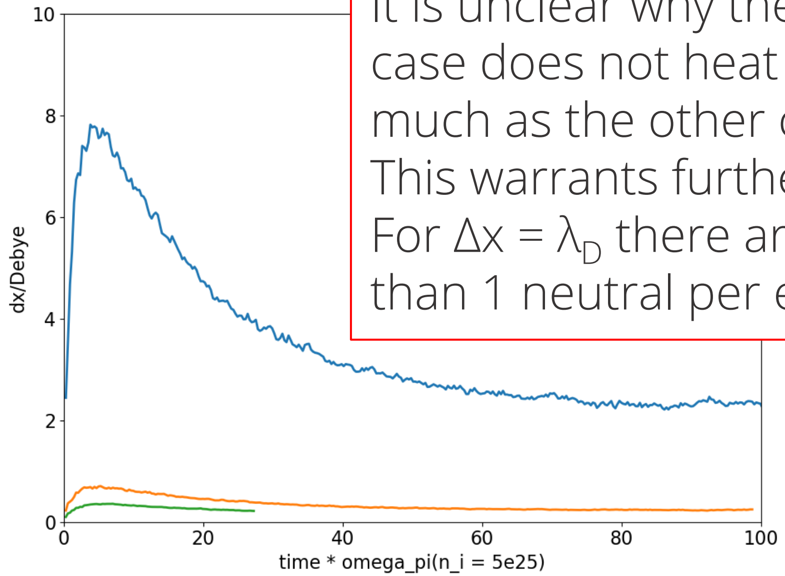
- Significant Disorder Induced Heating is seen to occur on the timescale of ~$50\omega_{pi}^{-1}$ as it takes time for the neutrals to expand and ω_{pi} is **not** constant!

- However! Given the large applied fields, the ion velocity distribution is NOT an equilibrium Maxwellian so "temperature" is not particularly meaningful in the usual sense.

- The $\Delta x = 20\lambda_D(n_i = 5\times10^{25}\ m^{-3}, T_i=2000K)$ case does not actually ever reach a mesh that is 20× Debye as the ions are rapidly heating (similarly for all mesh sizes)

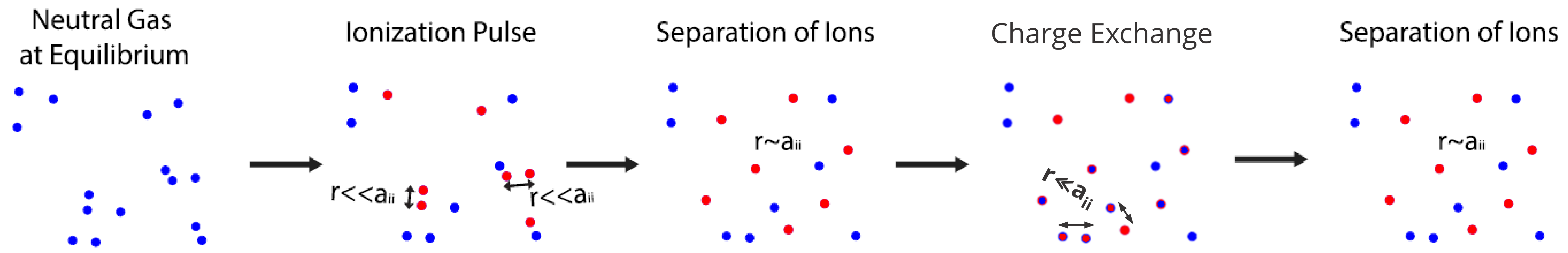
- Ion and neutral temperatures do not reach equilibrium as they expand into the vacuum and the collision rates are not fast enough to fully equilibrate



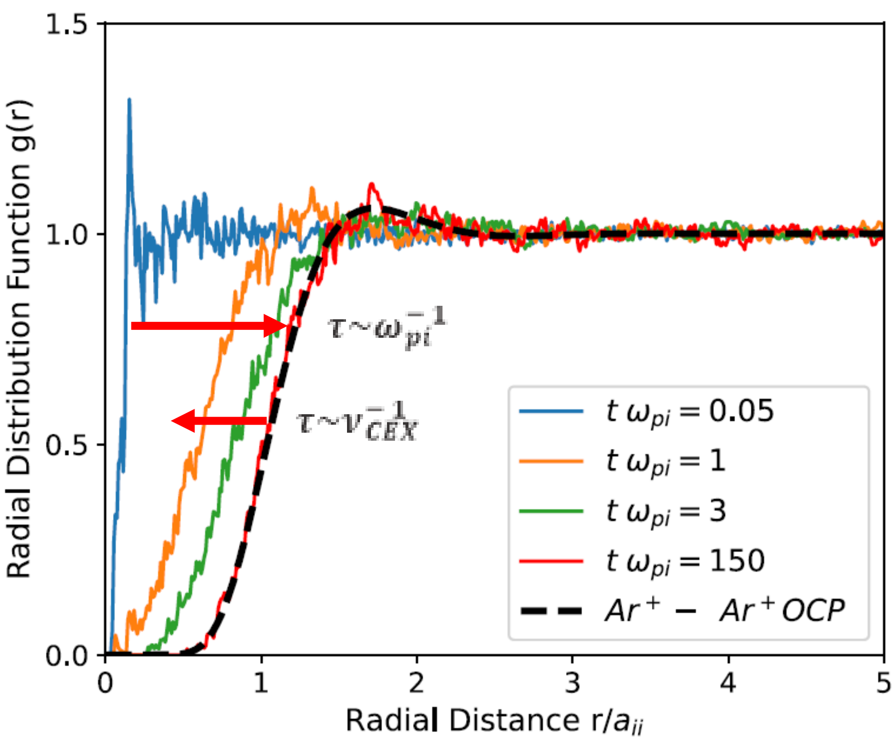


It is unclear why the $\Delta x = \lambda_D$ case does not heat quite as much as the other cases. This warrants further study. For $\Delta x = \lambda_D$ there are fewer than 1 neutral per element.

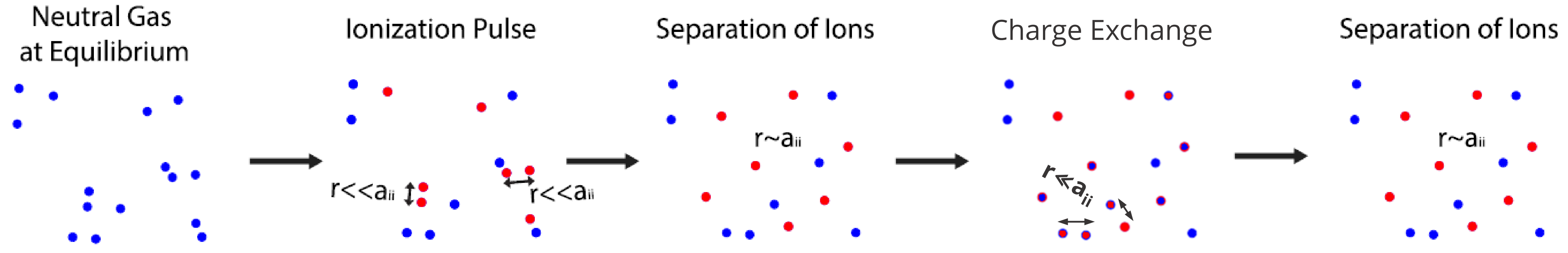
Disorder Induced Heating with Charge Exchange



- As ionization occurs the ions are too close together – some fraction of their positions are based on the former-neutral locations
- The ions fly apart due to Coulomb repulsion on the ion plasma period timescale and the ions gain thermal energy
- At the same time, charge exchange (tunneling of charge to the neutral) occurs as ions and neutrals pass closely by each other
- This results in more uncorrelated ions again and additional heating!



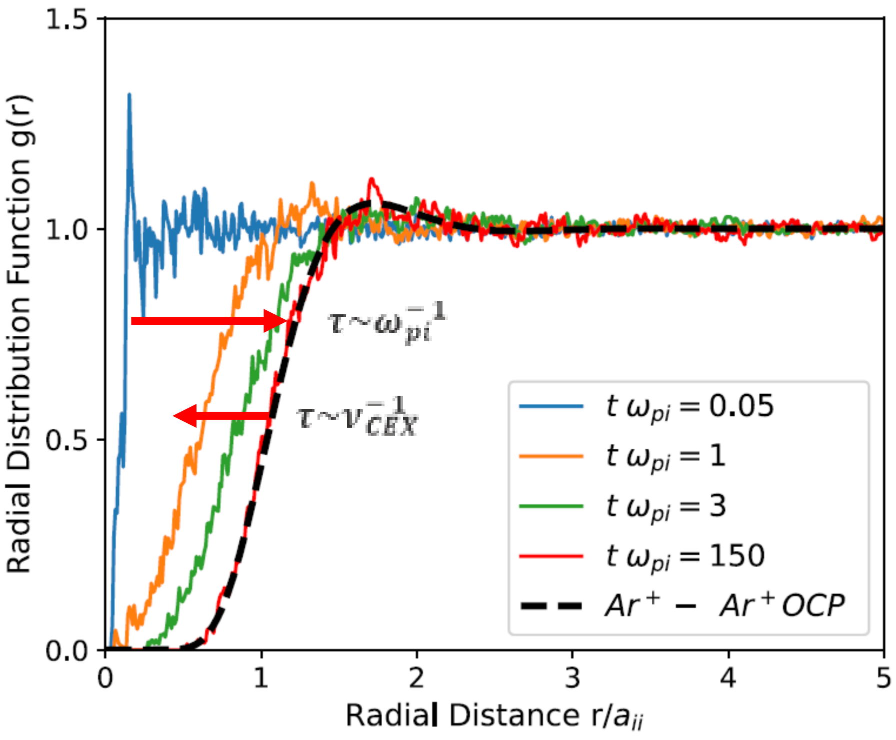
Disorder Induced Heating with Charge Exchange



- Will this just continue forever and T → ∞ ?
- No, for at least two reasons:

$$\sigma_{CEX} \sim \frac{1}{I_B}\left(C_1 - C_2 ln(v)\right)^2, C_1 = 6.5\times10^{-7}, C_2 = 3\times10^{-8}$$

- So as the temperature increases, ν_{CEX} will decrease
- Second, the densities rapidly decrease as the gas/plasma expands into the vacuum further decreasing $\nu_{CEX}(n_i)$ (faster than $\omega_{pi}\left(\sqrt{n_i}\right)$)

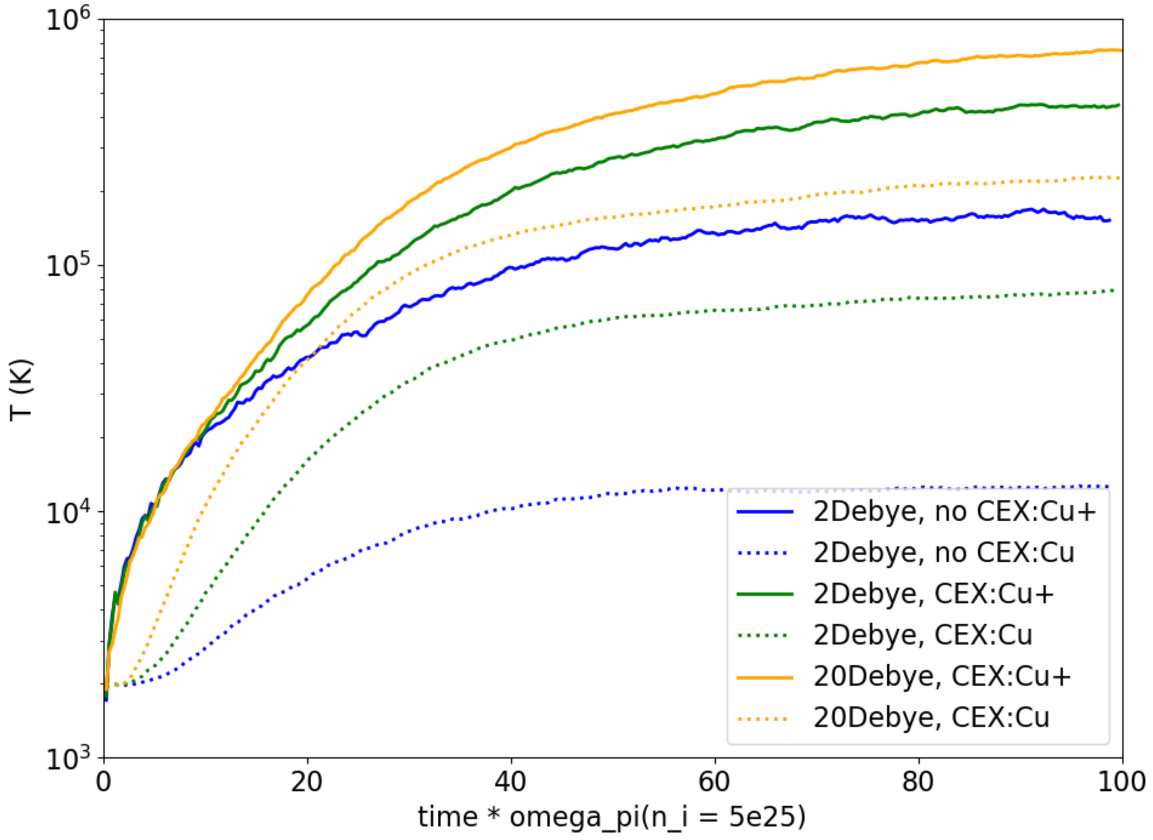


Results: With Charge Exchange

- As expected allowing charge exchange does result in additional DIH

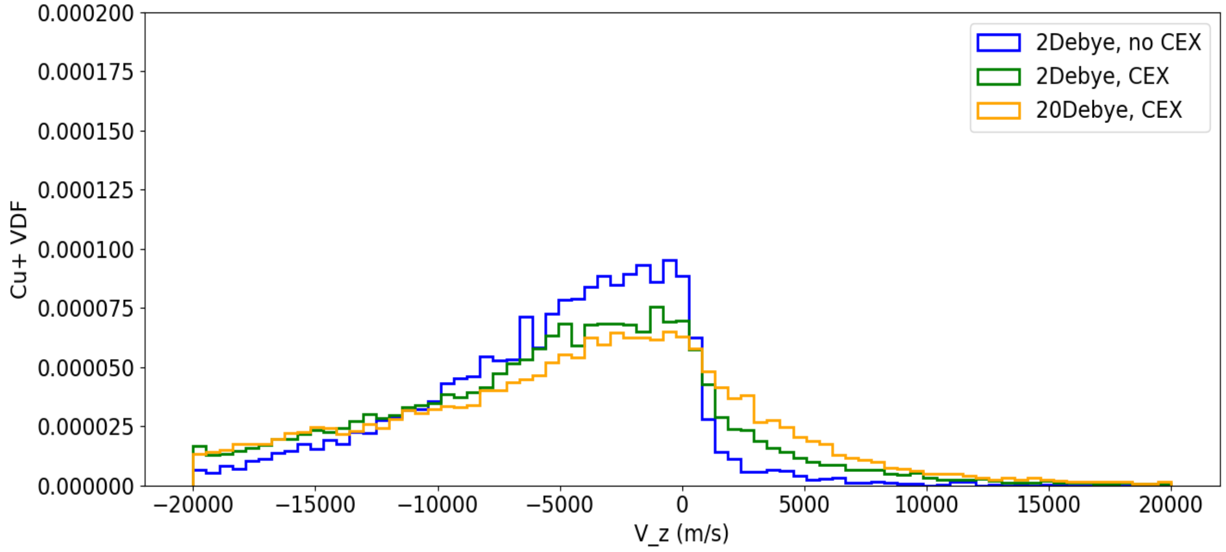
- Furthermore, as we decrease the size of the mesh, the additional DIH decreases (versus the no charge exchange case)
  - Due to charge exchange distances that scale with Δx

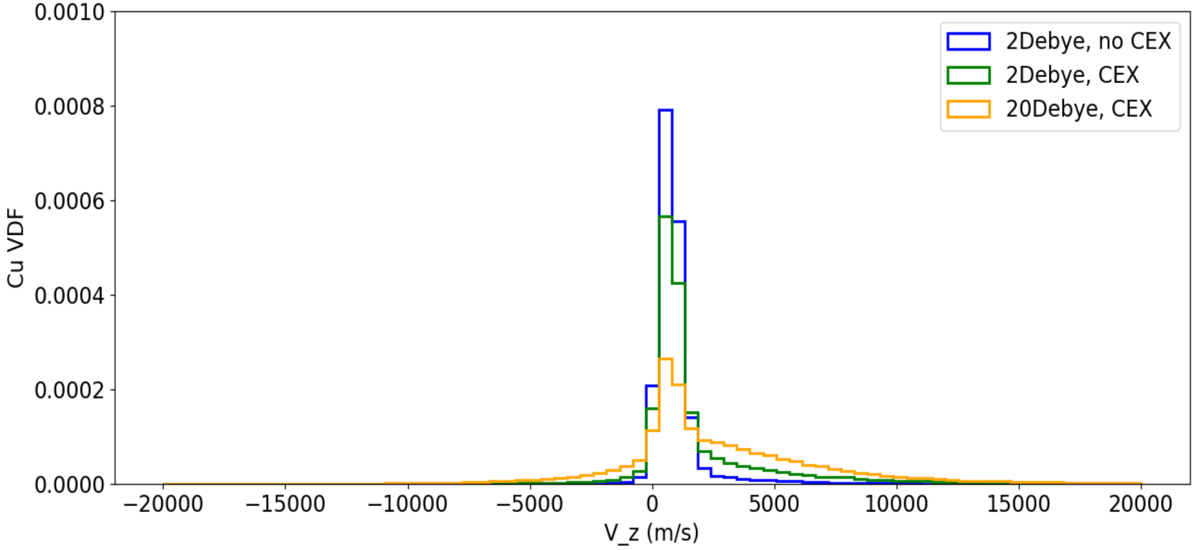
- Note, we did not include Cu^{++} charge exchange in the model; however there is increased Cu^{++} DIH due field interactions with the Cu^{+}



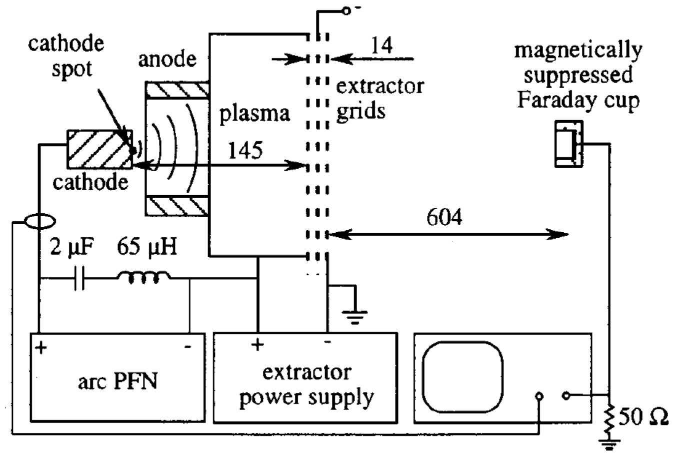
Results: With Charge Exchange

t=83.5ps -- $\omega_{pi}t$ ~ 98



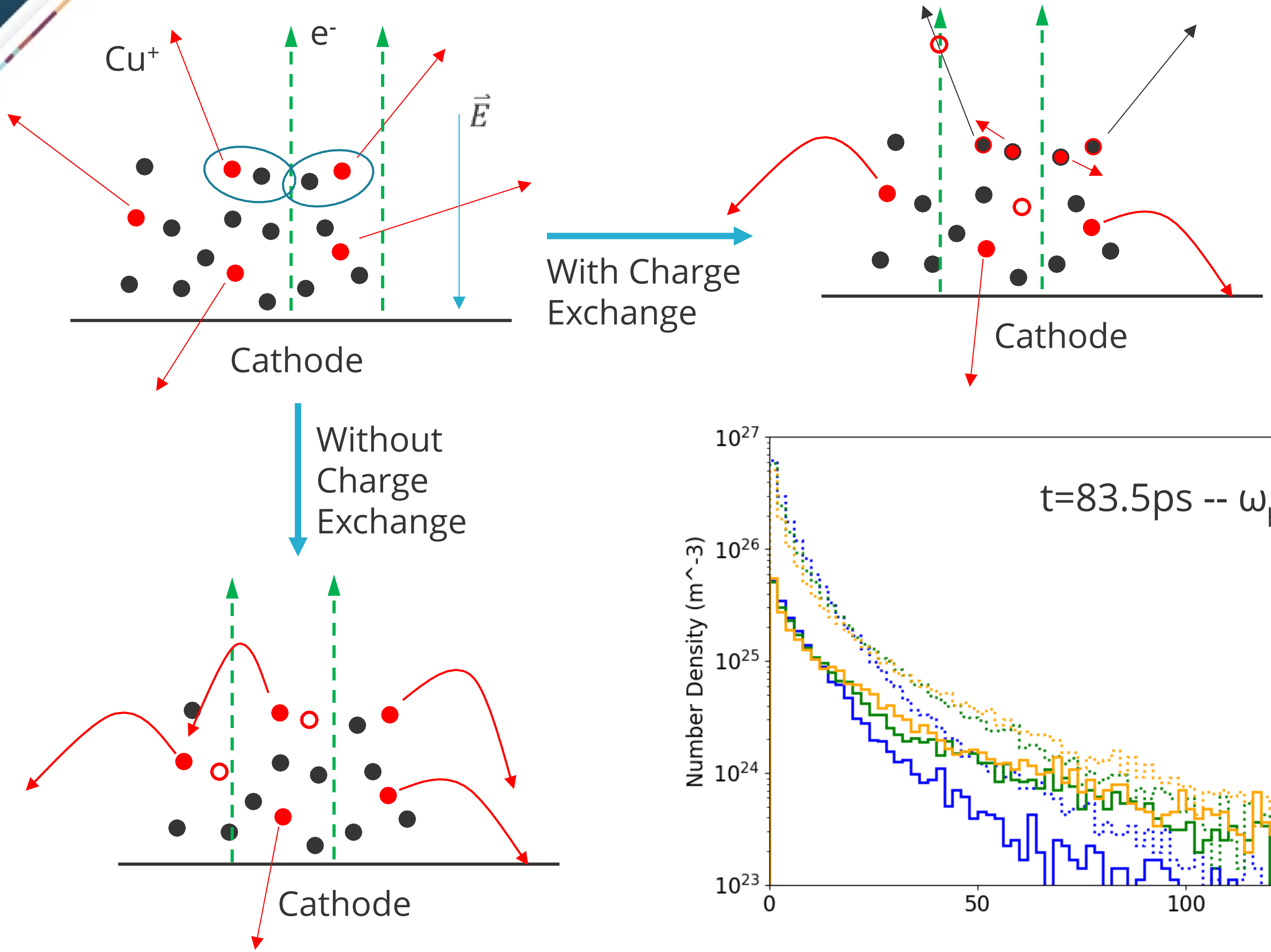


- With charge exchange we now get a non-negligible population of ions with large velocities (5-10km/s) away from the cathode
- Ions are rapidly accelerated via DIH and then charge exchange results in a fast neutral which is later ionized after traveling some distance from the cathode spot
- Similar in magnitude to the mean 12.8km/s Cu^+ velocity (for the ions that escape the cathode spot) reported in Yushkov et al. (2000)

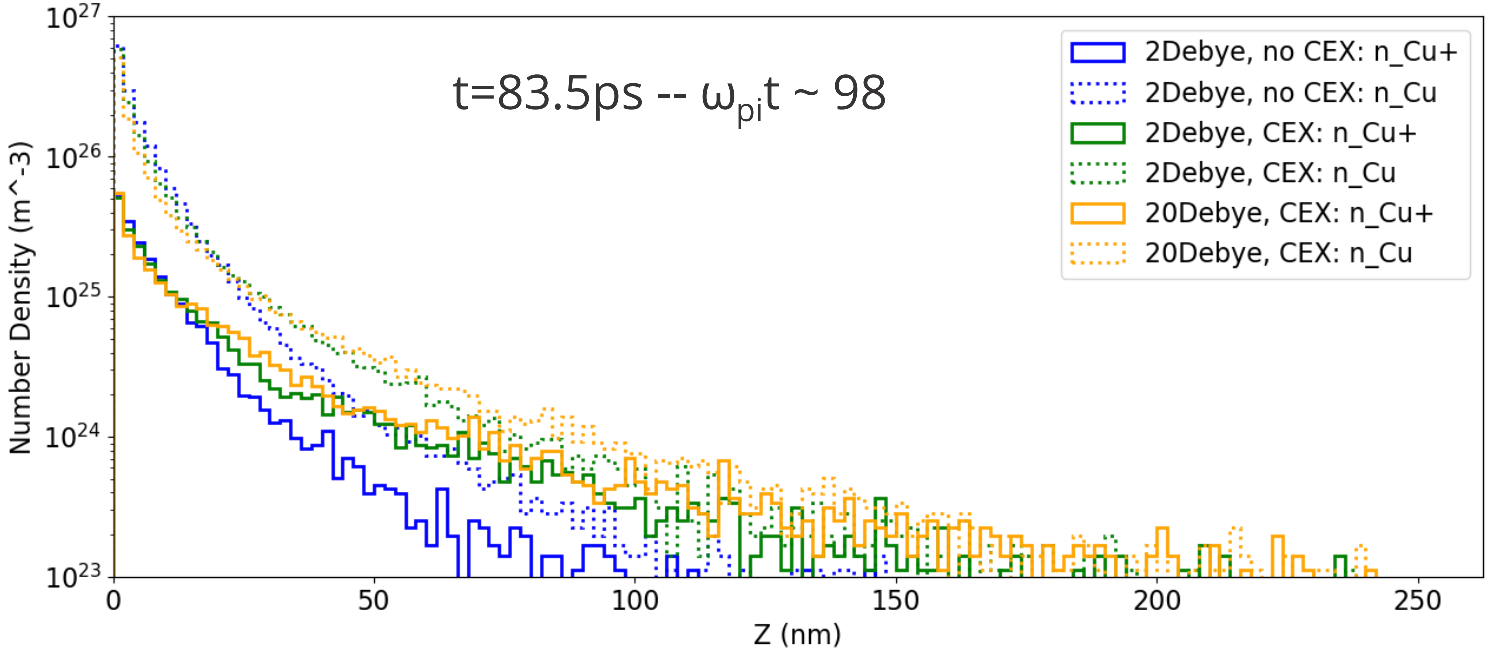


Yushkov, et al., JAP **83**, 10, 5618-5622 (2000)

Results: With Charge Exchange



- Ions are rapidly accelerated via DIH
- Charge exchange results in a fast neutrals and additional DIH
- The neutrals are then ionized after traveling some distance from the cathode spot
- →Faster expansion of the plasma away from the cathode



Conclusions

- The cathode spot plasma in a vacuum arc is very likely a SCP (this is not really "news") and thus we have several physical mechanisms we need to account for that are not present for ideal plasmas. At the very least be aware of:
  - Pressure Ionization (covered by Anders, et al., PSST **1**, 263-270 (1992))
  - Disorder Induced Heating

- DIH can result in much higher ion (and neutral) temperatures than present in the vaporizing cathode material surface temperature

- DIH (especially with charge exchange) can provide some explanation for the observed ion expansion velocity *away* from the cathode

- Modeling Strongly Coupled Plasmas with traditional PIC-DSMC is challenging at best, and should really only be attempted for short timescales.
  - → See M.D. Acciarri *et al*, "When should PIC simulations be applied to atmospheric pressure plasmas? Impact of correlation heating", PSST *under peer review* -- arXiv:2403.00656

- To model component-scales we will need a meso-scale model for the cathode material supply that accounts for SCP effects in the very-near (<1μm) cathode region!