

# Addressing Challenges to Simulating Breakdown and Arc Evolution in Vacuum and Low Pressure Systems

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National Nuclear Security Administration

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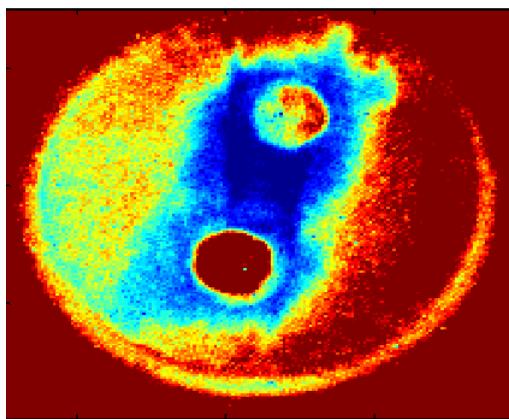
# Introduction

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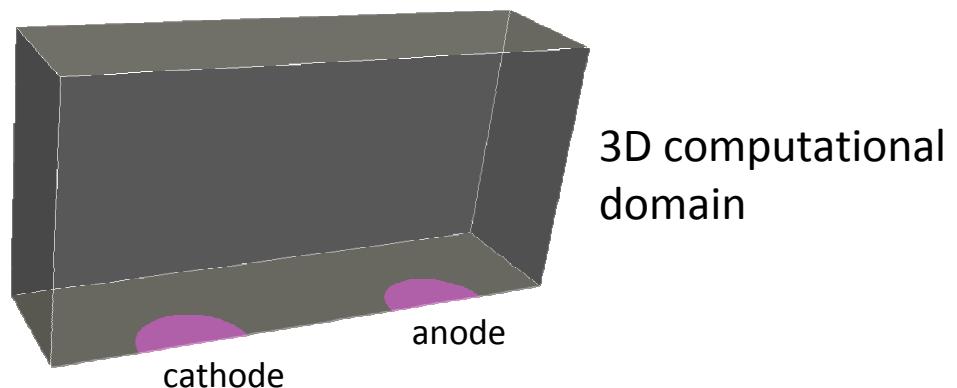
Vacuum arc discharge is a dominant failure mechanism in many vacuum electronic devices. The same basic failure mechanism is also described as high voltage breakdown (HVB), or electrostatic discharge (ESD). There are also numerous devices that operate based on intended discharge of an arc, e.g., plasma switches, spark plugs, and ion sources. In an effort to better understand the initiation process and post-breakdown evolution to a steady arc, we have developed a 3D massively parallel electrostatic low temperature plasma simulation tool, *Aleph*. *Aleph* includes a number of algorithm and model advances to understand the mechanisms and key phases of vacuum arc discharge. Our long-term goal is to provide predictive capability for breakdown in complex 3D vacuum devices in a production environment.

The spatial, temporal, and model capability demands for simulating vacuum arc discharges are enormous. The simulation must evolve from an initial collisionless vacuum (or near vacuum) state through a sputtering phase with surface interaction and low collisionality and ionization, into a growing quasi-neutral plasma with increasing collisionality and ionization, to an explosive growth electron avalanche process, and finally to a steady current-carrying arc plasma. The modeling demands change drastically as each of these phases is encountered. We describe a number of model advances to address these challenges.

# Typical Application



- In vacuum or 4 Torr Ar background
- 1.5 mm inner-to-inner distance
- 0.75 mm diameter electrodes
- Copper electrodes (this picture is Cu-Ti)
- 2 kV drop across electrodes
- $20\Omega$  resistor in series
- Steady conditions around 50V, 100A
- Breakdown time  $\ll 100\text{ns}$
- To meet an ionization mean free path of 1.5 mm at maximum  $\sigma$ ,  $n_i \sim 10^{16} - 10^{17} \text{ #}/\text{cm}^3$



# Description of *Aleph*

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- 1, 2, or 3D Cartesian
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Hybrid PIC + DSMC (PIC-MCC)
- Electrostatics
- Fixed B field
- Solid conduction
- e- approximations (quasi-neutral ambipolar, Boltzmann)
- Dual mesh (Particle and Electrostatics/Output)
- Advanced surface (electrode) physics models
- Collisions, charge exchange, chemistry, excited states, ionization
- Advanced particle weighting methods
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for extending BCs, post-processed quantities, etc.
- Currently utilizing up to 64K processors (>1B elements, >1B particles)

# Description of Aleph

Basic algorithm for one time step of length  $\Delta t$ :

- Given known electrostatic field  $\mathbf{E}^n$  move each particle for  $\frac{\Delta t}{2}$  via:

$$v_i^{n+1/2} = v_i^n + \frac{\Delta t}{2} \left( \frac{q_i}{m_i} \mathbf{E}^n \right)$$

$$x_i^{n+1} = x_i^n + \Delta t v_i^{n+1/2}$$

- Compute intersections (non-trivial in parallel).
- Transfer charges from particle mesh to static mesh.
- Solve for  $\mathbf{E}^{n+1}$

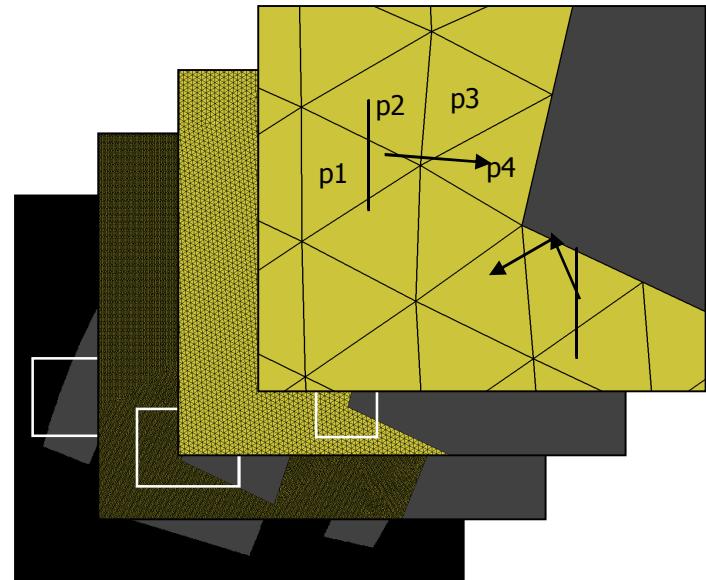
$$\nabla \cdot (\epsilon \nabla V^{n+1}) = -\rho(\mathbf{x}^{n+1})$$

$$\mathbf{E}^{n+1} = -\nabla V^{n+1}$$

- Transfer fields from static mesh to dynamic mesh.
- Update each particle for another  $\frac{\Delta t}{2}$  via:

$$v_i^{n+1} = v_i^{n+1/2} + \frac{\Delta t}{2} \left( \frac{q_i}{m_i} \mathbf{E}^{n+1} \right)$$

- Perform DSMC collisions: sample pairs in element, determine cross section and probability of collision. Roll a digital die, and if they collide, re-distribute energy.
- Perform chemistry: for each reaction, determine expected number of reactions. Sample particles of those types, perform reaction (particle creation/deletion).
- Reweighting particles.
- Compute post-processing and other quantities and write output.
- Rebalance particle mesh if appropriate (variety of determination methods).



# Simulation Requirements

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Temporal scales dominated by plasma electron frequency  $\omega_p$ , CFL, and collision frequency  $\nu_c$  at different phases of breakdown:

$$\Delta t < \min \left( \frac{2}{\omega_p}, \frac{\Delta x}{\sqrt{\frac{m_e \Delta v}{2q_e}}}, \frac{1}{n_n \sigma \bar{\nu}} \right)$$

Spatial scales dominated by Debye length  $\lambda_D$  and collision mean free path  $\lambda_{mfp}$  at different phases of breakdown:

$$\Delta x < \min \left( \lambda_D, \frac{1}{n_n \sigma} \right)$$

Number densities increase from “0” to  $10^{17}$  #/cm<sup>3</sup>. Using same fixed particle weight  $p_{weight}$  isn’t an option.

# Typical Vacuum Arc Progression

A: Initial injection  
of e- (no  
plasma yet)

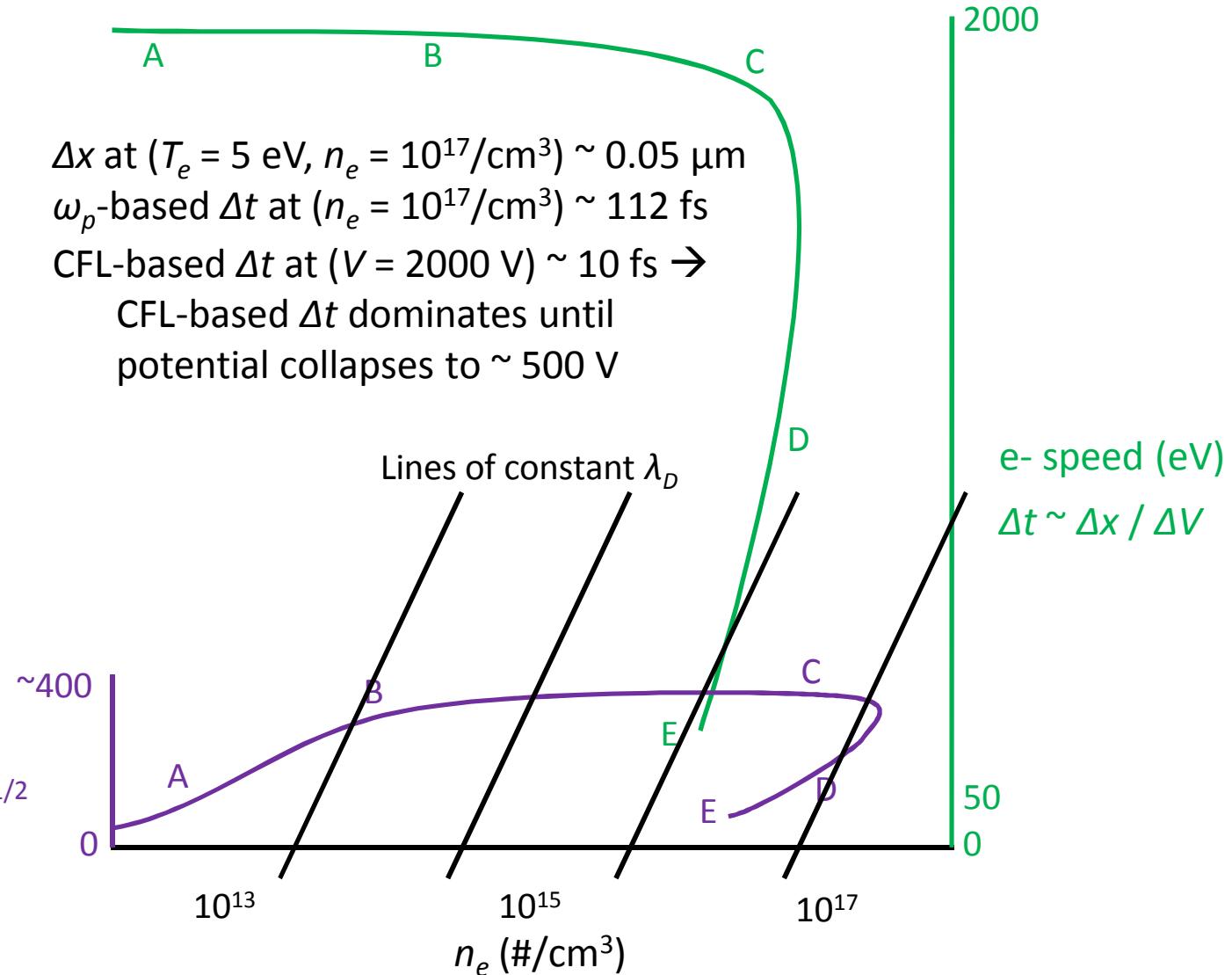
B: Growth of  
cathode plasma

C: Breakdown

D: Relax to steady  
operation ( $\Delta V$   
drops to  $\sim 50$  V)

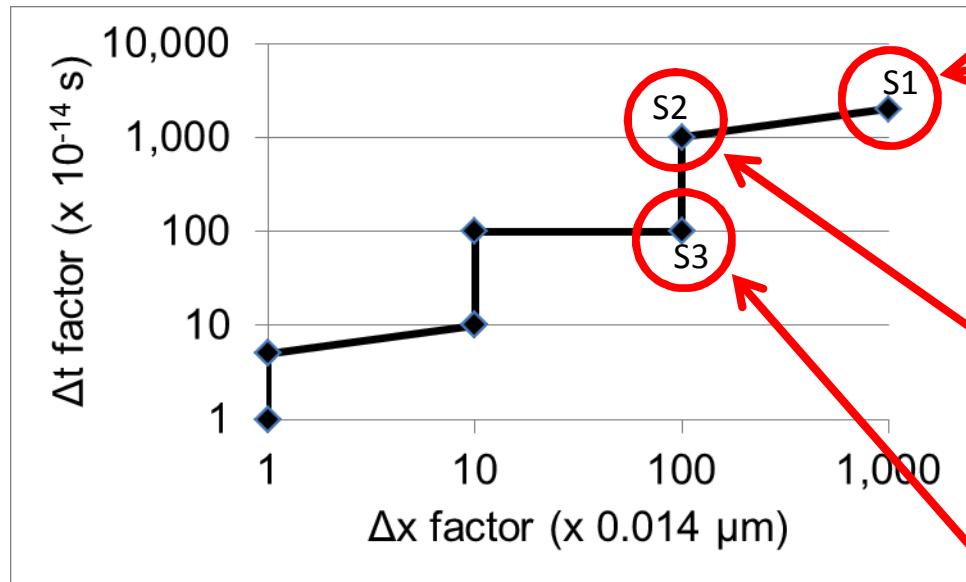
E: Steady  
operation ( $\Delta V$   
 $\sim 50$  V,  $I \sim 100$  A)

$$\begin{aligned} \text{plasma } T_e \text{ (eV)} \\ \Delta x \sim \lambda_D \sim (T_e/n_e)^{1/2} \\ \Delta t \sim \omega_p^{-1} \sim n_e^{-1/2} \end{aligned}$$



# Managing $\Delta x, \Delta t$ : Successive Refinement

Discretely refine in  $(\Delta x, \Delta t)$  by stopping simulation near stability/fidelity limits and perform full particle restart on  $\Delta x$ - and/or  $\Delta t$ -refined simulation. A typical progression to  $(\Delta x, \Delta t) = (0.014 \text{ } \mu\text{m}, 10 \text{ fs})$  looks like:



S1:  $(\Delta x, \Delta t) = (0.014 \text{ mm}, 20 \text{ ps})$ , or 2,000,000 x less work than final solution steps.

... after 160 ns, both  $\lambda_D$  and  $\omega_p$  are being challenged, so move to ...

S2:  $(\Delta x, \Delta t) = (0.0014 \text{ mm}, 10 \text{ ps})$ . ... after another 190 ns, only  $\omega_p$  is being challenged, so move to ...

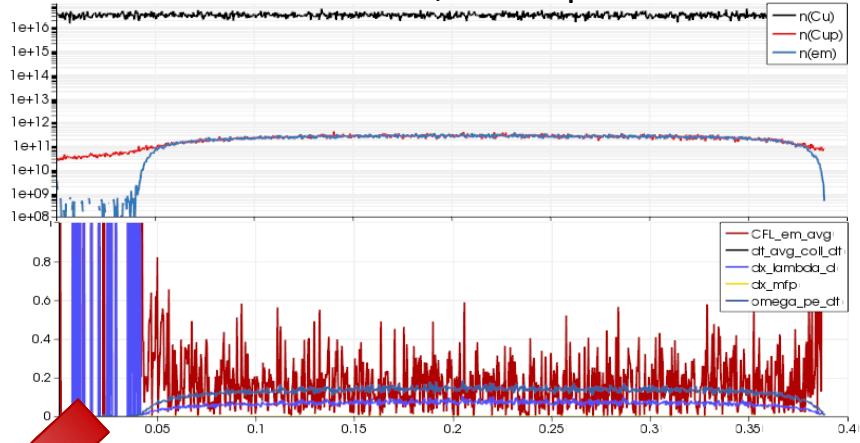
S3:  $(\Delta x, \Delta t) = (0.0014 \text{ mm}, 1 \text{ ps})$ .

... and continue ... (right now this is manual, want to automate termination ...)

Total savings to 1.35  $\mu\text{s}$  (this case) is tremendous, but still need many small steps on small mesh at end...

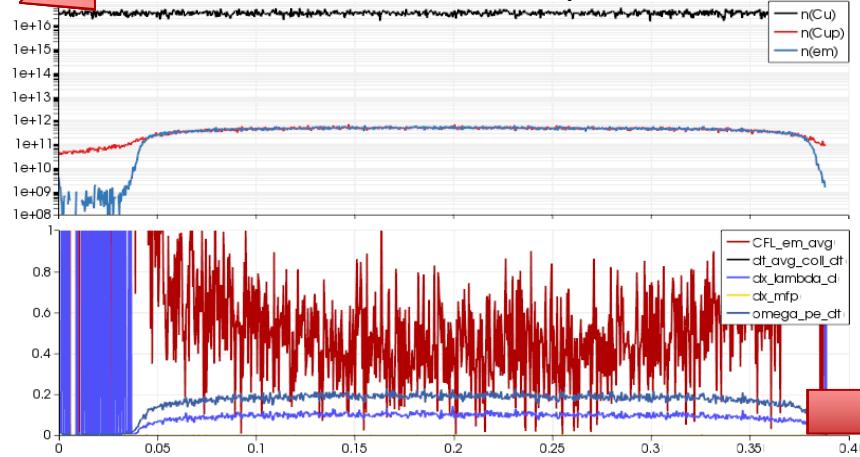
# Managing $\Delta x$ , $\Delta t$ : Successive Refinement

$t = 166 \text{ ns}, \Delta t = 5 \text{ ps}$



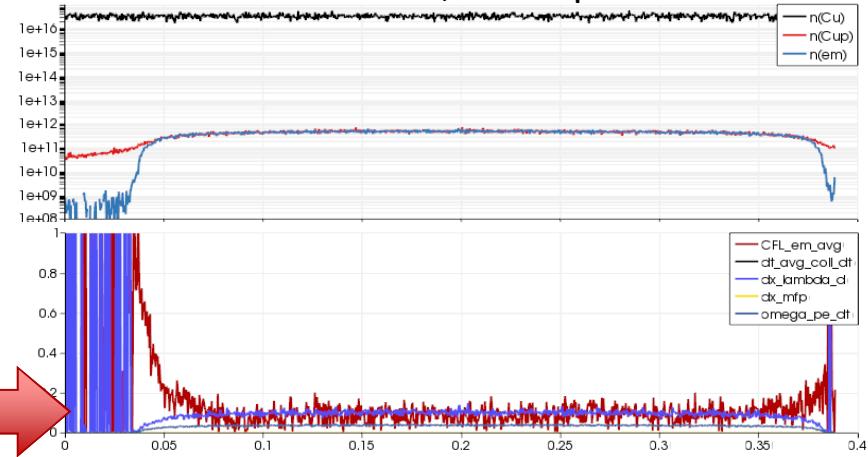
Cathode on left, anode on right,  
120 V drop across 3.88 mm,  
1 Torr background Cu,  
Trickle influx of cold e- ( $10^{10} \text{ #}/\text{cm}^2/\mu\text{s}$ ),  
300 K Cu “sputters” at:  
1% vs. e-,  
100% vs. Cu and Cu+,  
1 eV SEE from Cu+ impact,  
 $\Delta x = 1.38 \mu\text{m}$ , 2812 cells.

$t = 236 \text{ ns}, \Delta t = 5 \text{ ps}$



Growing average e- CFL prompts restarting with smaller  $\Delta t$ .

$t = 236 \text{ ns}, \Delta t = 1 \text{ ps}$



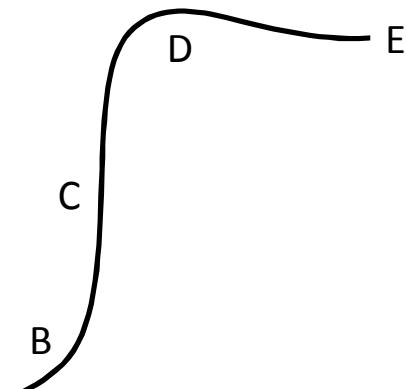
# Managing $\Delta t$ : Quasi-Static Acceleration

$n_e$

To accelerate through Phase A, we take large neutral steps with “equilibration” of ions and electrons, including accounting for proper collision opportunities, e.g.,

A

time



For each of 400  $\Delta t_{neutral}$  steps,  
move neutrals  
neutral-neutral interactions  
for each of 10  $\Delta t_{ion}$  steps,  
move ions  
ion-neutral interactions  
ion-ion interactions  
for each of 10  $\Delta t_{electron}$  steps,  
move electrons  
enhanced electron-\* interactions

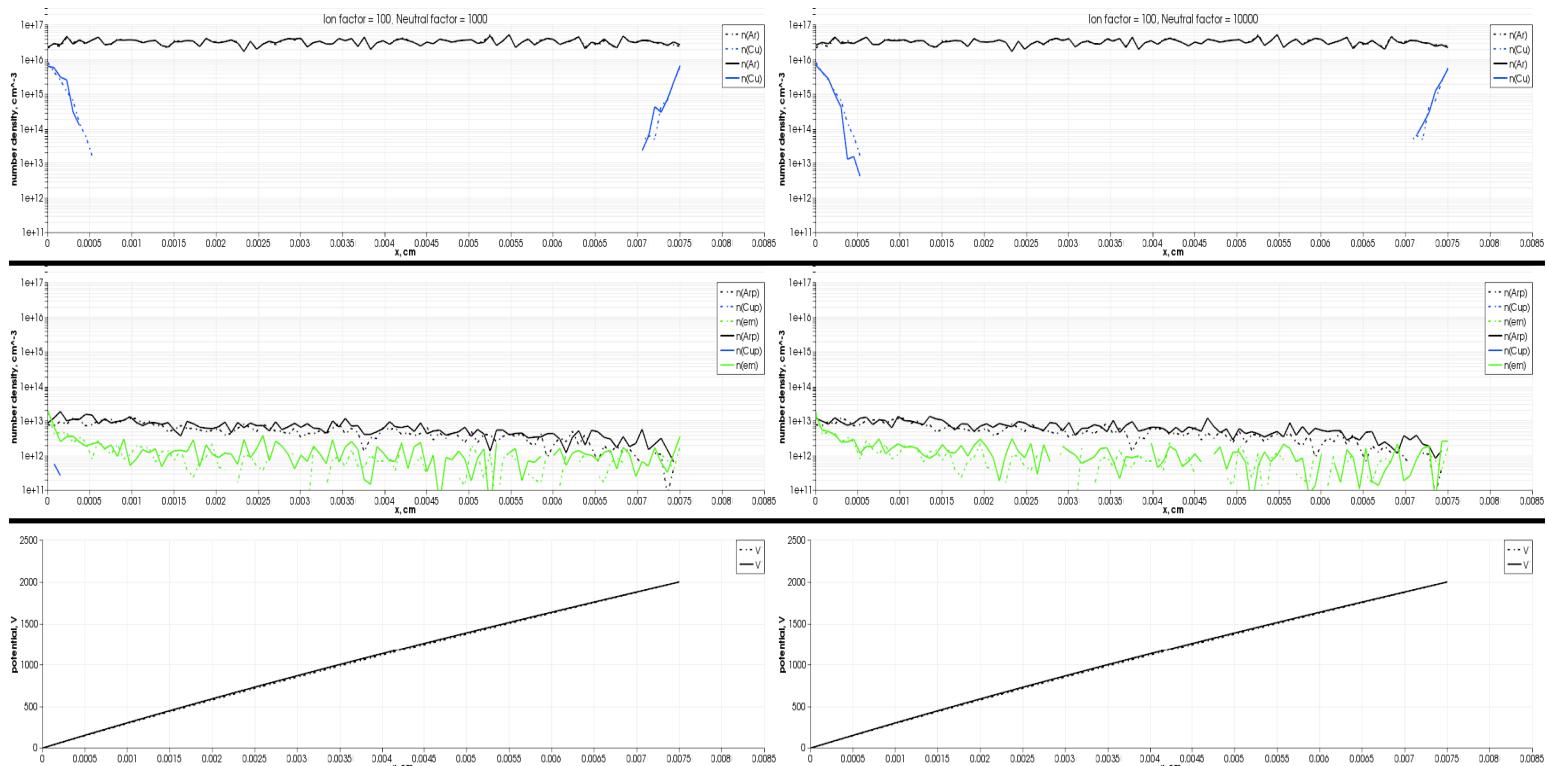
and

For each of 40 10 x  $\Delta t_{neutral}$  steps,  
move neutrals  
neutral-neutral interactions  
for each of 100  $\Delta t_{ion}$  steps,  
move ions  
ion-neutral interactions  
ion-ion interactions  
for each of 10  $\Delta t_{electron}$  steps,  
move electrons  
enhanced electron-\* interactions

# Managing $\Delta t$ : Quasi-Static Acceleration

- Dashed lines are no acceleration.
- Neutral sputtering BC's.
- Cathode on left, anode on right.
- Influx of  $e^-$  from cathode.

$n_n$   
 Ar background  
 Cu from surface



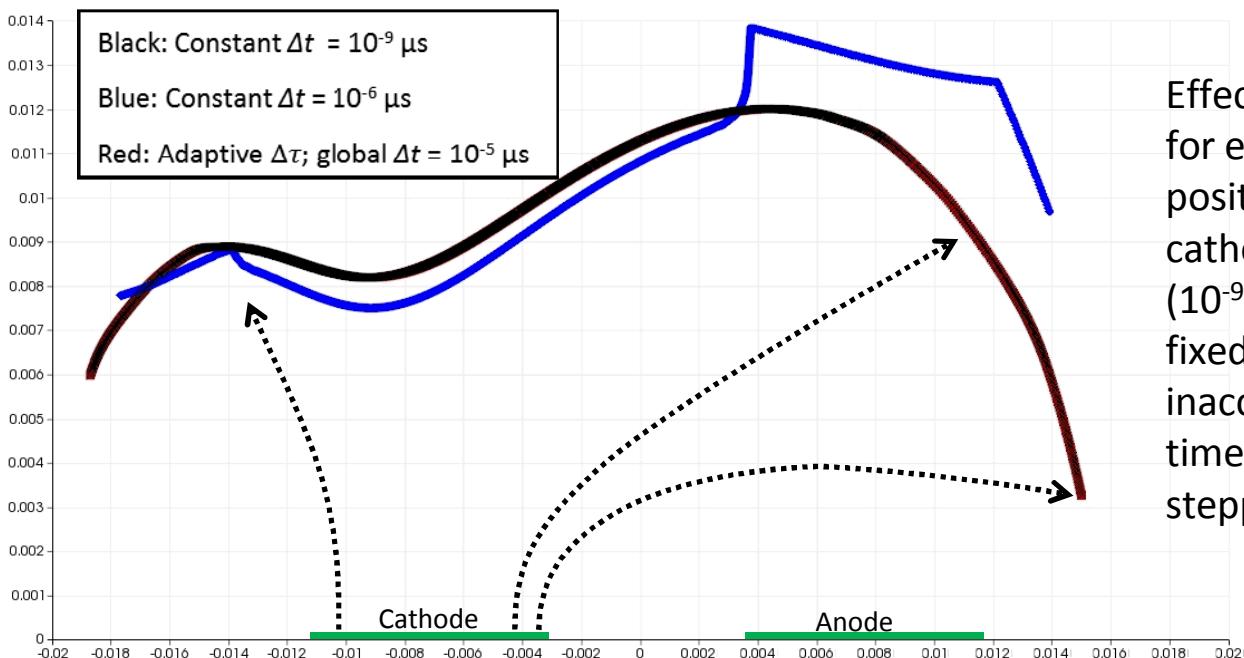
400 neutral steps

10x speed up!

40 (larger) neutral steps

# Managing $\Delta t$ : Explicit Adaptive Time-Stepping

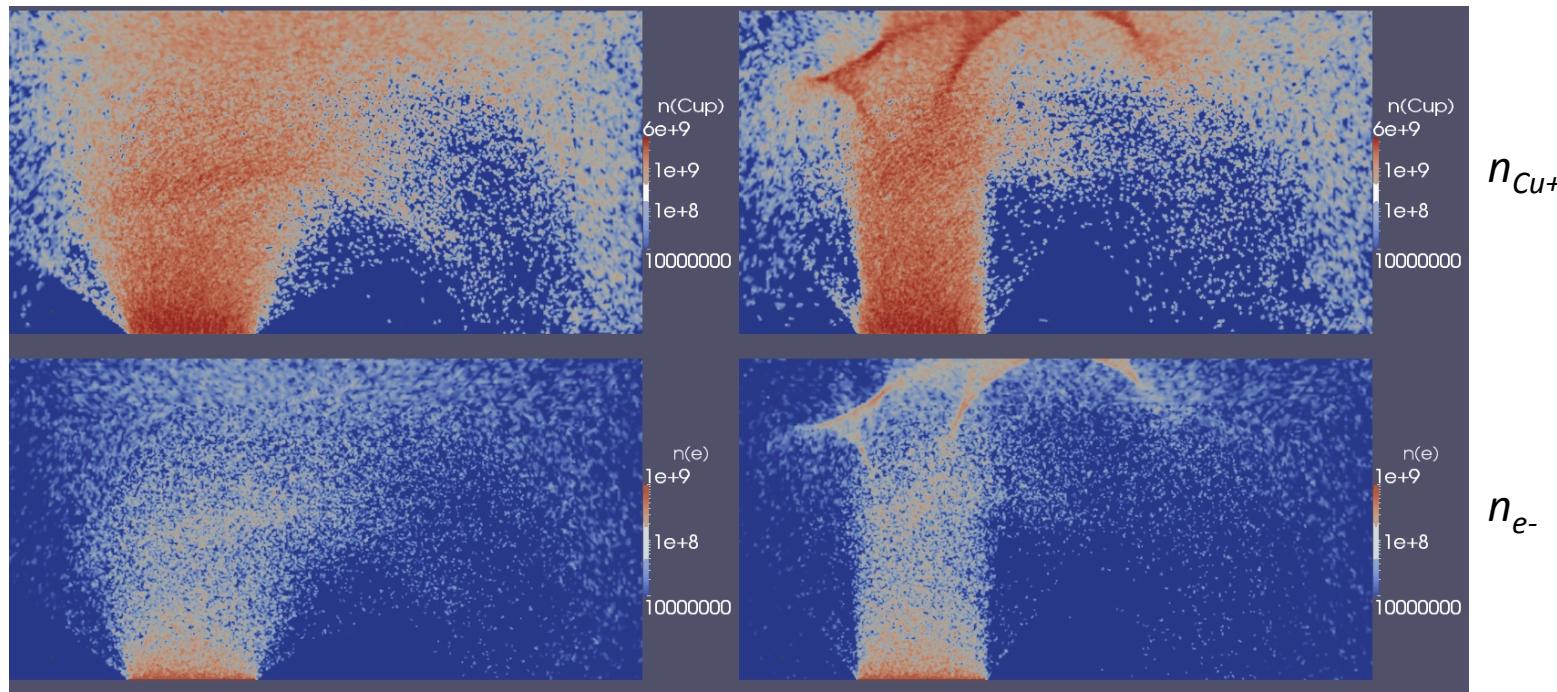
In many initiation processes there is no significant space charge – only the initial applied field is relevant. In these cases we only need to accurately integrate particle trajectories. To mitigate the cost of using the most restrictive CFL-based  $\Delta t$ , we use a large “global” timestep  $\Delta t$  and force individual particles to use smaller adaptive timesteps  $\{\Delta\tau_{i,j}\}$  within the global step ( $\sum_j \Delta\tau_{i,j} = \Delta t$ ).  $\Delta\tau_{i,j}$  is a function of particle velocity  $v_i$ , and the field  $\mathbf{E}$  and field gradient  $\nabla\mathbf{E}$  along the particle trajectory.



Effect of using adaptive time-stepping for e- trajectories. Thick lines are final positions of e- injected along the cathode after  $10^{-5} \mu\text{s}$ . Small fixed time ( $10^{-9} \mu\text{s}$ ) gives correct answer. Larger fixed time ( $10^{-6} \mu\text{s}$ ) is significantly inaccurate. Using an even larger global timestep ( $10^{-5} \mu\text{s}$ ) but adaptive time-stepping again gives correct answer.

# Managing $\Delta t$ : Explicit Adaptive Time-Stepping

2D domain with  $\sim 3$  Torr background neutral gas – consistent with experiments. Small flux of  $e^-$  from cathode, should ionize background gas. Ions can generate electrons at cathode. Run 3 cases out to  $1.5 \times 10^{-3} \mu\text{s}$ . Constant  $\Delta t = 10^{-8} \mu\text{s}$  and adaptive  $\Delta t = 10^{-5} \mu\text{s}$  results overlap.



Constant  $\Delta t = 10^{-8} \mu\text{s}$  runtime 24.6 hours  
 Adaptive  $\Delta t = 10^{-5} \mu\text{s}$  runtime 1.6 hours  
 (solutions essentially identical)

Constant  $\Delta t = 10^{-5} \mu\text{s}$  -- 0.024 hours

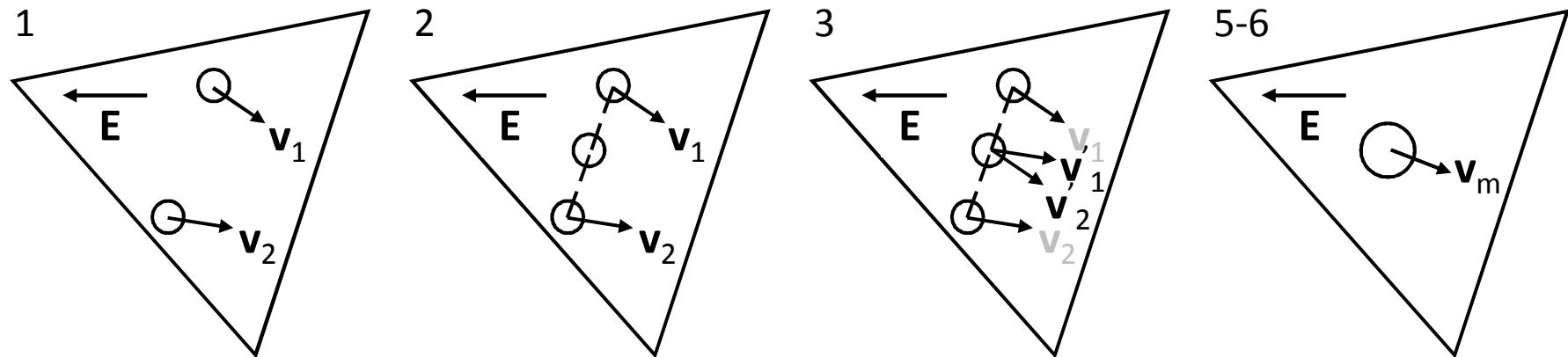
15x speed up!

# Managing $p_{weight}$ : Particle Merging

We assume the discrete particle sample is the best representation of the “true” particle distribution. This drives us to use particle-only merge methods.

1. Choose a random pair of species  $S$  particles in the cell.
2. Compute center of mass position.
3. Compute modified velocities at the center of mass by accounting for displacement in the potential field.
4. If velocities are “too different,” reject pair and repeat 1-3.
5. Calculate average velocity, conserving momentum.
6. Adjust (to target) weight and record difference in kinetic energy.

Repeat 1-6 until target number or limiter is met.



# Managing $p_{weight}$ : Particle Merging

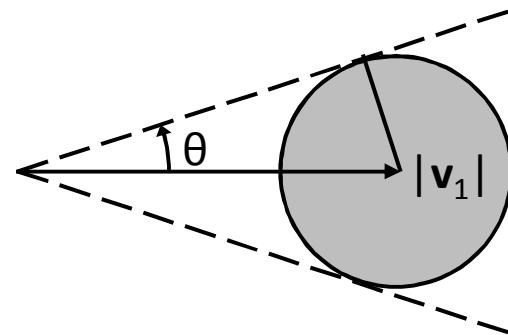
Only approve merge pairs that are close in both position and velocity.

- The spatial bin is the element, approves any pair.
- The velocity bin has many options. We use velocity interval, since it is easy to compute and adjusts based on local temperature.

Much faster to sort particles in element by speed, then choose one at random and check neighbors for valid merge partner.

Velocity Sphere

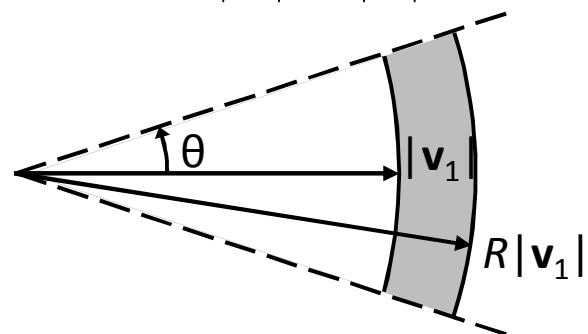
$$|\mathbf{v}_2 - \mathbf{v}_1| < |\mathbf{v}_1| \sin(\theta)$$



Velocity Proportion

$$\mathbf{v}_1 \cdot \mathbf{v}_2 > |\mathbf{v}_1| |\mathbf{v}_2| \cos(\theta)$$

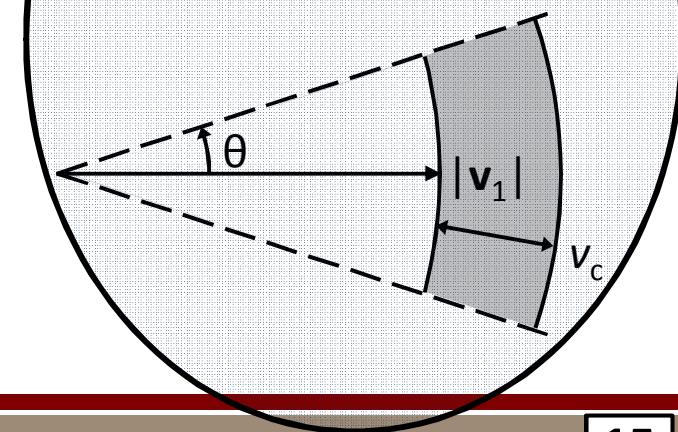
$$|\mathbf{v}_2| < R |\mathbf{v}_1|$$



Velocity Interval

$$\mathbf{v}_1 \cdot \mathbf{v}_2 > |\mathbf{v}_1| |\mathbf{v}_2| \cos(\theta)$$

$$|\mathbf{v}_2| - |\mathbf{v}_1| < v_c = \alpha \sqrt{k_B T / m}$$



# Managing $p_{weight}$ : Particle Merging

Example of using dynamic particle weighting is a growing Xenon sheath.

## Injection

$$V = 5 \text{ V}$$

$$n_{Xe^+} = n_e = 10^{10} \text{ #/cm}^3 \text{ to } 10^{12} \text{ #/cm}^3 \text{ over 20 ion transit times}$$

$$v_D = 3 \text{ cm/}\mu\text{s}$$

$$T_e = 1 \text{ eV}$$

$$T_{Xe^+} = 300 \text{ K}$$

## Side walls

$$dV/dn = 0$$

specular

## Wall

$$V = 0 \text{ V}$$

$$\Delta x \{ \text{[yellow bar]} \}$$

$(10 \text{ to } 100)\lambda_D = 300\Delta x$

## Bulk plasma parameters

$$v_{Bohm} = 0.086 \text{ cm/}\mu\text{s}$$

$$\lambda_D = 7.4 \times 10^{-3} \text{ cm to } 7.4 \times 10^{-4} \text{ cm}$$

$$\Delta x = 2.5 \times 10^{-4} \text{ cm}$$

$$\Delta t = 20 \text{ ps}$$

$$\lambda_D / \Delta x = 30 \text{ to } 3$$

$$\omega_p \cdot \Delta t = 0.11 \text{ to } 1.1$$

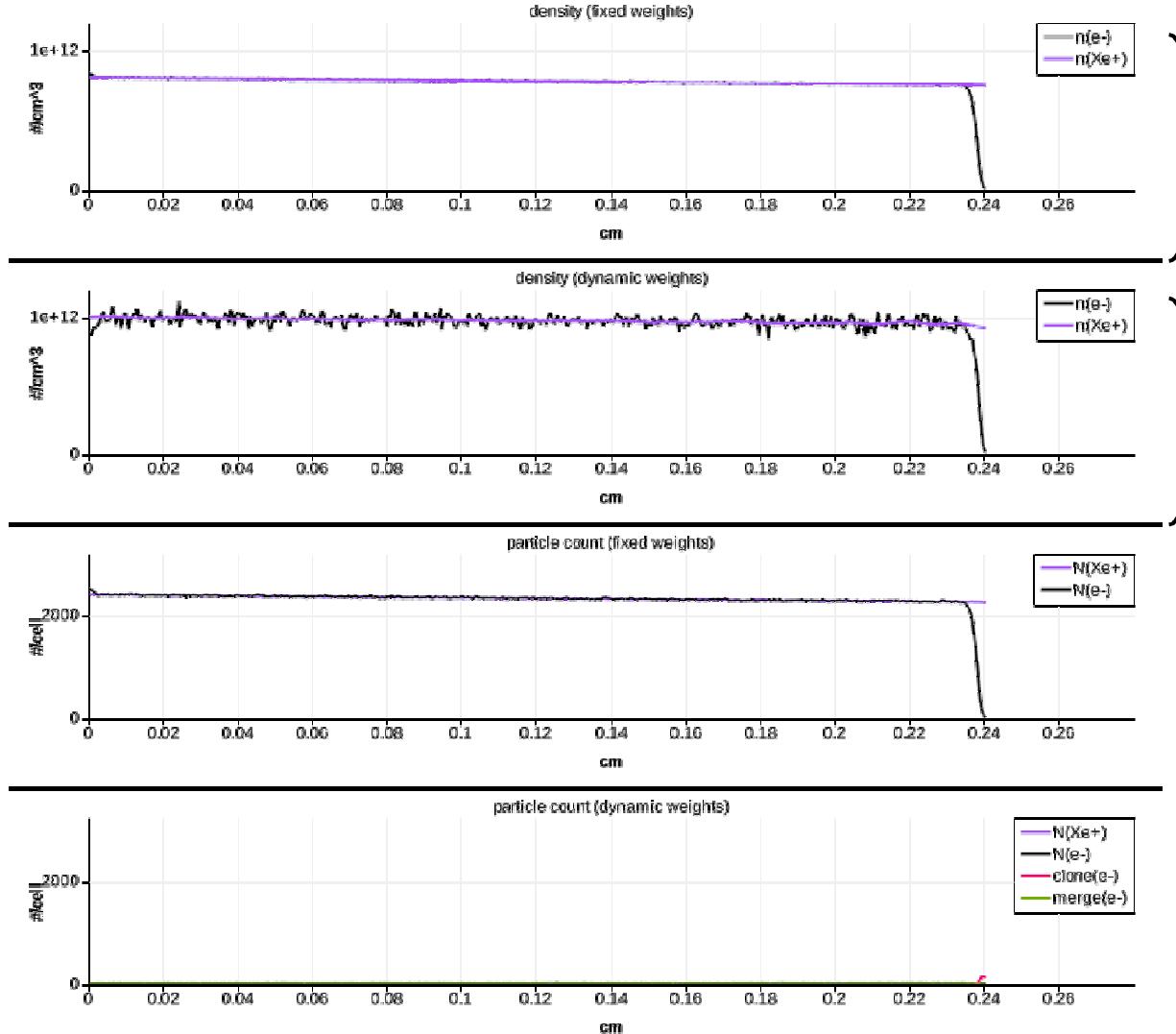
Two solutions:

- Fixed particle weight
- Dynamic particle weight (merging)

Small weight vs. large weight vs.  
requirements...

# Managing $p_{weight}$ : Particle Merging

Solution at high end,  $n_{Xe^+} = 10^{12} \text{ #}/\text{cm}^3$ .



Runtime 147371 secs

# particles = 11M

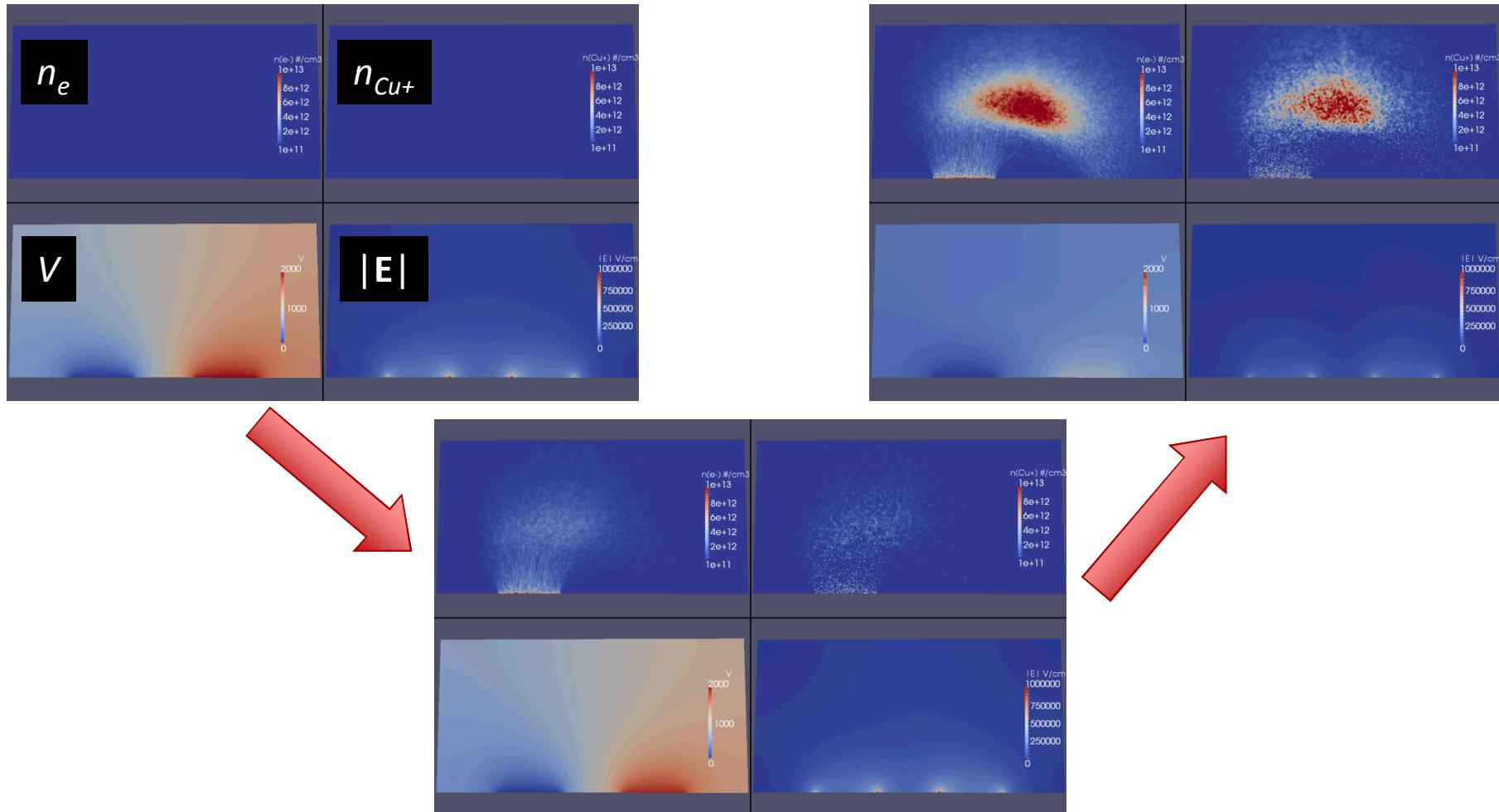
Runtime 7435 secs

# particles = 150K

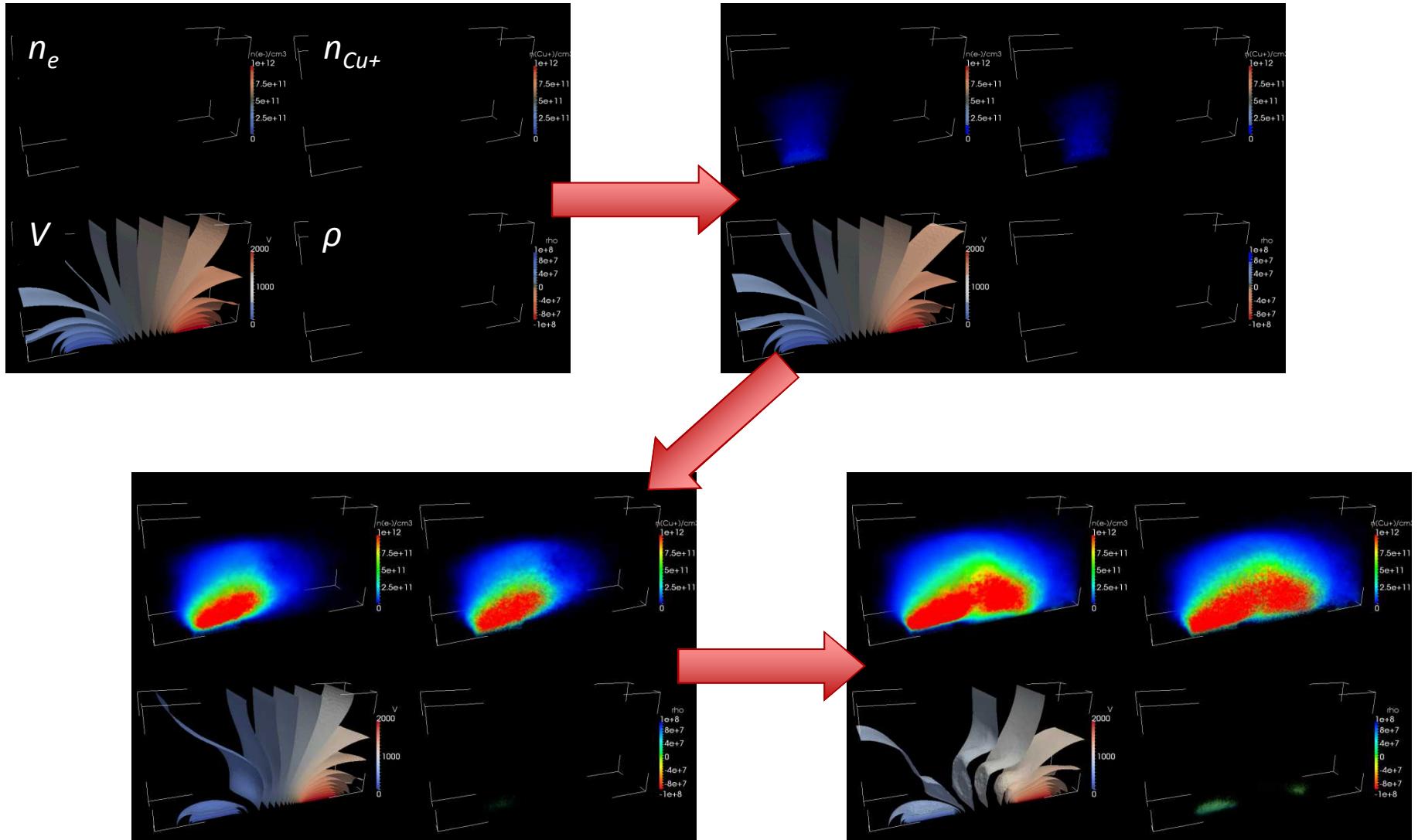
20x speed up!

# 3D Simulation

A  $1/10^{\text{th}}$  reduced size 3D simulation was performed. It is still under-resolved in  $\Delta x$  resulting in “correct” solution blow-up when  $\lambda_D \sim \Delta x$  (not shown here).



# 3D Simulation



# Conclusions & Other Pursuits

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Simulating vacuum arcs is *extremely* expensive with vanilla PIC/DSMC methods. We are concurrently pursuing better physics models (not presented here) and more efficient algorithms with acceptable approximation errors to address these extreme simulation challenges.

Other areas we are pursuing / have pursued include:

- Implicit kinetic methods
- Oct-tree DSMC collision mesh separate from PIC mesh
- Particle-Particle Particle-Mesh ( $P^3M$ ) methods
- Dynamic load balancing and other scaling improvements
- Stochastic cathode hot spot models
- Photoionization, photoemission

For more information, contact [mmhopki@sandia.gov](mailto:mmhopki@sandia.gov).

# Upcoming Related Conference

**Mechanisms of Vacuum Arcs-4**





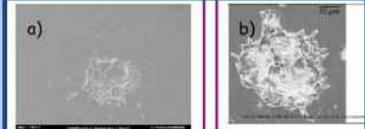
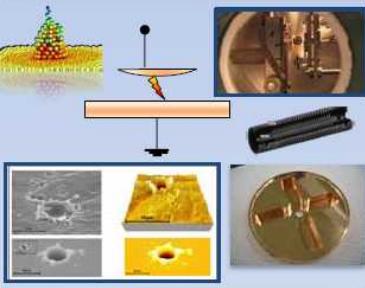
5-7 November, 2013

The workshops aims to combine the efforts of researchers in the different fields to understand the mechanisms underlying the highly intriguing phenomenon of electrical breakdown.

This workshop will cover **rf** and **dc** types of electrical breakdowns, both theoretically and experimentally. A one-day satellite school "**Introduction to rf-acceleration**" will be organized on the Monday, preceding the workshop.

**Topics**

1. **Experiments:** vacuum arcs, dc spark systems, *rf*-accelerating structures, materials, diagnostics, techniques and technologies for high gradients, arcing in fusion devices.
2. **Theory and simulations:** Surface modification under electric and electromagnetic fields, dislocation activity, PIC plasma simulations, plasma-wall interactions, surface damage and other.
3. **Applications:** Particle accelerators, fusion devices, satellites and industrial.


**Venue**

The workshop will be held in the spectacular mountain resort area Chamonix (about 1,5 hour ride from the Geneva airport with the direct shuttle).

**Organizers:**

Walter Wuensch, Sergio Calatroni  
CERN, Switzerland

Flyura Djurabekova  
HIP, University of Helsinki, Finland

Matthew Hopkins  
Sandia National Laboratories, USA

**Contact:**  
[mmhopki@sandia.gov](mailto:mmhopki@sandia.gov)  
 Also a 1-day class on  
*rf* accelerator basics!

<http://indico.cern.ch/conferenceDisplay.py?confId=246618>