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Ingredients for 3D Vacuum Arc Discharge Simulation

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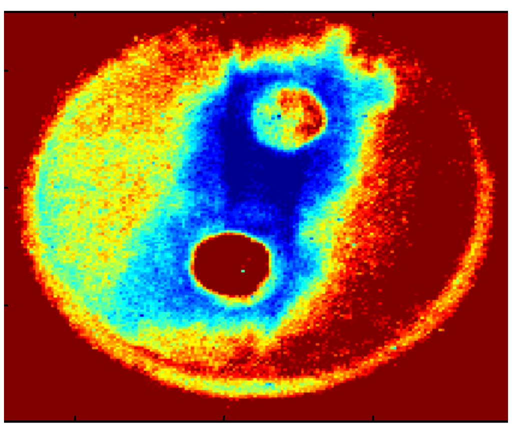
Physical System



In vacuum

1.5 mm inner-to-inner distance

0.75 mm diameter electrodes

Copper electrodes (this picture is Cu-Ti)

2 kV drop across electrodes

20Ω resistor in series

Steady conditions around 50V, 100A

Breakdown time << 100ns

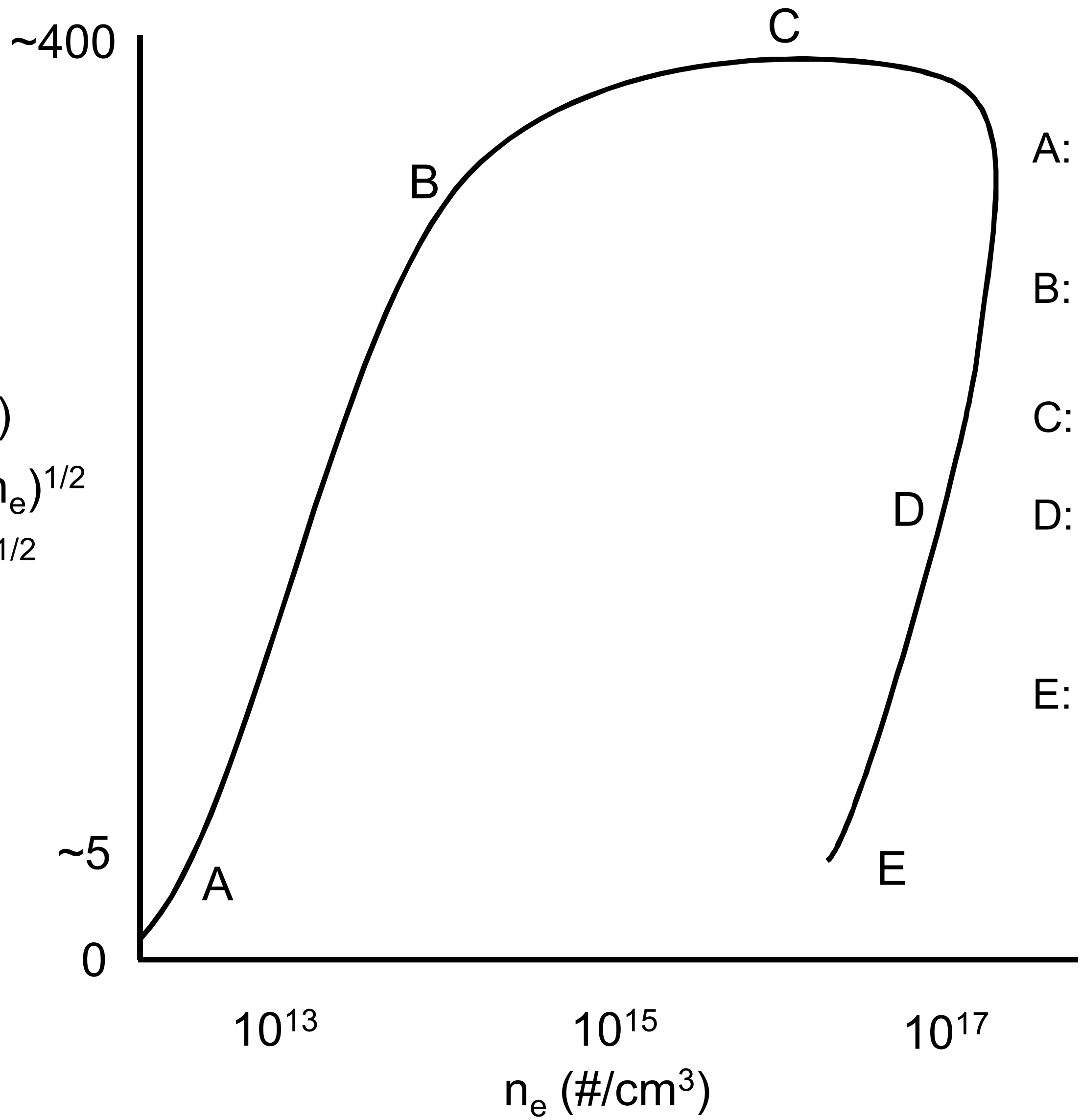
To meet an ionization mean free path of 1.5 mm at maximum σ, $n_i \sim 10^{16} - 10^{17}$ #/cm^3

Build-up, Breakdown, and Evolution Path

plasma T_e (eV)

$\Delta x \sim \lambda_D \sim (T_e/n_e)^{1/2}$

$\Delta t \sim \omega_p^{-1} \sim n_e^{-1/2}$



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

B: Growth of cathode plasma

C: Breakdown

D: Relax to steady operation (ΔV drops to ~50V)

E: Steady operation (ΔV ~50V, I ~100A)

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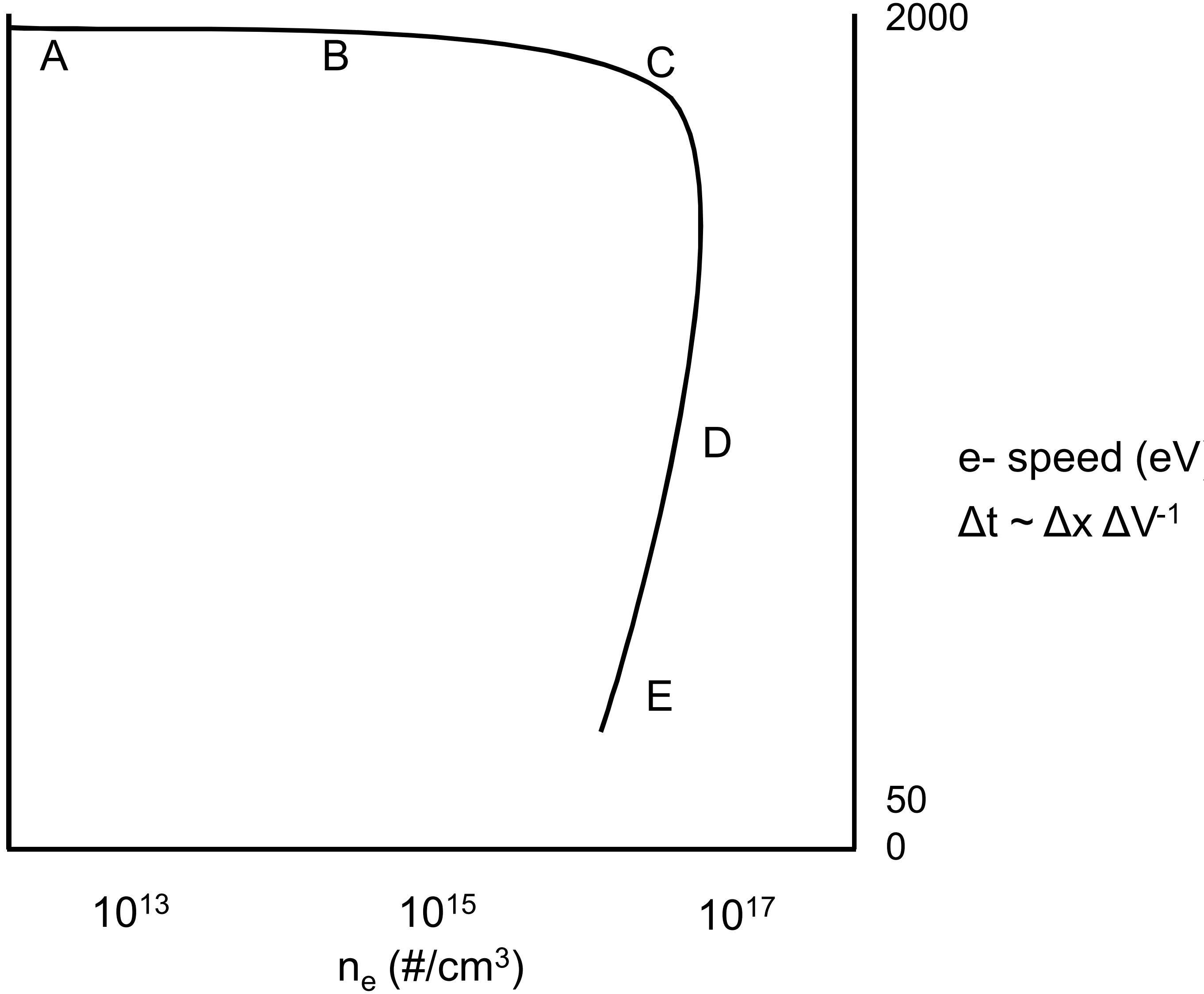

Approximate Simulation Demands

Approximate smallest Δx at (Te = 10 eV, $n_e = 10^{16}$) ~ 0.25 μm
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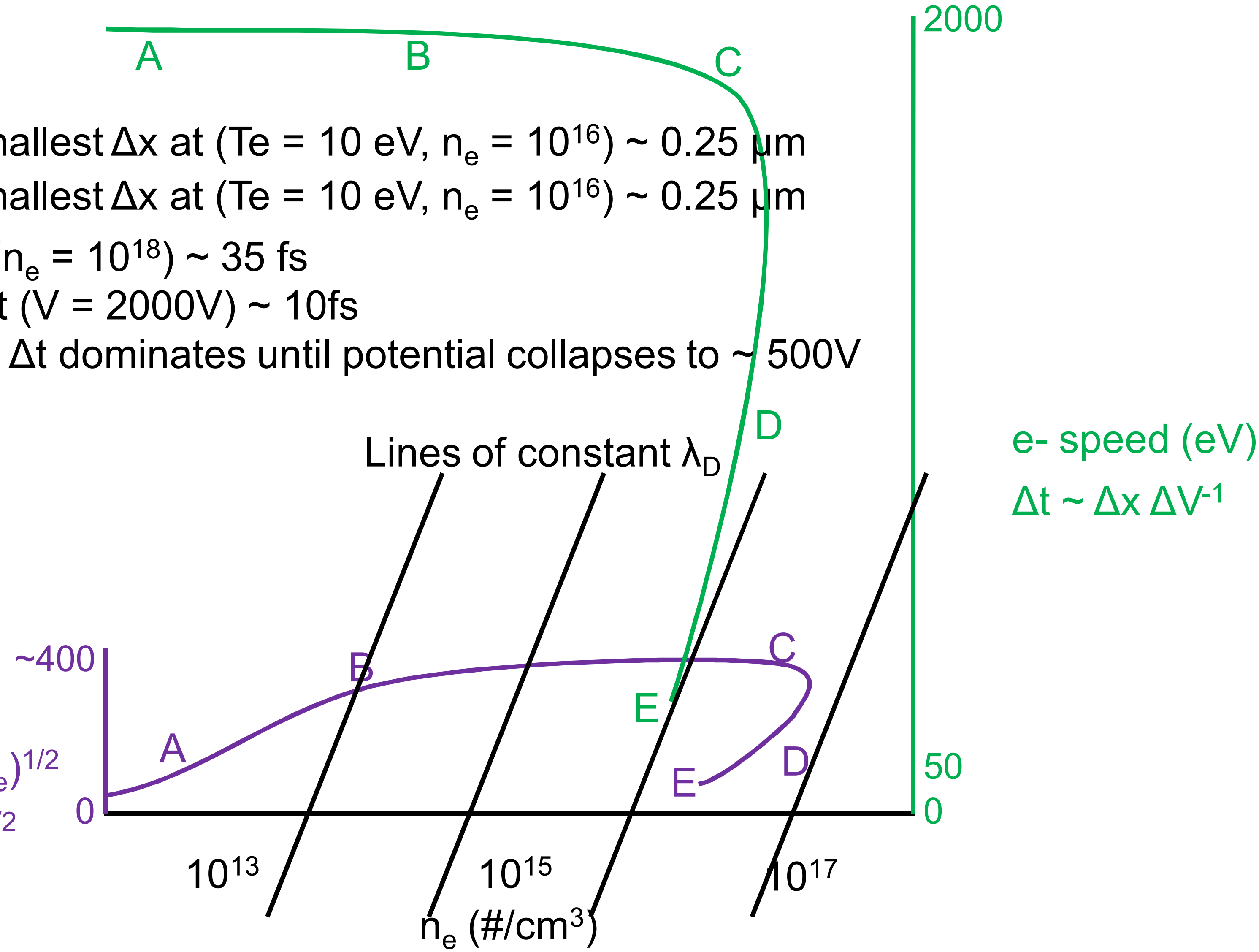
ω_p-based Δt at ($n_e = 10^{18}$) ~ 35 fs
CFL-based Δt at (V = 2000V) ~ 10fs
→ CFL-based Δt dominates until potential collapses to ~ 500V



Approximate Simulation Demands

$4\ mm \times 1.5\ mm \times 2\ mm = 24\ mm^3$

\+ $vol_E = 0.1\ \mu m^3$

~ 100B elements

~ 10 ns breakdown time at $\Delta t = 10$ fs

\+ ~ 100 ns evolution time at $\Delta t = 100$ fs

2M timesteps

3 x (~10) particles/cell in breakdown region

\+ ~ 5% of cells in breakdown region

~ 150B particles

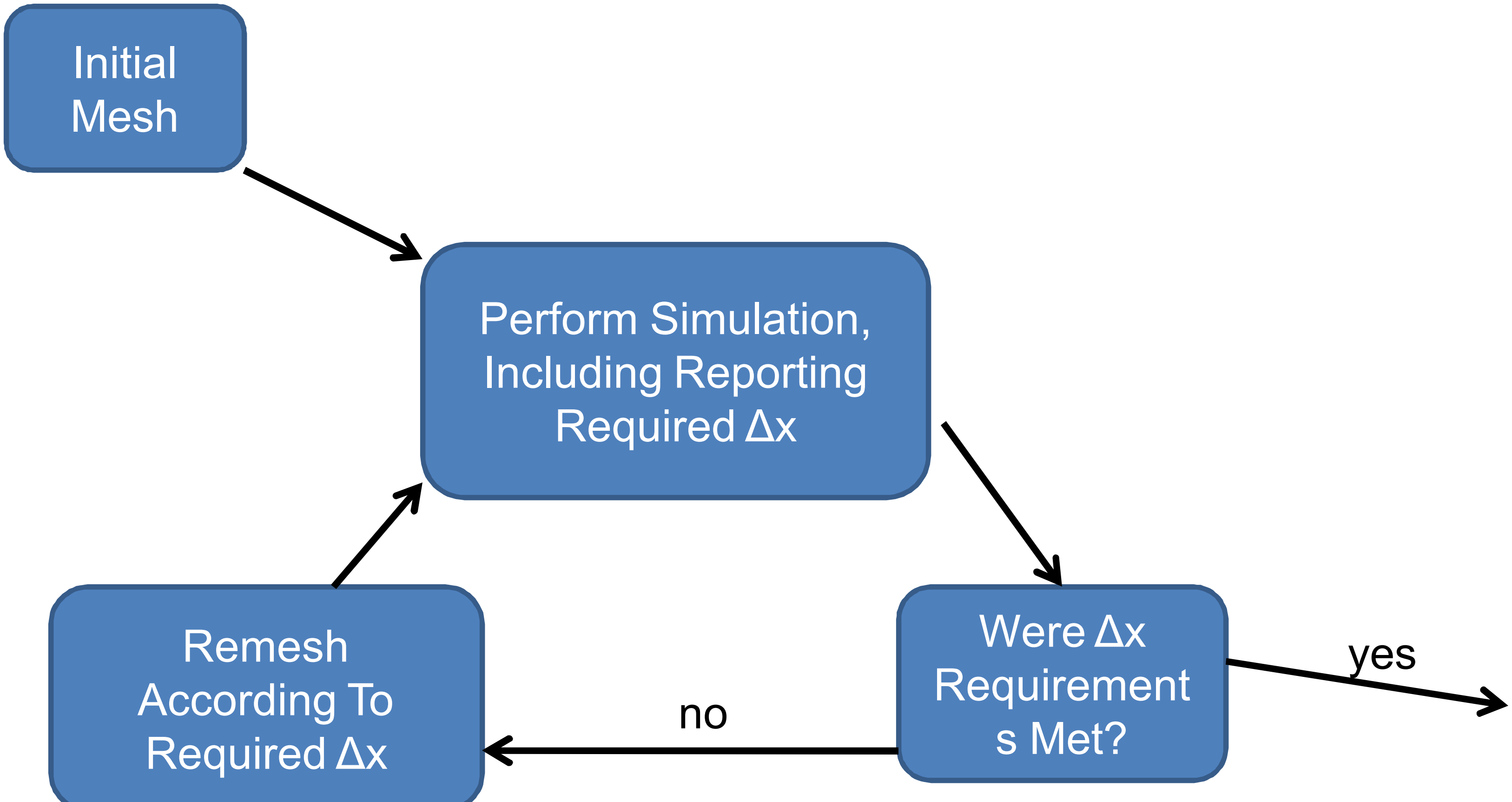
Performing the build-up, breakdown, and evolution of vacuum arc discharge in 3D is extremely challenging! We are employing and/or developing a number of mitigation technologies to address the challenges. What follows is a number of these ingredients for our overall 3D vacuum arc discharge modeling work. Some are fully developed and in use; others are in progress...

Ingredient: Unstructured Mesh

Need to use very small cells only where they are necessary – Cartesian meshes are problematic. Real arcs have complicated geometry requiring cut cells and/or stairstepping, etc. Currently working on getting large unstructured meshes – have 1B cells, need more

Ingredient: Sizing Cells As Large As Possible

“Poor Man’s” Automatic Mesh Refinement procedure:



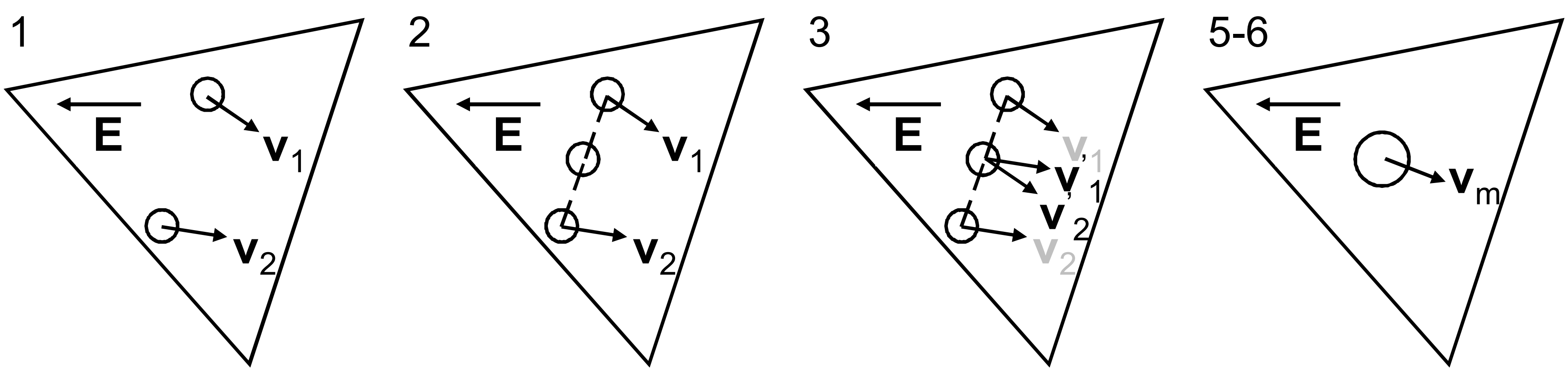
Ingredient: Dynamic Particle Weighting

To manage the increase in number density over many orders of magnitude (6 or 7 minimum), we have developed multiple approaches to merging particles. In particular, we have a *separate weight for every computational particle*, and a *target weight for each cell* that evolves in time.

Merge Procedure:

1. Choose a random pair of *S* particles.
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.

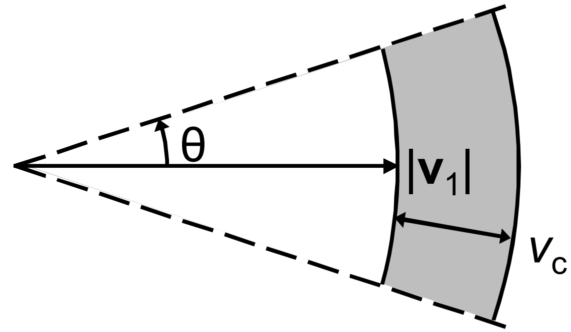


Velocity Phase Space Acceptance Criteria:

Velocity Interval

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

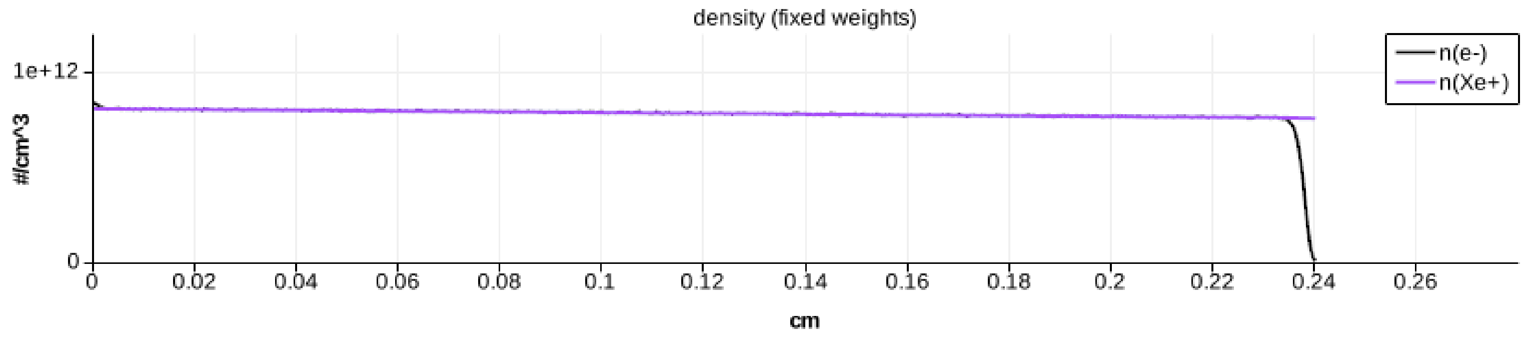
$$|\mathbf{v}_2| - |\mathbf{v}_1| < v_c = \alpha\sqrt{k_B T / m}$$



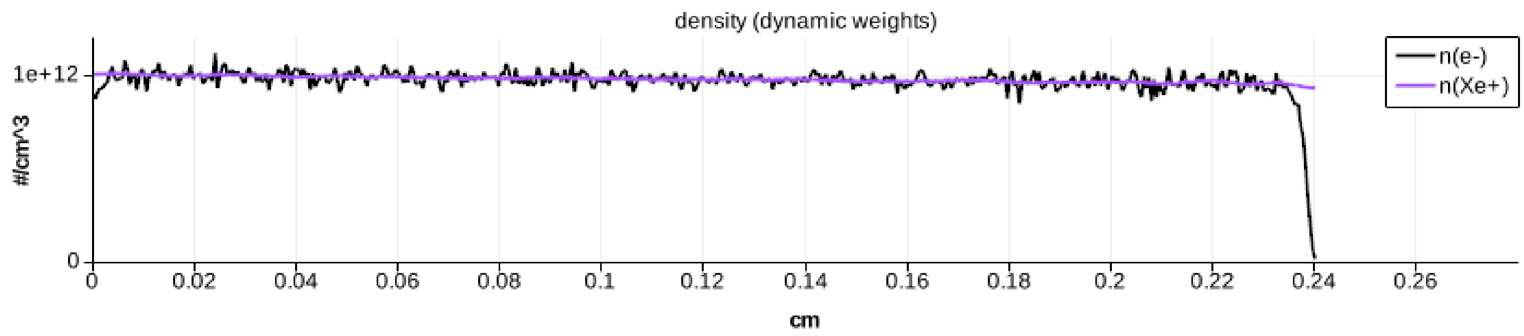
Successful test problems:

- Box of plasma
- Neutral Injection (constant or increasing flux)
- Sheaths (constant or growing density)
- 1D arcs (similar to work here)

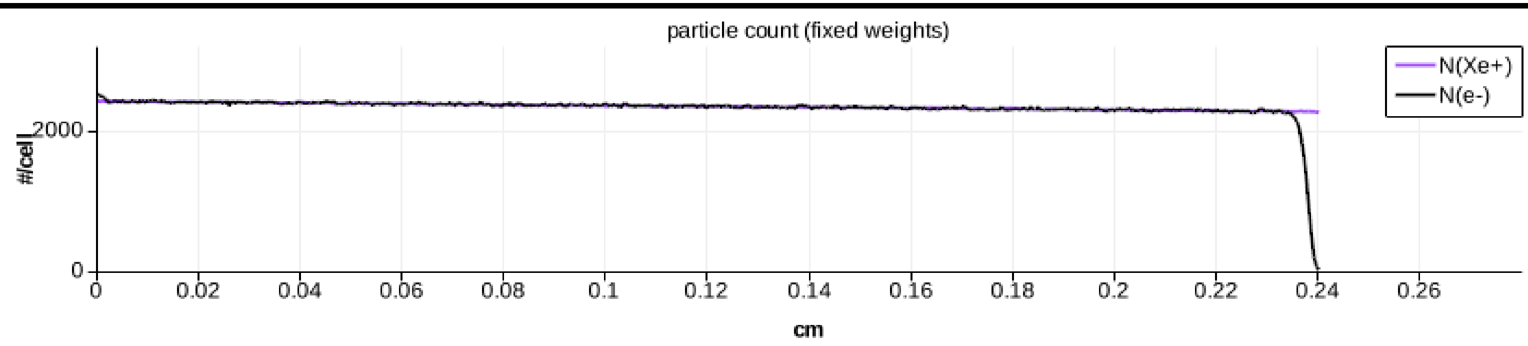
Next slide is “Xe Sheath With Growing Density”



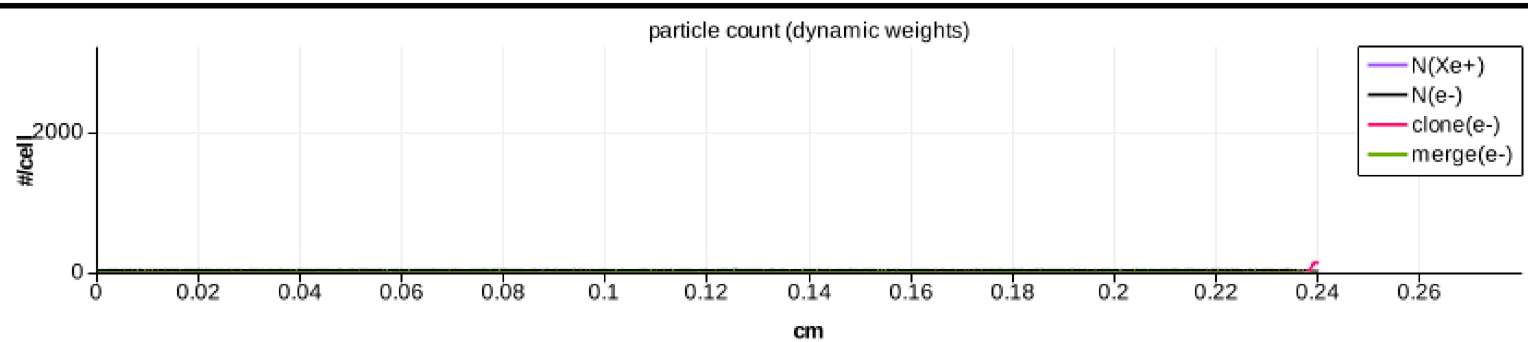
147371s,
= 11M



7435s,
= 150k



95% runtime redu



Ingredient: Multiple Time Scales

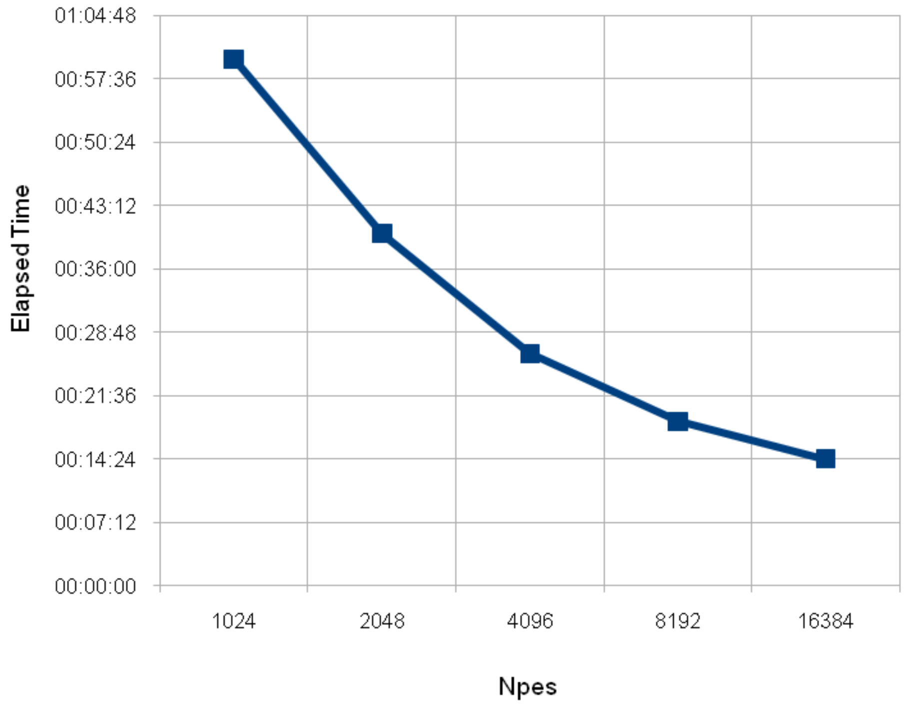
We plan on implementing either fixed regions with separate Δt, or advanced particle moves (similar to event driven methods).

Ingredient: Model Switching

At some point in arc evolution electrons no longer need to be modeled as particles everywhere. By employing other electron transport models we will loosen some length and time constraints. Candidates currently include: implicit kinetic methods, Boltzmann electrons, and quasi-neutral ambipolar approximations. A difficult challenge is to decide when, where, and how to switch models (say, from full kinetic → implicit kinetic → Boltzmann → ambipolar).

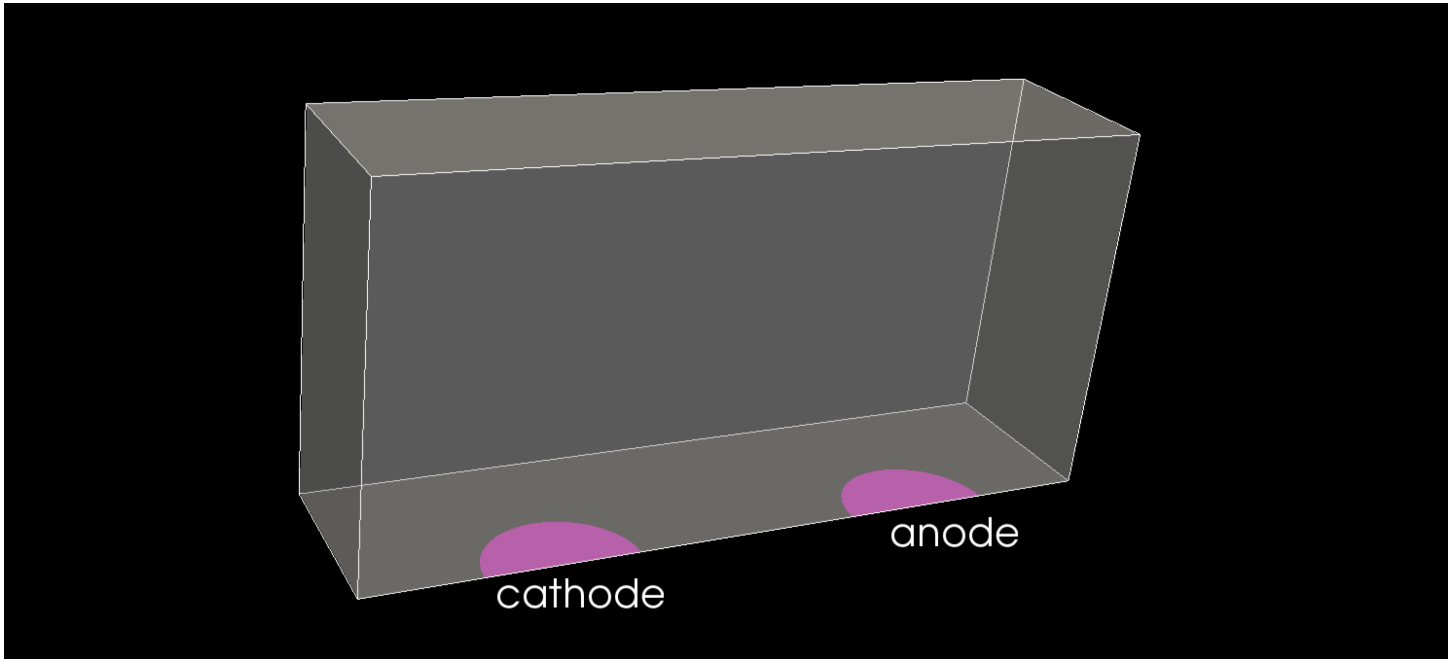
Ingredient: High Performance Computing And Efficient Scaling

We are currently communications and data movement limited at large scales, but have successfully scale to 10K's of cores:



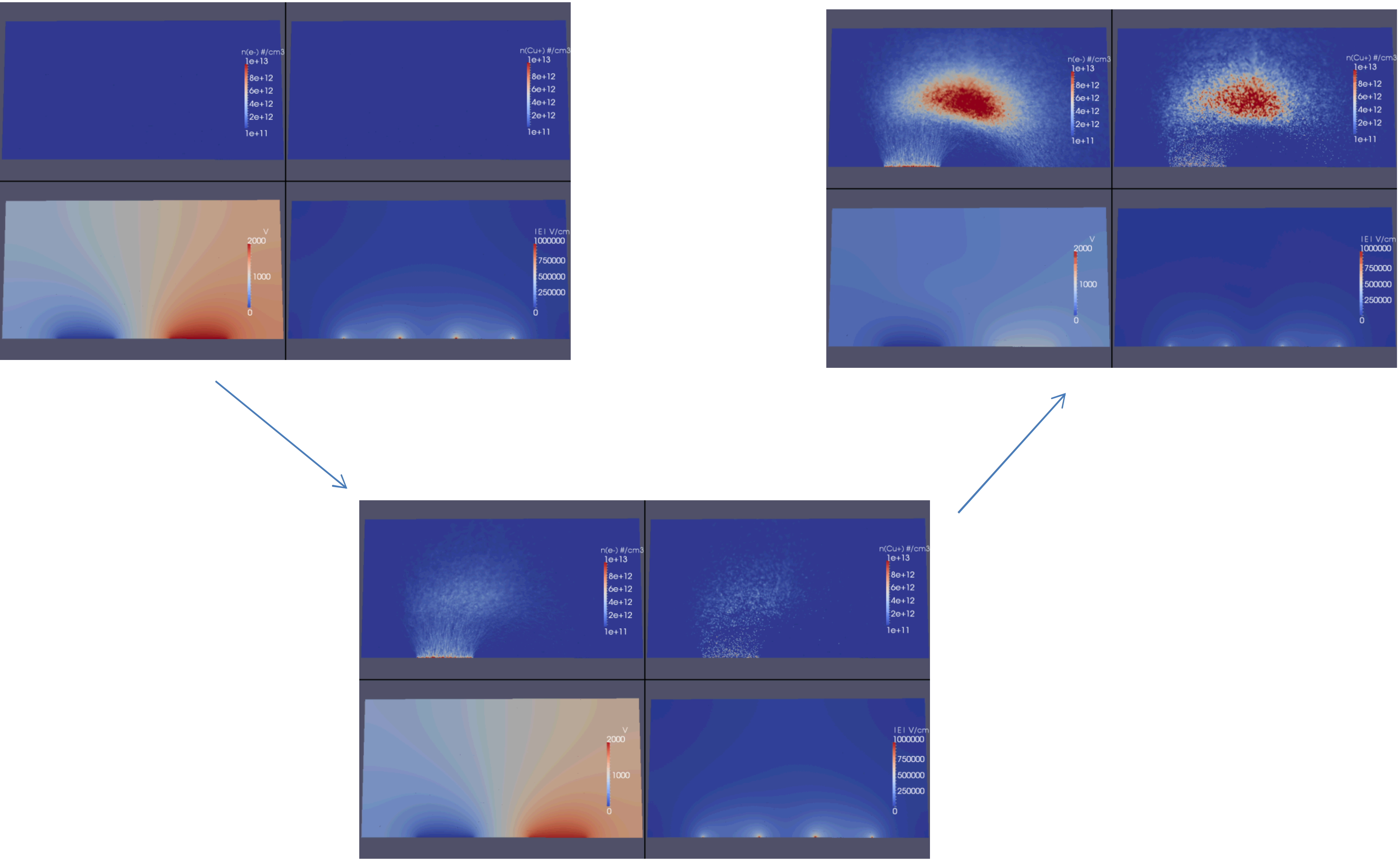
Strong scaling for 16M cell problem on Cielo.

Recent Computational Model



Caveats:

- Smaller domain size (1/10th)
- Cells are too large, leading to correct blow-up
- Not vacuum, background = 10^{18} Cu/cm^3


n(e-) #/cm3
1e+13
8e+12
6e+12
4e+12
2e+12
1e+11
n(Cu+) #/cm3
1e+13
8e+12
6e+12
4e+12
2e+12
1e+11
V
2000
1000
0
IEI V/cm
1000000
750000
500000
250000
0
n(e-) #/cm3
1e+13
8e+12
6e+12
4e+12
2e+12
1e+11
n(Cu+) #/cm3
1e+13
8e+12
6e+12
4e+12
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V
2000
1000
0
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1000000
750000
500000
250000
0
n(e-) #/cm3
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n(Cu+) #/cm3
1e+13
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V
2000
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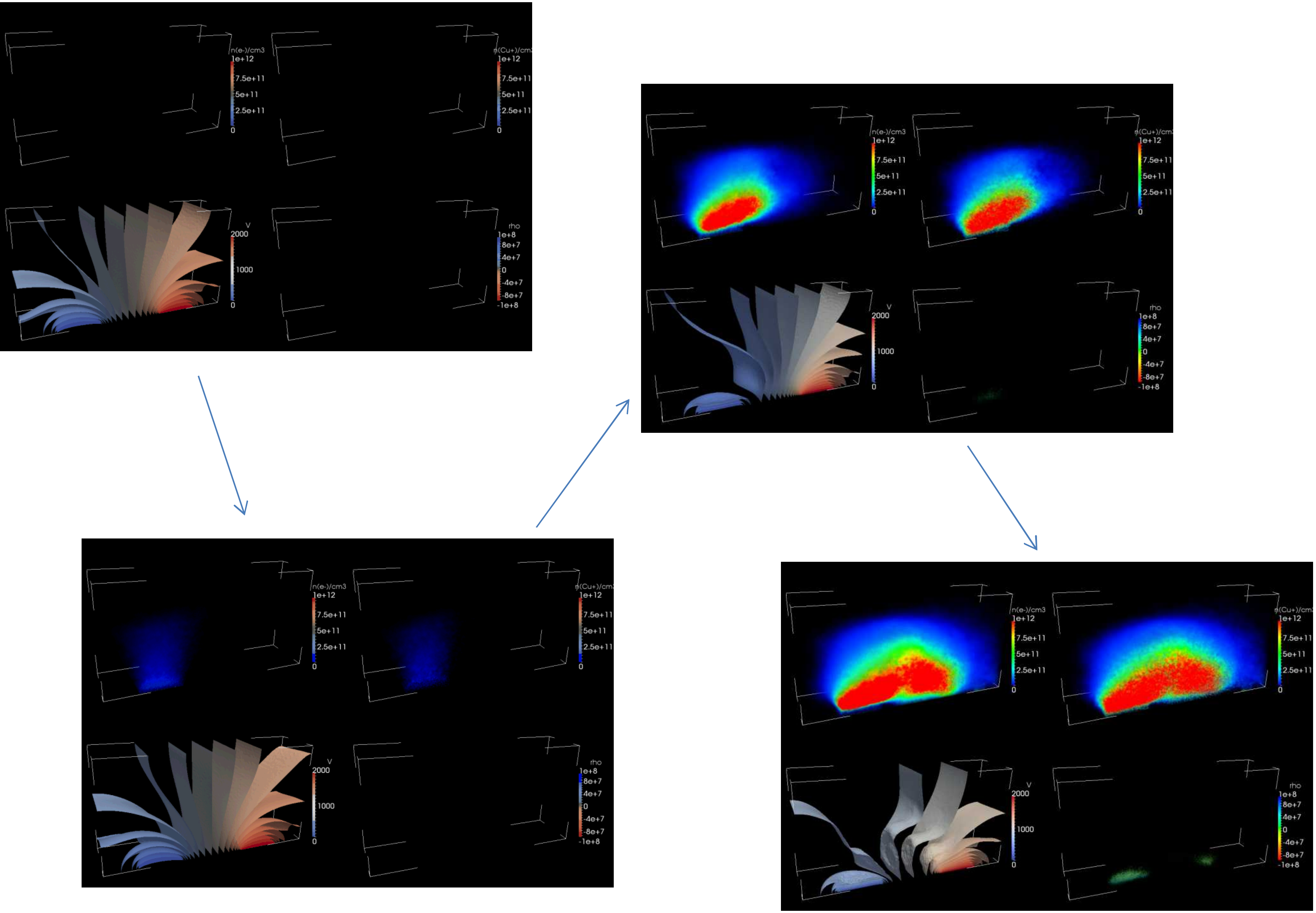

n(e-)/cm3
1e+12
7.5e+11
5e+11
2.5e+11
0
n(Cu+)/cm3
1e+12
7.5e+11
5e+11
2.5e+11
0
v
2000
1000
0
rho
1e+8
8e+7
4e+7
0
-4e+7
-8e+7
-1e+8