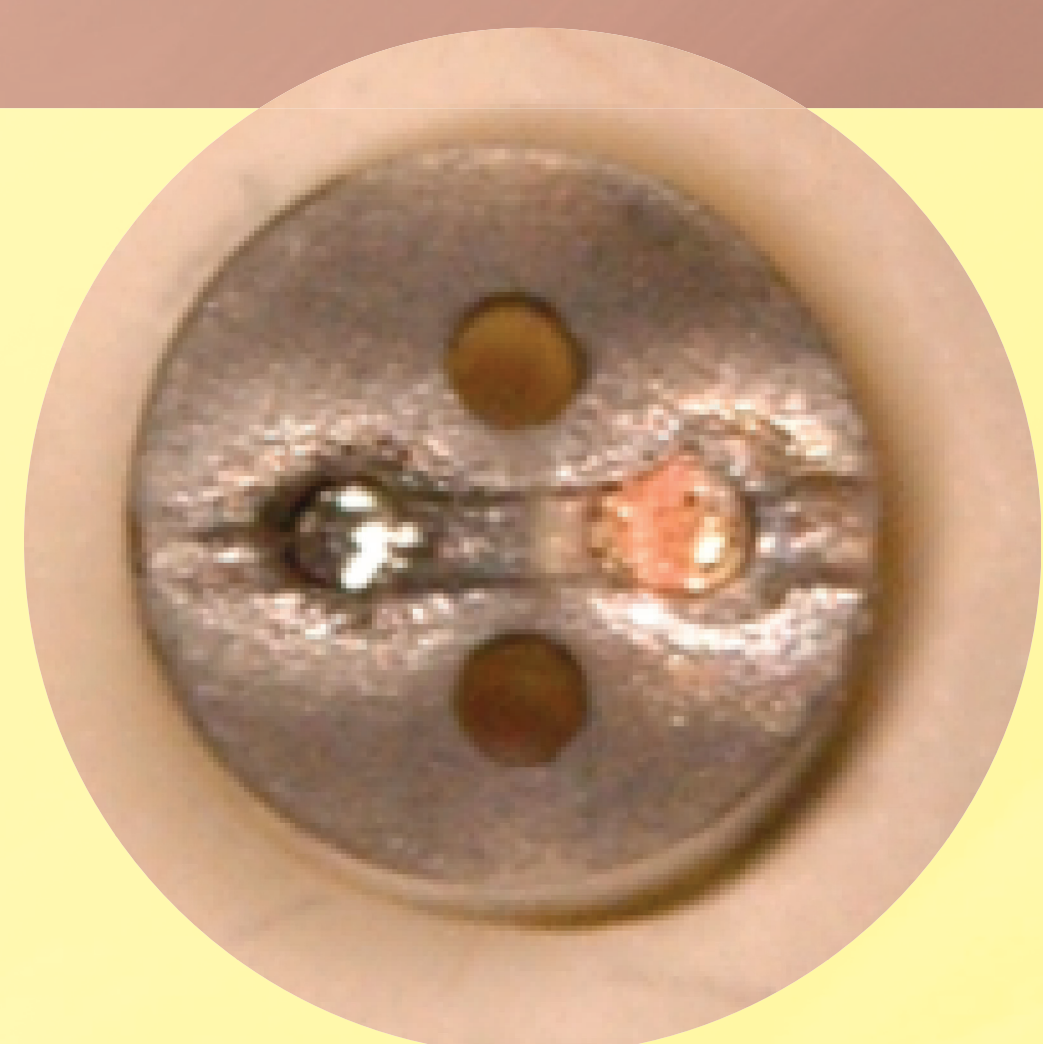# Ingredients for 3D Vacuum Arc Discharge Simulation
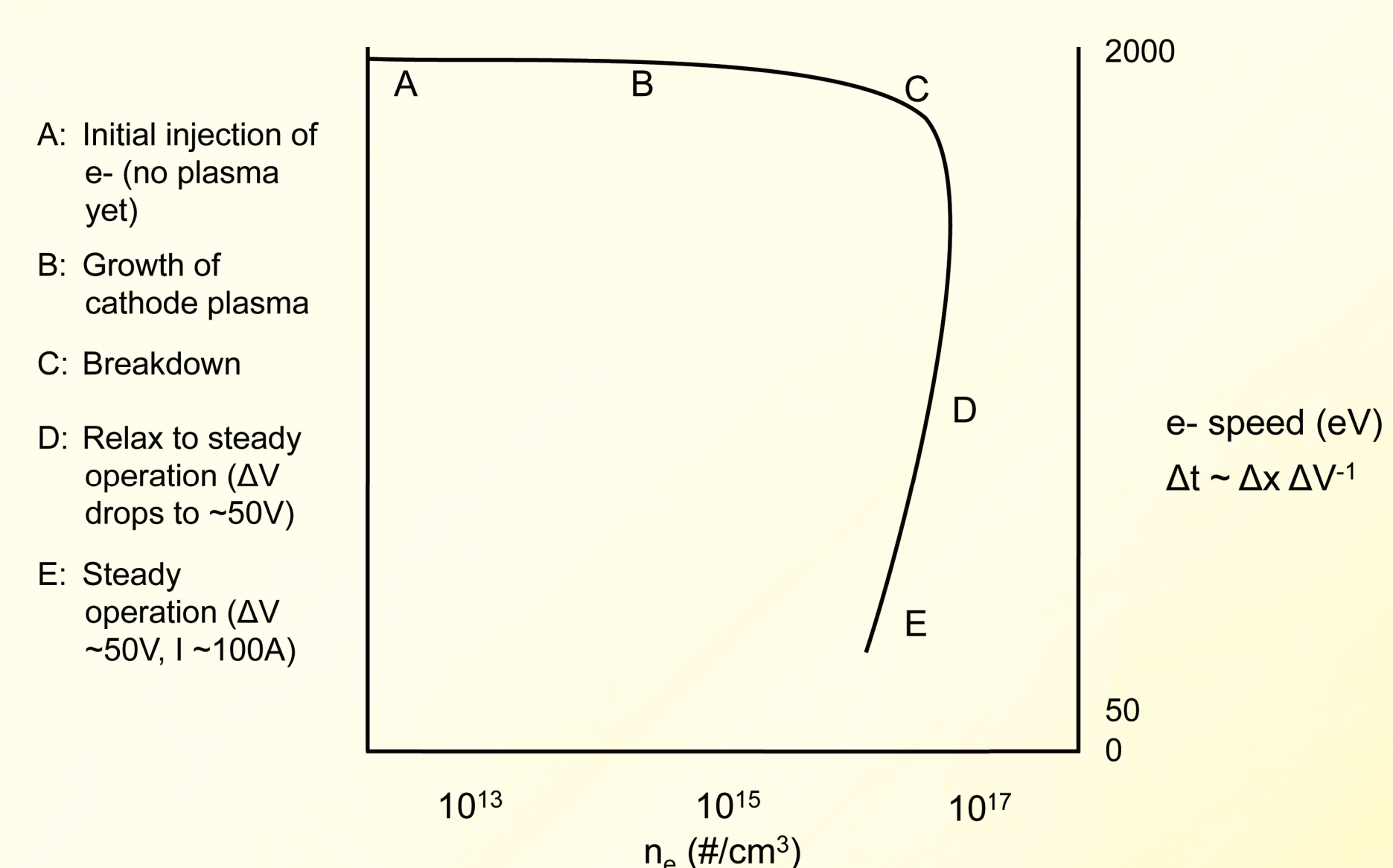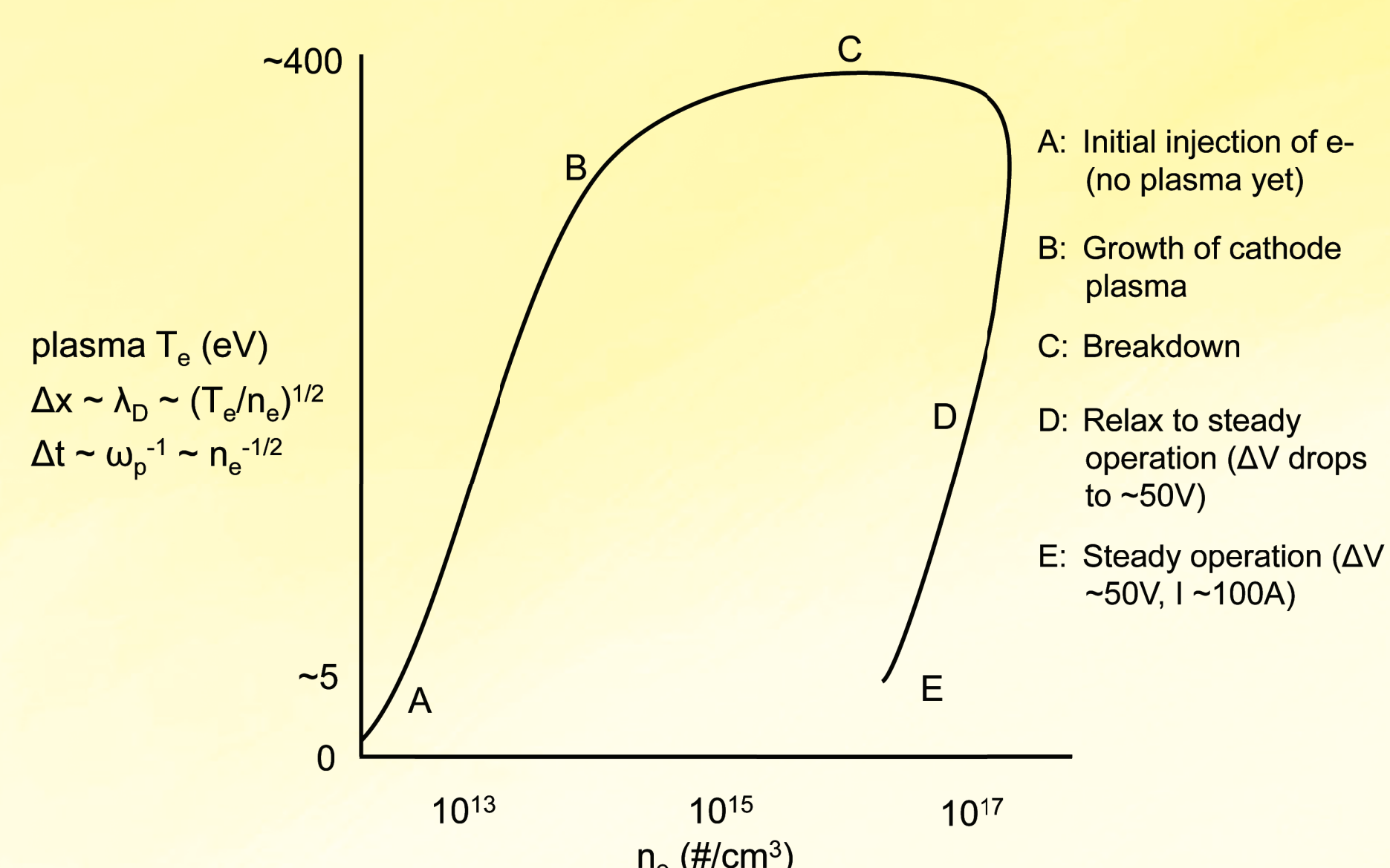
M. M. Hopkins, P. S. Crozier, J. J. Boerner, L. C. Musson, T. P. Hughes, R. Hooper, E. V. Barnat, M. T. Bettencourt, Sandia National Laboratories

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...
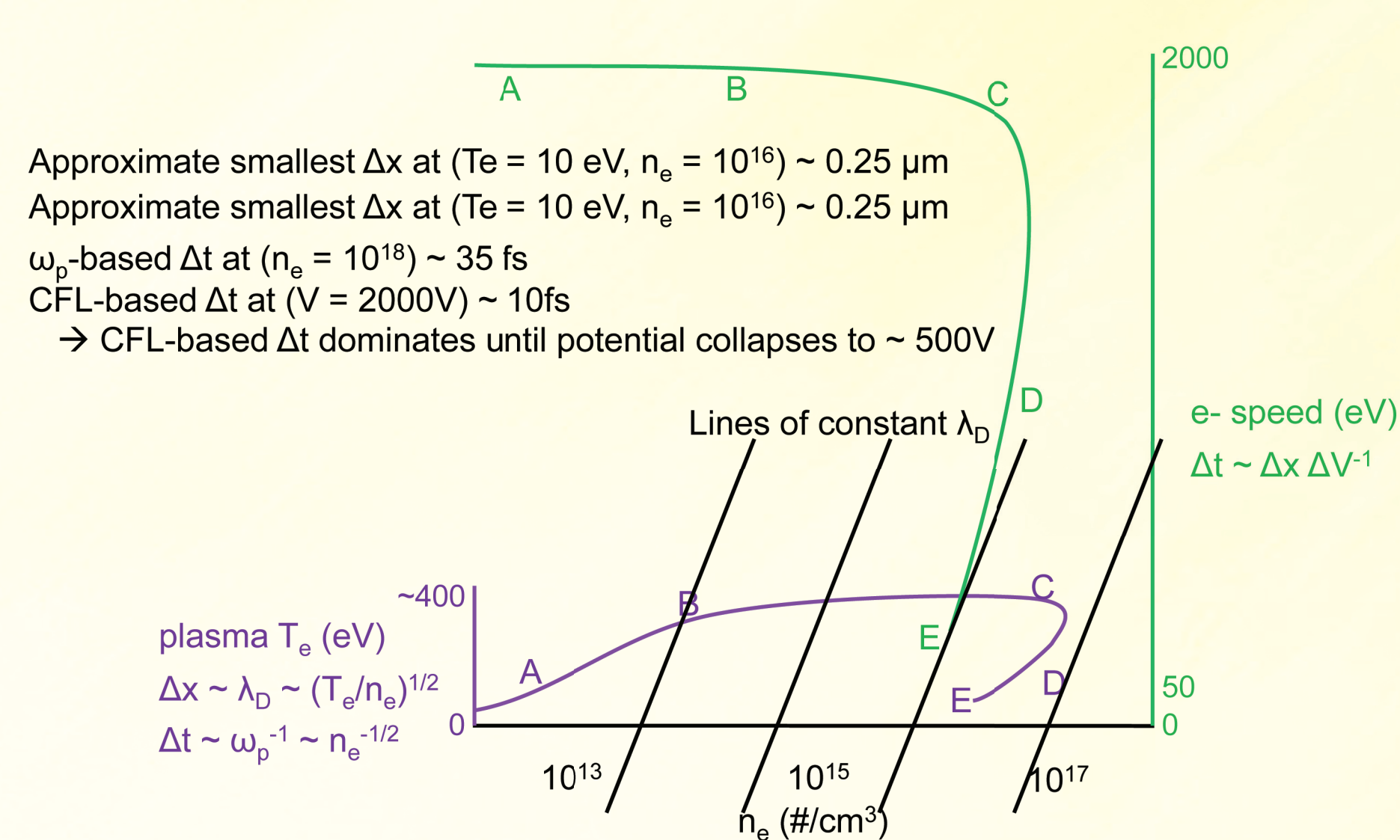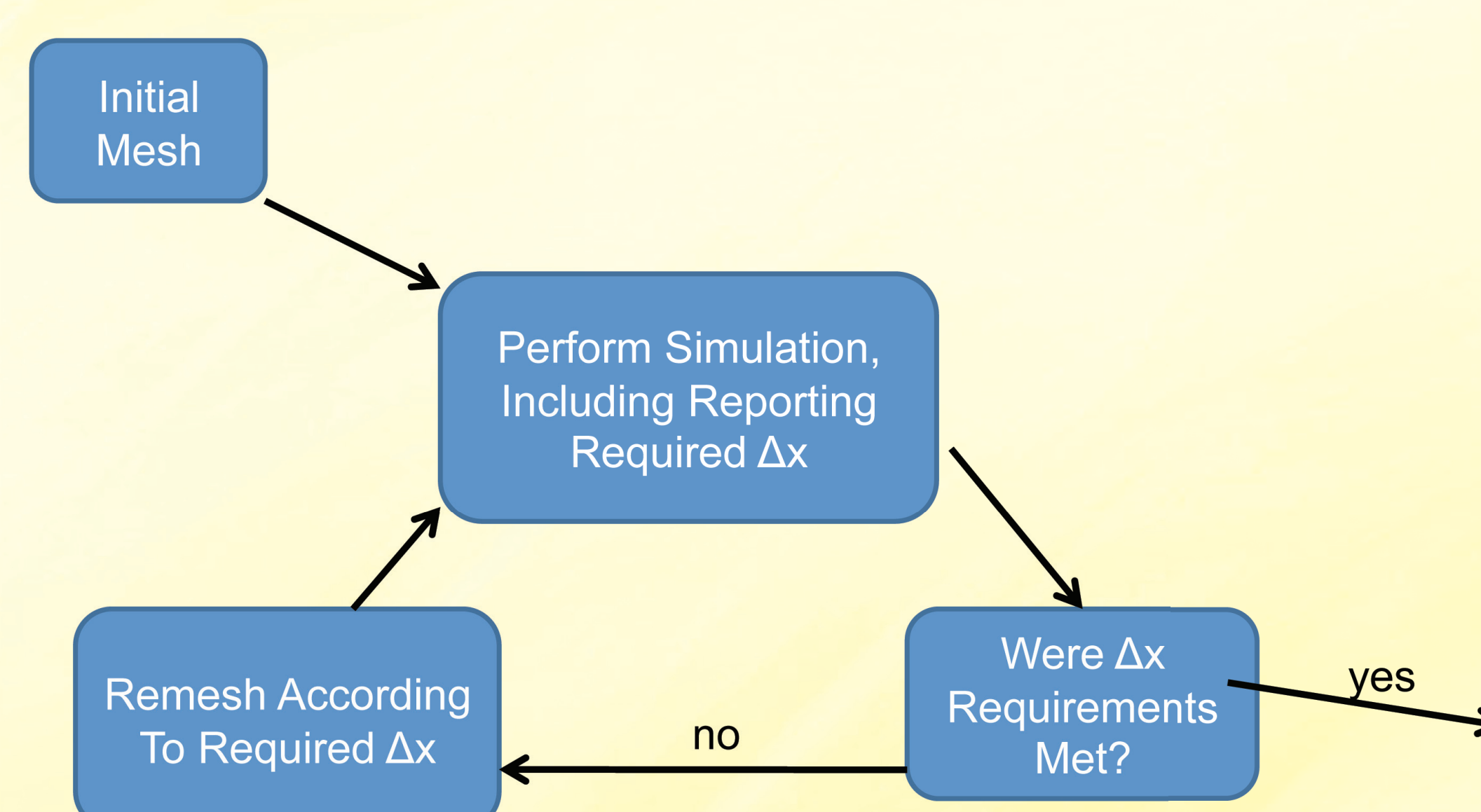
Physical System

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, $n_i \sim 10^{16} - 10^{17}$ #/cm³

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)

A: Initial injection of e- (no plasma yet)
B: Growth of cathode plasma
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e- speed (eV)
$\Delta t \sim \Delta x \, \Delta V^{-1}$

Approximate Simulation Demands

Approximate smallest Δx at (T_e = 10 eV, $n_e = 10^{16}$) ~ 0.25 μm
Approximate smallest Δx at (T_e = 10 eV, $n_e = 10^{16}$) ~ 0.25 μm
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

Lines of constant λ_D

e- speed (eV)
$\Delta t \sim \Delta x \, \Delta V^{-1}$

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

4 mm x 1.5 mm x 2 mm = 24 mm³
+ vol_E = 0.1 μm³
~ 100B elements

~ 10 ns breakdown time at Δt = 10 fs
+ ~ 100 ns evolution time at Δt = 100 fs
2M timesteps

3 x (~10) particles/cell in breakdown region
+ ~ 5% of cells in breakdown region
~ 150B particles

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:

Initial Mesh → Perform Simulation, Including Reporting Required Δx → Were Δx Requirements Met? → yes
Were Δx Requirements Met? → no → Remesh According To Required Δx → Perform Simulation...

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.
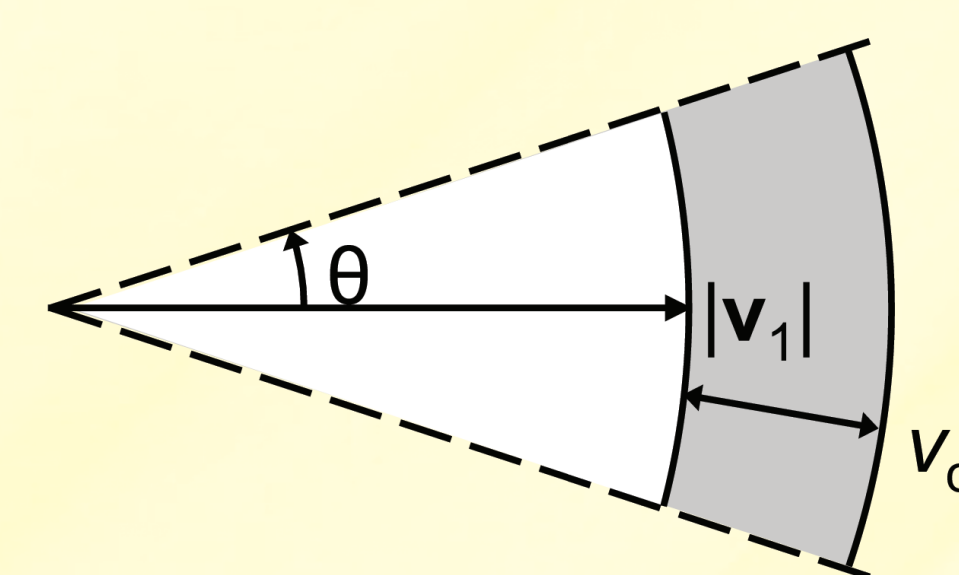Repeat 1-6 until target number or limiter is met.
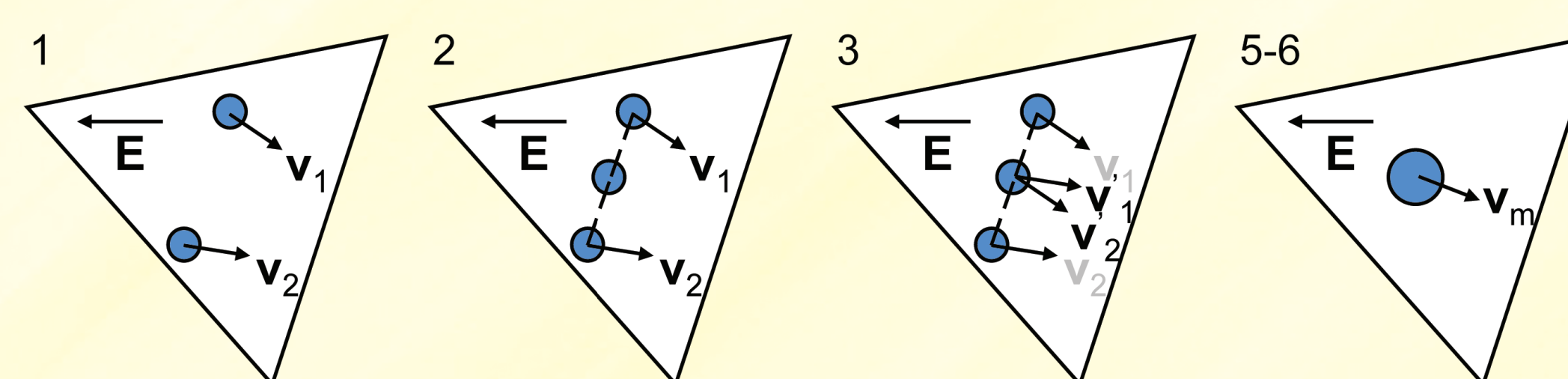
Velocity Phase Space Acceptance Criteria:

Velocity Interval
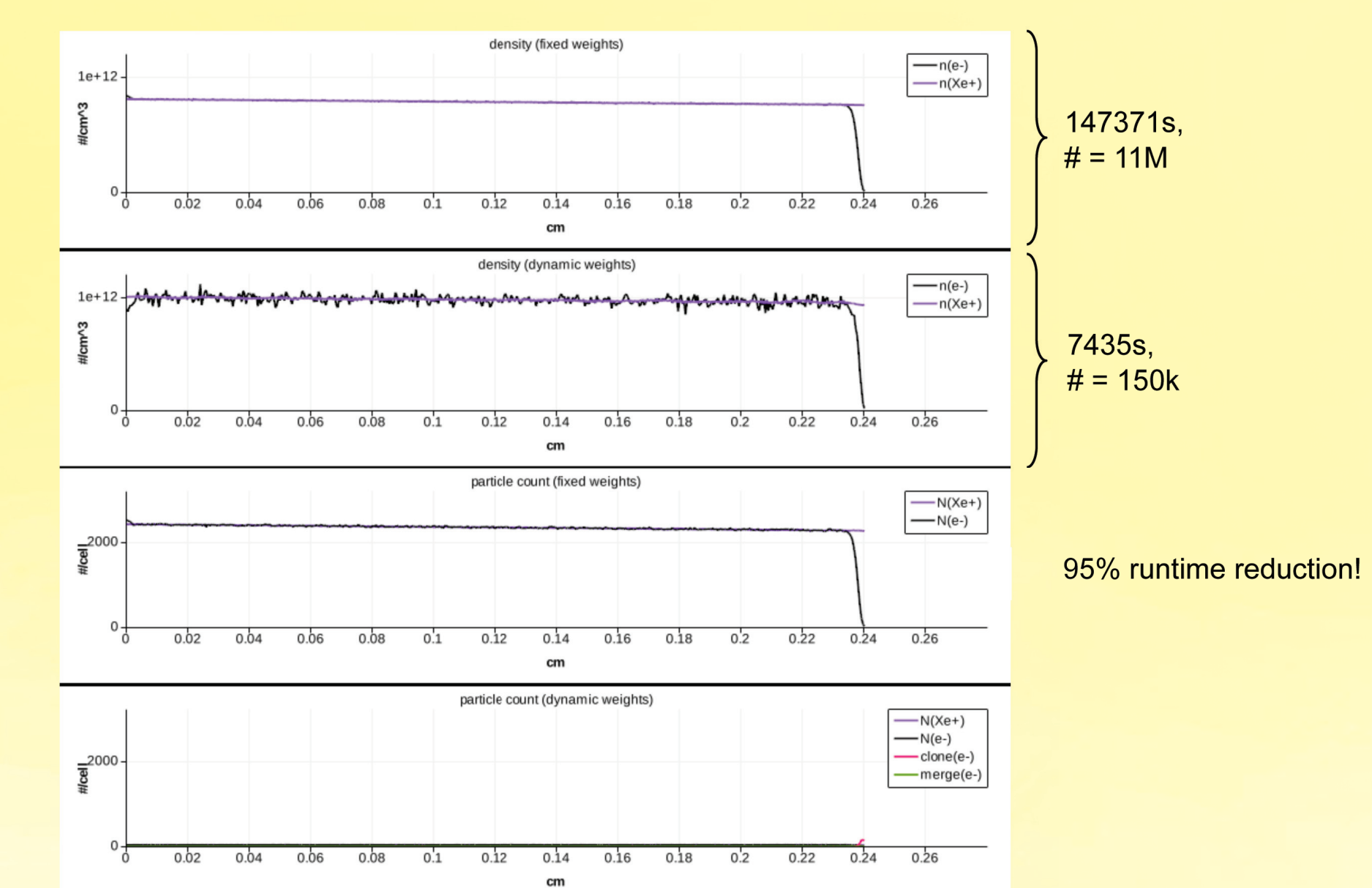$$\mathbf{v}_1 \cdot \mathbf{v}_2 > |\mathbf{v}_1|\|\mathbf{v}_2|\cos(\theta)$$
$$|\mathbf{v}_2| - |\mathbf{v}_1| < v_c = \alpha\sqrt{k_B T/m}$$

Successful test problems:
• Box of plasma
• Neutral Injection (constant or increasing flux)
• Sheaths (constant or growing density)
• 1D arcs (similar to work here)

Xe Sheath With Growing Density

147371s, # = 11M
7435s, # = 150k
95% runtime reduction!

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).
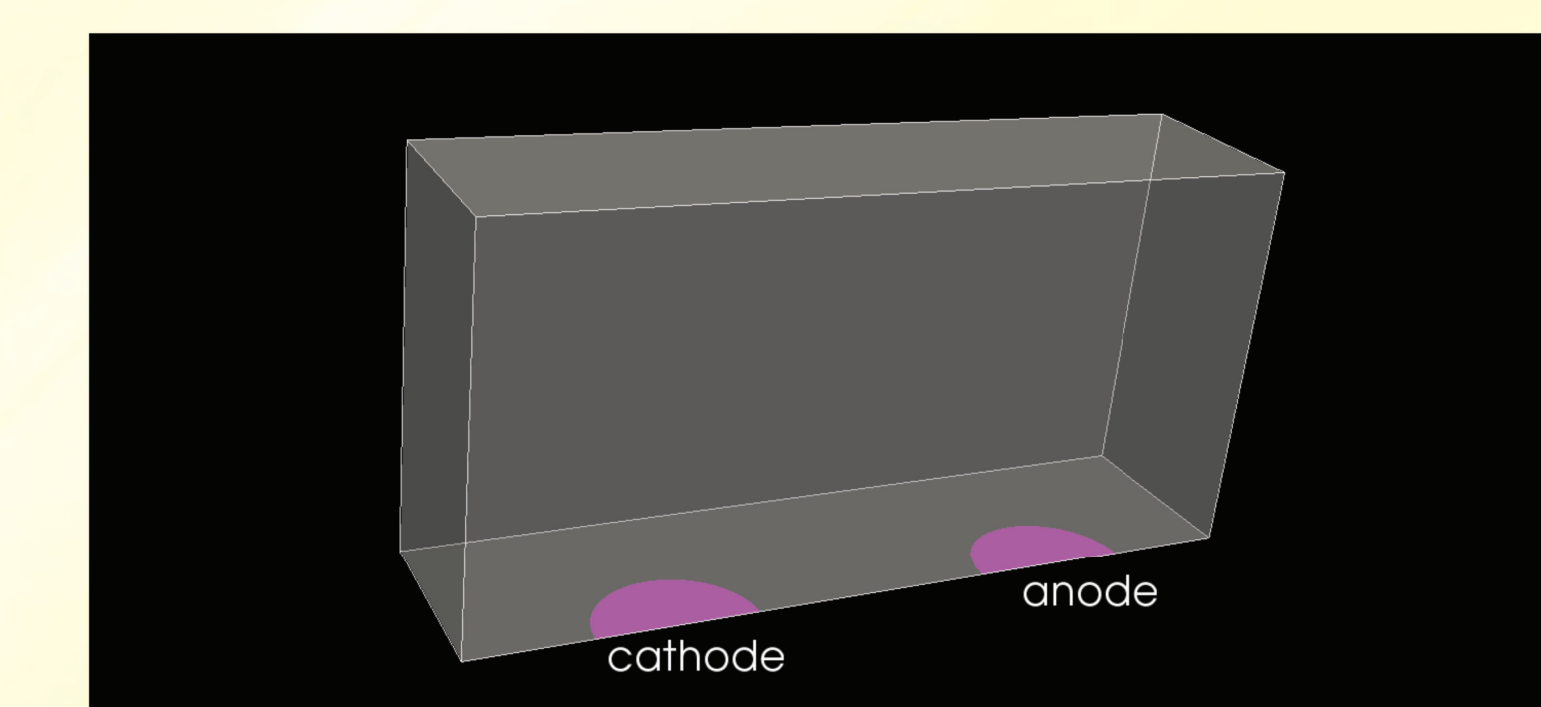
Ingredient: High Performance Computing And Efficient Scaling

We are currently communications and data movement limited at large scales, but have successfully scale to 10K's of cores:
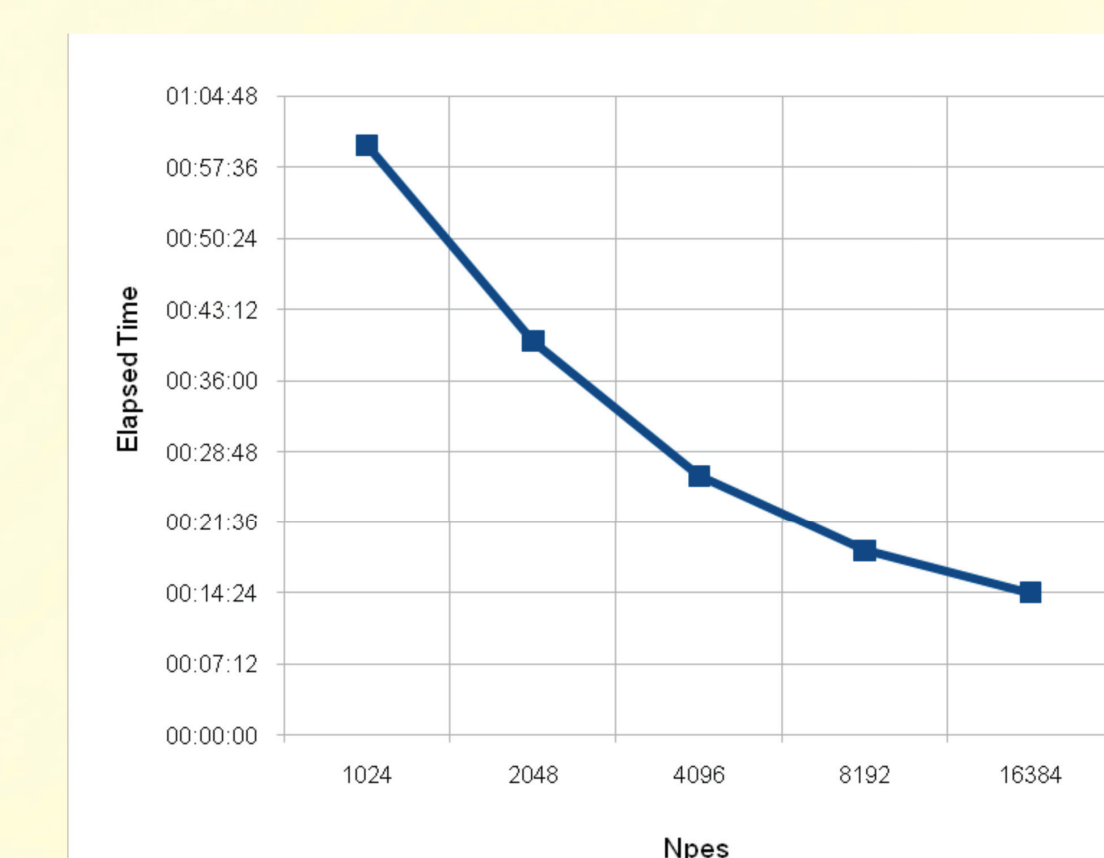
Strong scaling for 16M cell problem on Cielo.

Recent Computational Model

cathode   anode

Caveats:
• Smaller domain size (1/10th)
• Cells are too large, leading to correct blow-up
• Not vacuum, background = 10^{18} Cu/cm³

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