SAND2012-2894C

State of 3D Vacuum Arc Discharge Simulation via PIC-DSMC

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International Workshop on Breakdown Science and High Gradient Technology

KEK

Tsukuba, Japan

April 18-20, 2012

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

1. Our needs
2. Modeling tool, Aleph
3. Complex models need CV & V & SV & SA & UQ
4. Current 3D vacuum arc modeling

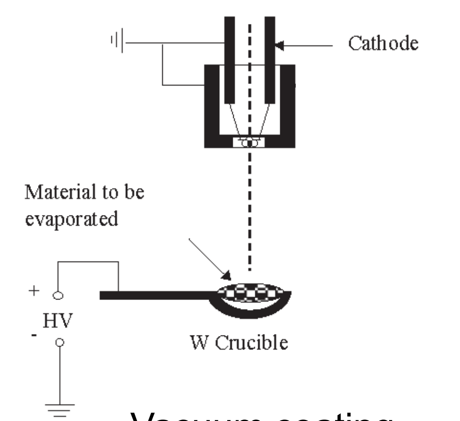
SNL Modeling Needs

We're interested in low temperature collisional plasma phenomena. Our applications generally share the following requirements:

- Kinetic description.
- Collisions/chemistry, including ionization (arcs). Neutrals are important.
- Very large variations in number densities over time and space.
- Sheaths.
- Real applications with complex geometry.

Examples:

- Vacuum arc discharge
- Plasma processing
- Spark gap devices
- Gas switches
- Ion and neutral beams

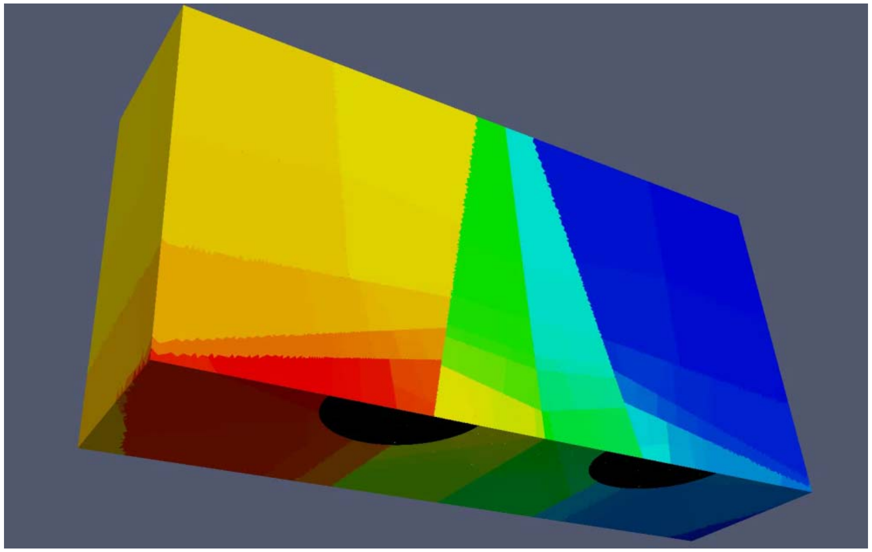


Vacuum coating

We are especially interested in the transient start-up of arc-based devices.

Description of Aleph

- 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 easily extending BCs, post-processed quantities, etc.
- Currently utilizing up to 32K processors (>100M elements, >1B particles)



256 core particle load balancing example

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CV & SV & V & SA & UQ

All Interesting Arc/Plasma Behavior Is Nonlinear And Coupled – How Can We Be Confident In Our Predictions?

CV: Code Verification. Necessary, woefully insufficient. Can test single simple capabilities.

SV: Solu
right

V: Valid
realit
solut

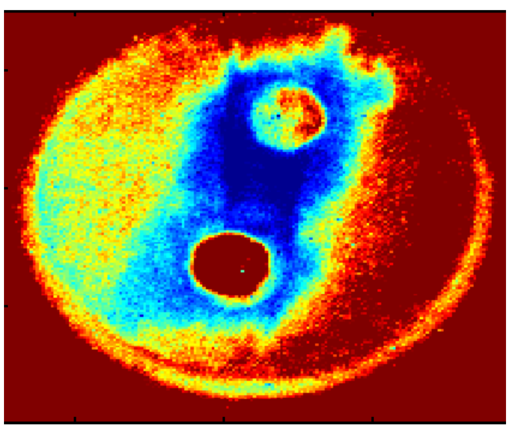
SA: Sens
Dete
prediction, experimental result, and/or validation comparison. Identifies problem areas and is a source of planning decisions/efficiency.

UQ: Uncertainty Quantification. Estimate uncertainty in a code prediction, usually without experimental comparator. Incorporates error estimation and quantified code prediction uncertainties.

ALL OF THIS IS MORE COMPLICATED BECAUSE OUR BASIC MODELING METHODS ARE STOCHASTIC (PIC, MCC, MD, ...) AND DO NOT HAVE TYPICAL “GRID CONVERGENCE” BEHAVIOR

Paul’s poster

3D Model of Cu-Cu Arc System



At 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

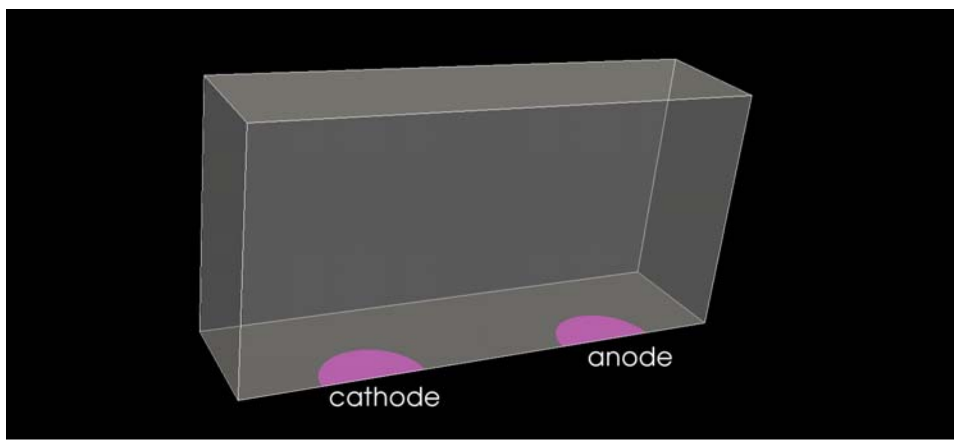
20Ω resistor in series

Steady conditions around 50V, 100A

Breakdown time << 100ns

Ionization mfp = 1.5 mm at maximum σ

→ $n_i \sim 10^{16} – 10^{17}$ #/cm^3

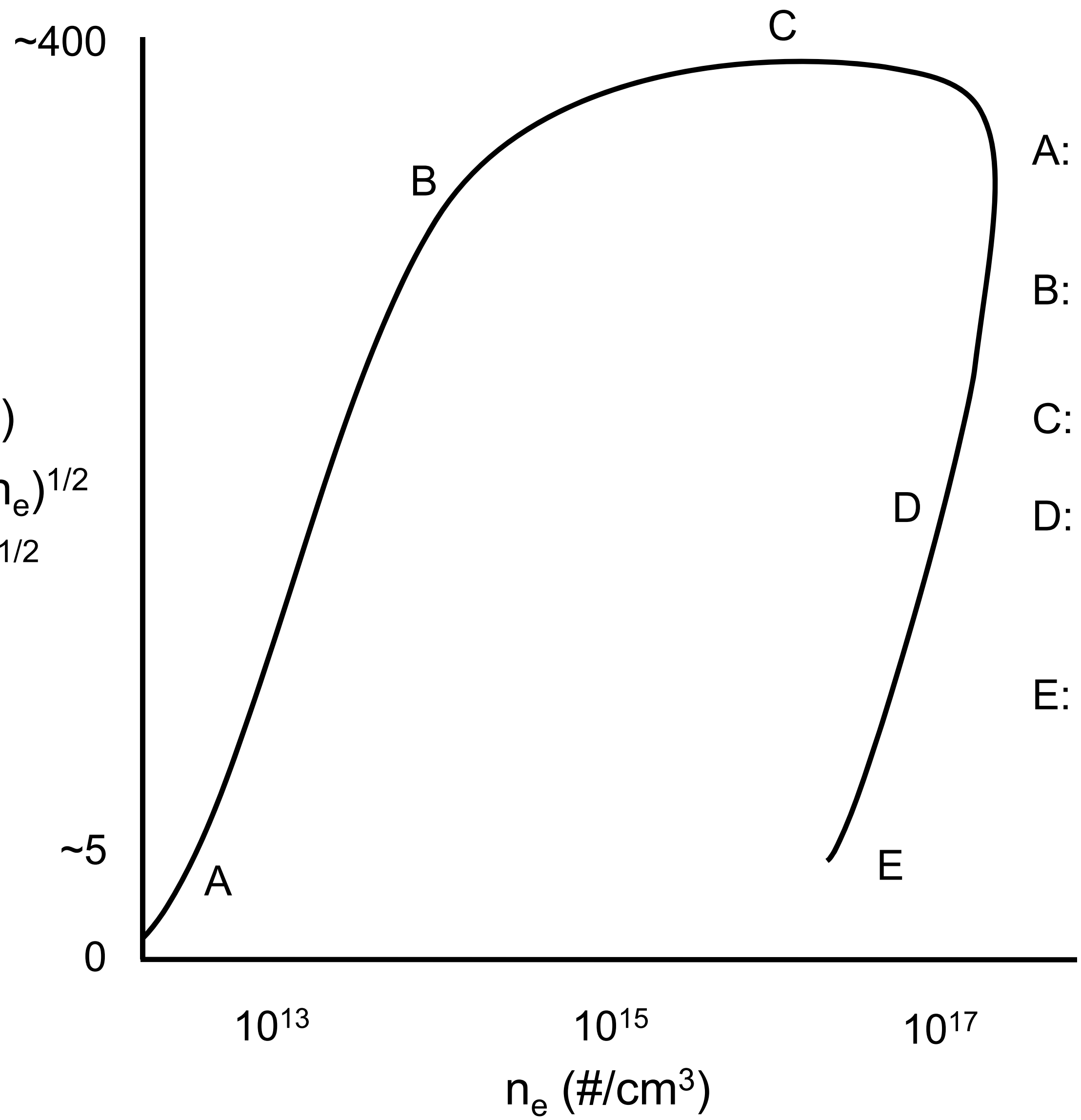


3D Model of Cu-Cu Arc System

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)

3D Model of Cu-Cu Arc System

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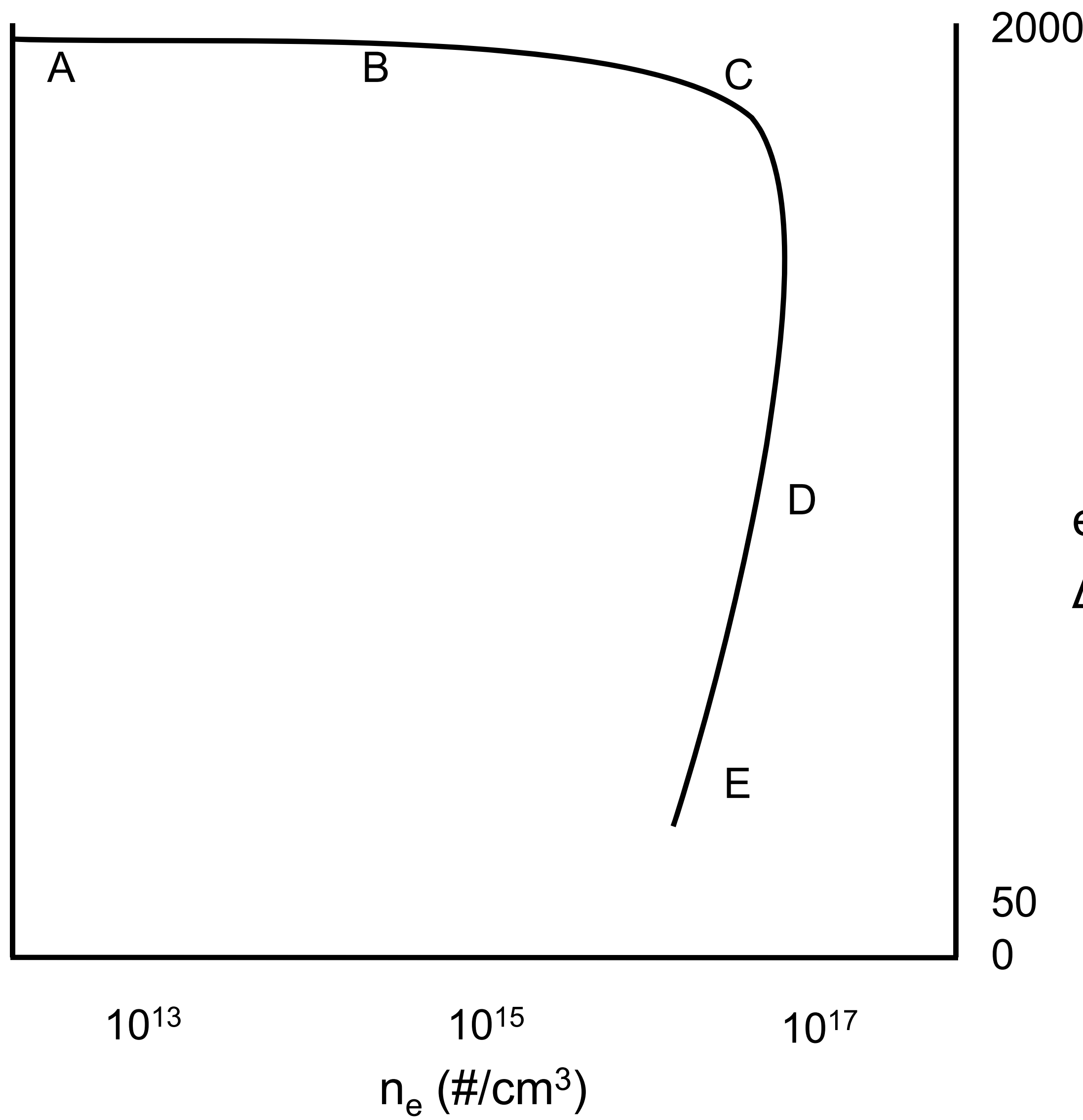


e- speed (eV)

$\Delta t \sim \Delta x \, \Delta V^{-1}$

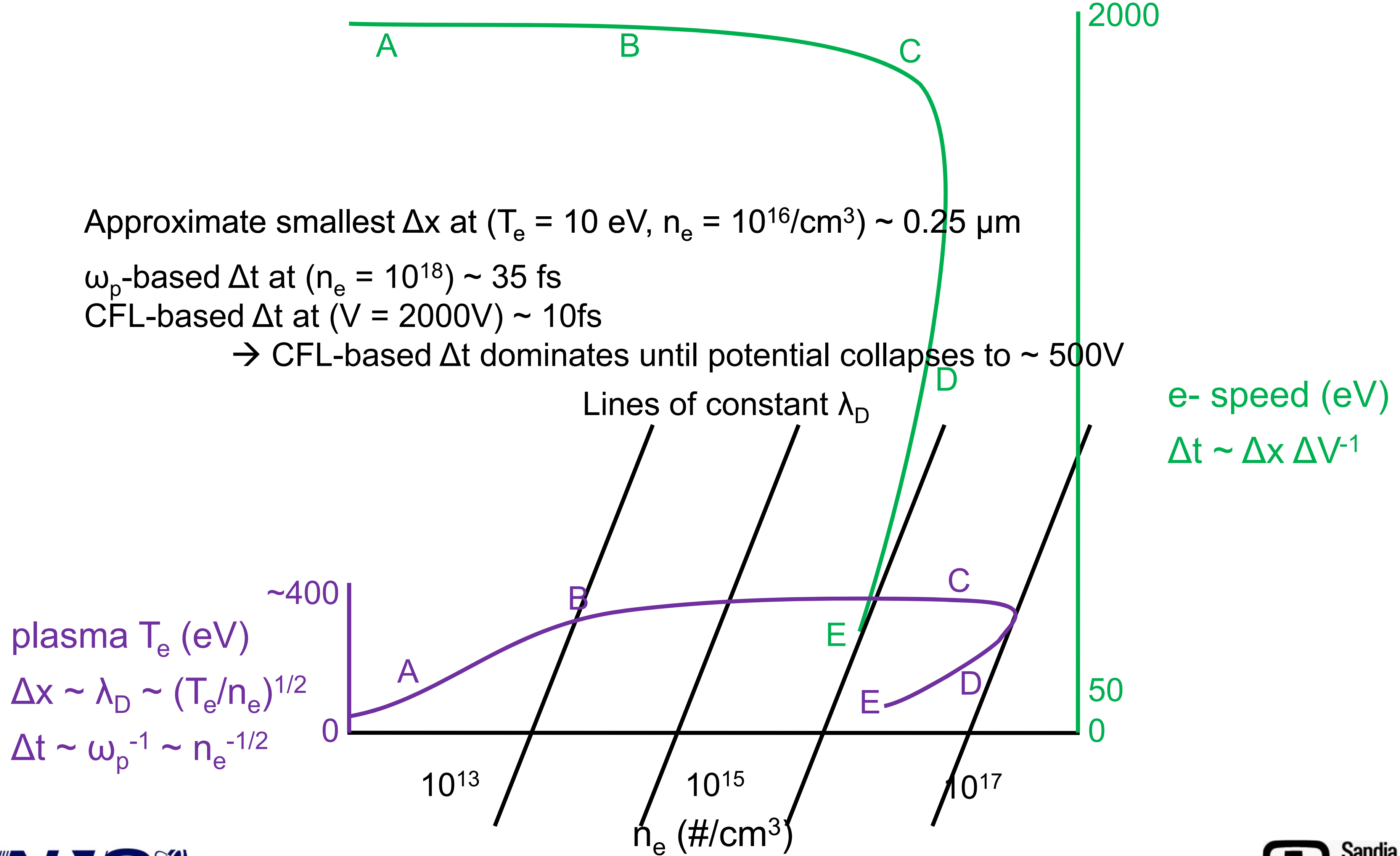
3D Model of Cu-Cu Arc System

Approximate smallest Δx at (T_e = 10 eV, $n_e = 10^{16}/cm^3$) ~ 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



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3D Model of Cu-Cu Arc System

4 mm x 1.5 mm x 2 mm = 24 mm^3

+ vol_E = 0.1 μm^3

+ ~ 5% of volume is at smallest Δx

~ 5B elements

~ 10 ns breakdown time at Δt = 10 fs

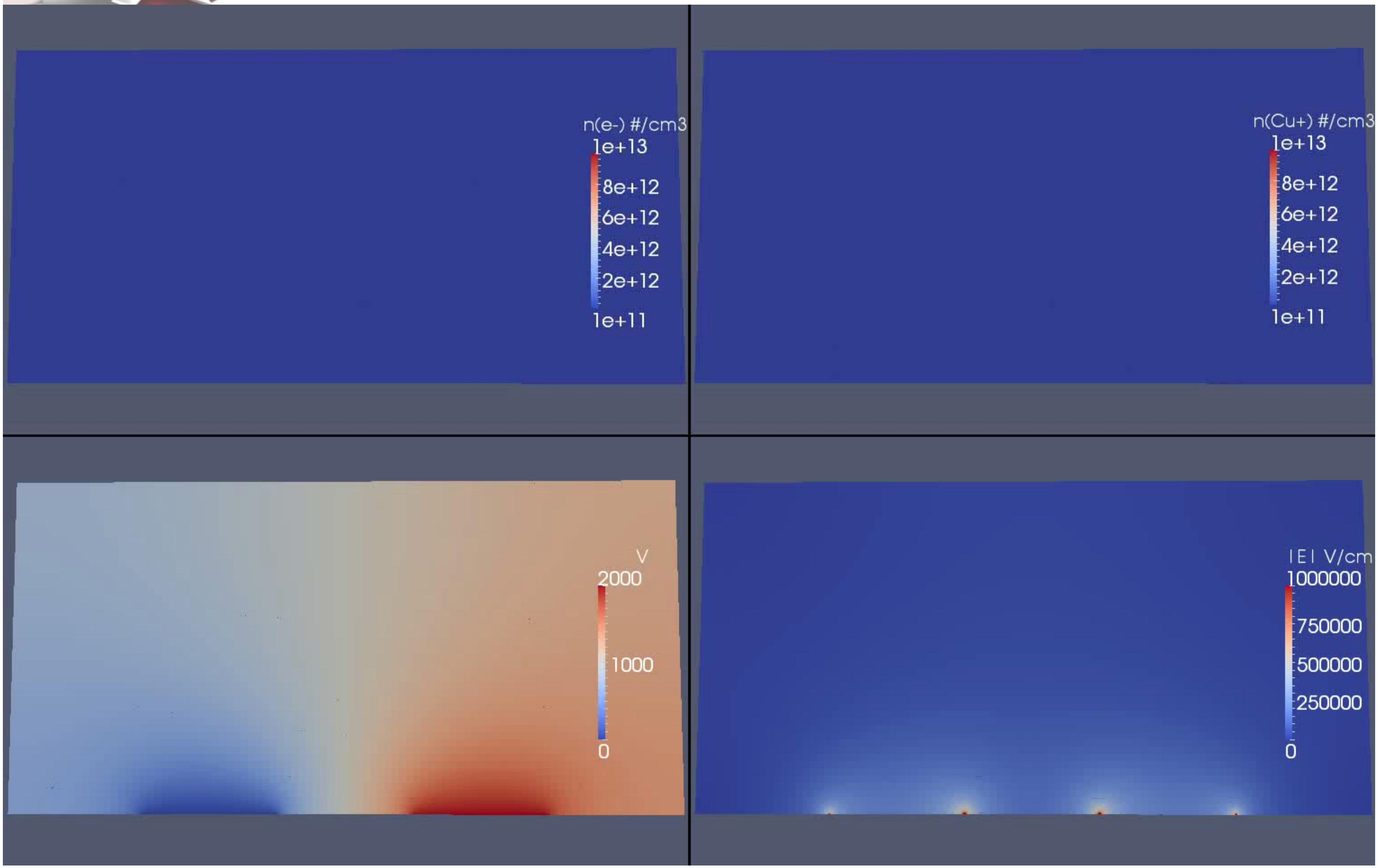
+ ~ 100 ns evolution time at Δt = 100 fs

+ ~ 5% of volume is at smallest Δx

2M timesteps

... assuming fixed work per timestep, which is why we developed dynamic particle weighting (keep # particles/element fixed)

... not there, yet. Results are 1/10th domain size, 2x Δx, 10^{18} background Cu ... on 256 cores ... awaiting better meshing capability ...



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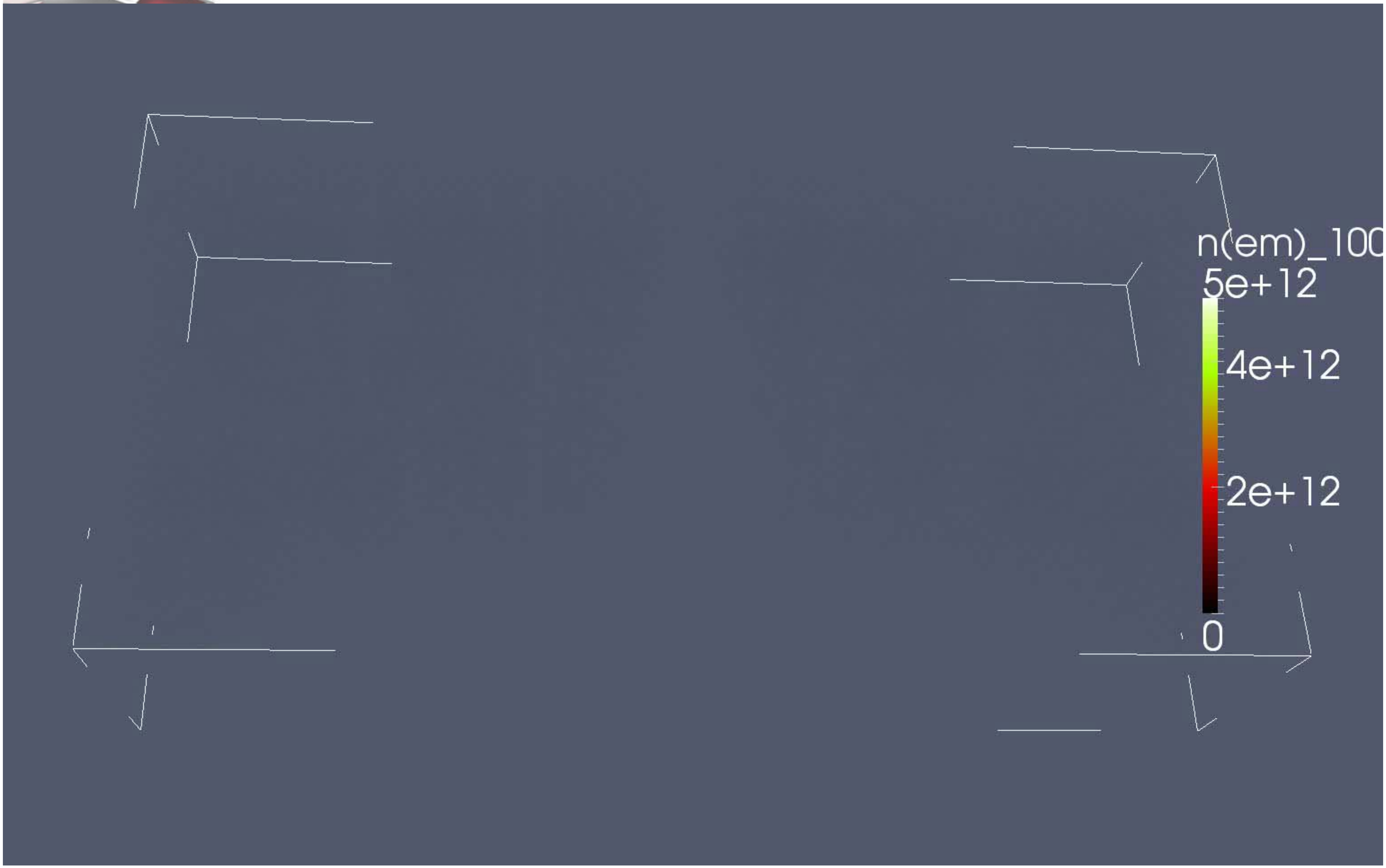
n(em)_10
5e+12
4e+12
2e+12
0

The End

Description of Aleph

Basic algorithm for one time step of length Δt:

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

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

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

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

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

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

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

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

7. 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.
8. Perform chemistry: for each reaction, determine expected number of reactions. Sample particles of those types, perform reaction (particle creation/deletion).
9. Reweight particles.
10. Compute post-processing and other quantities and write output.
11. Rebalance particle mesh if appropriate (variety of determination methods).