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3D Vacuum Arc Breakdown Simulation: Many Challenges and Some Solutions

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[3]Scalable Algorithms,
[4]Advanced Device Technologies,
[5]Scientific Apps and User Support,
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Albuquerque, NM, USA

39th IEEE International Conference on Plasma Science
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Edinburgh, Scotland, U.K.

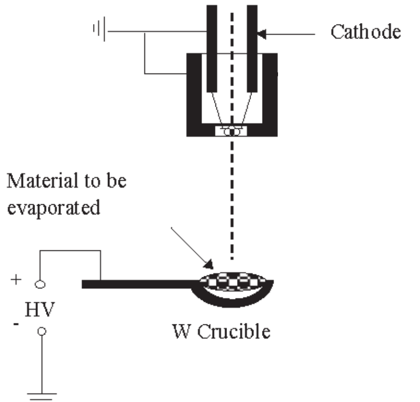
Modeling Needs and Challenges

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:

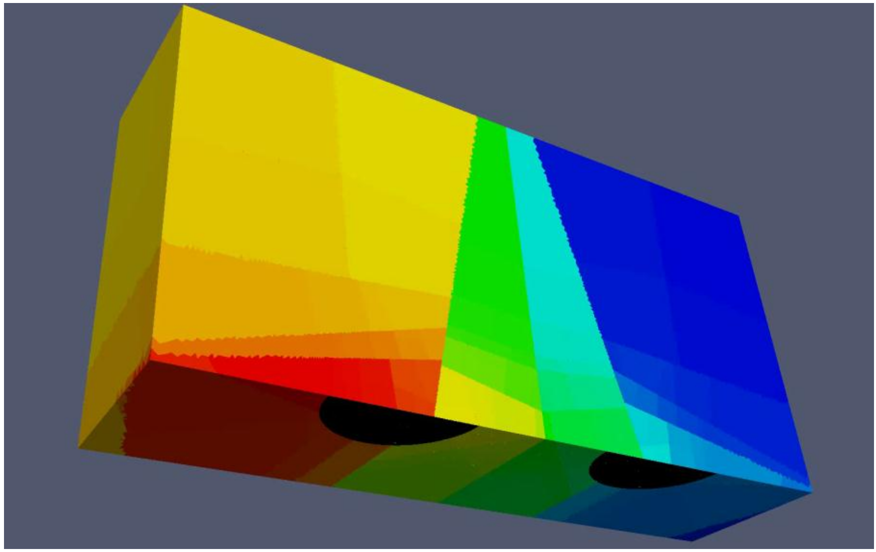
- Vacuum arc discharge
- Plasma processing
- Spark gap devices
- Gas switches
- Ion and neutral beams



Vacuum coating

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

Description of Aleph



256 core particle load balancing example

- 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 64K processors (>1B elements, >1B particles)

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

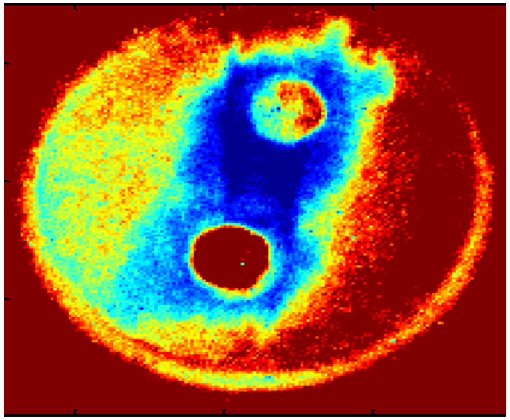
20Ω resistor in series

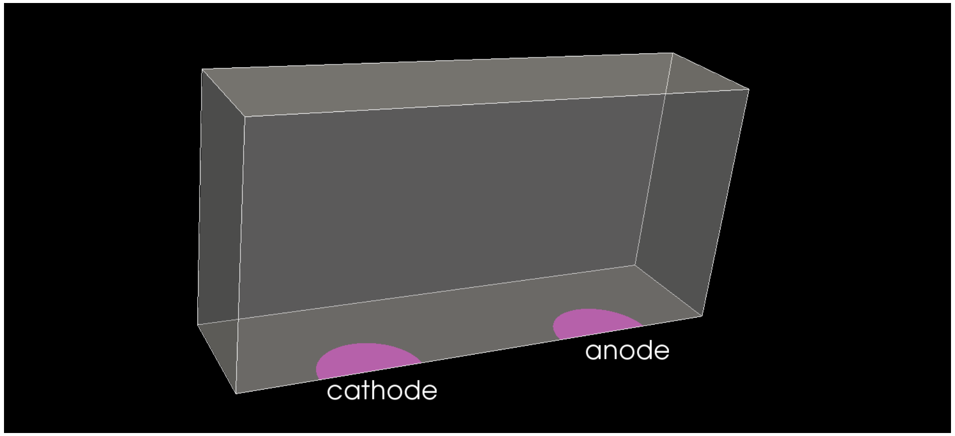
Steady conditions around 50V, 100A

Breakdown time << 100ns

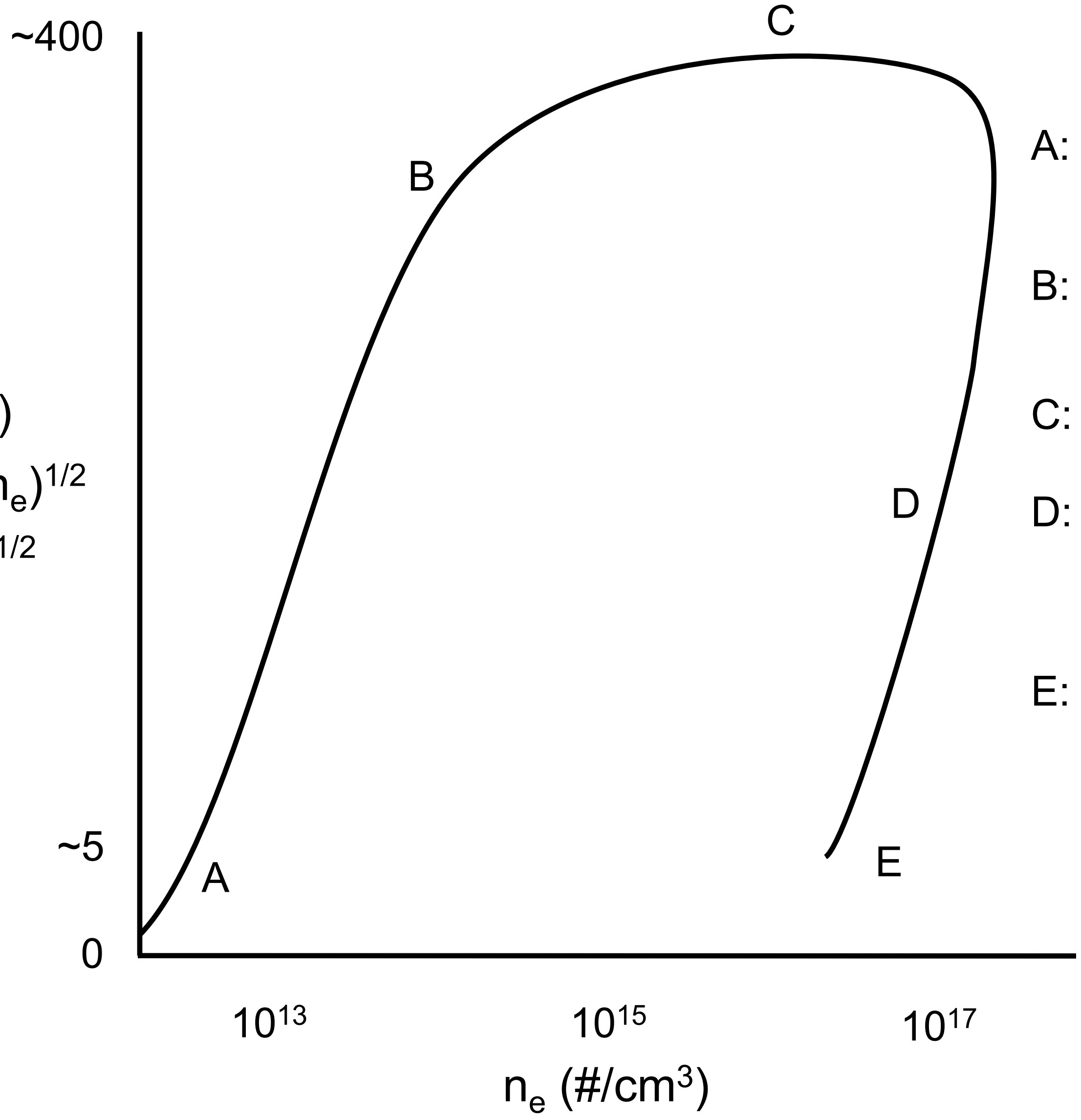
Ionization mfp = 1.5 mm at maximum σ

→ $n_i \sim 10^{16} - 10^{17}$ #/cm^3





3D Model of Cu-Cu Arc System



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

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

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

B: Growth of cathode
plasma

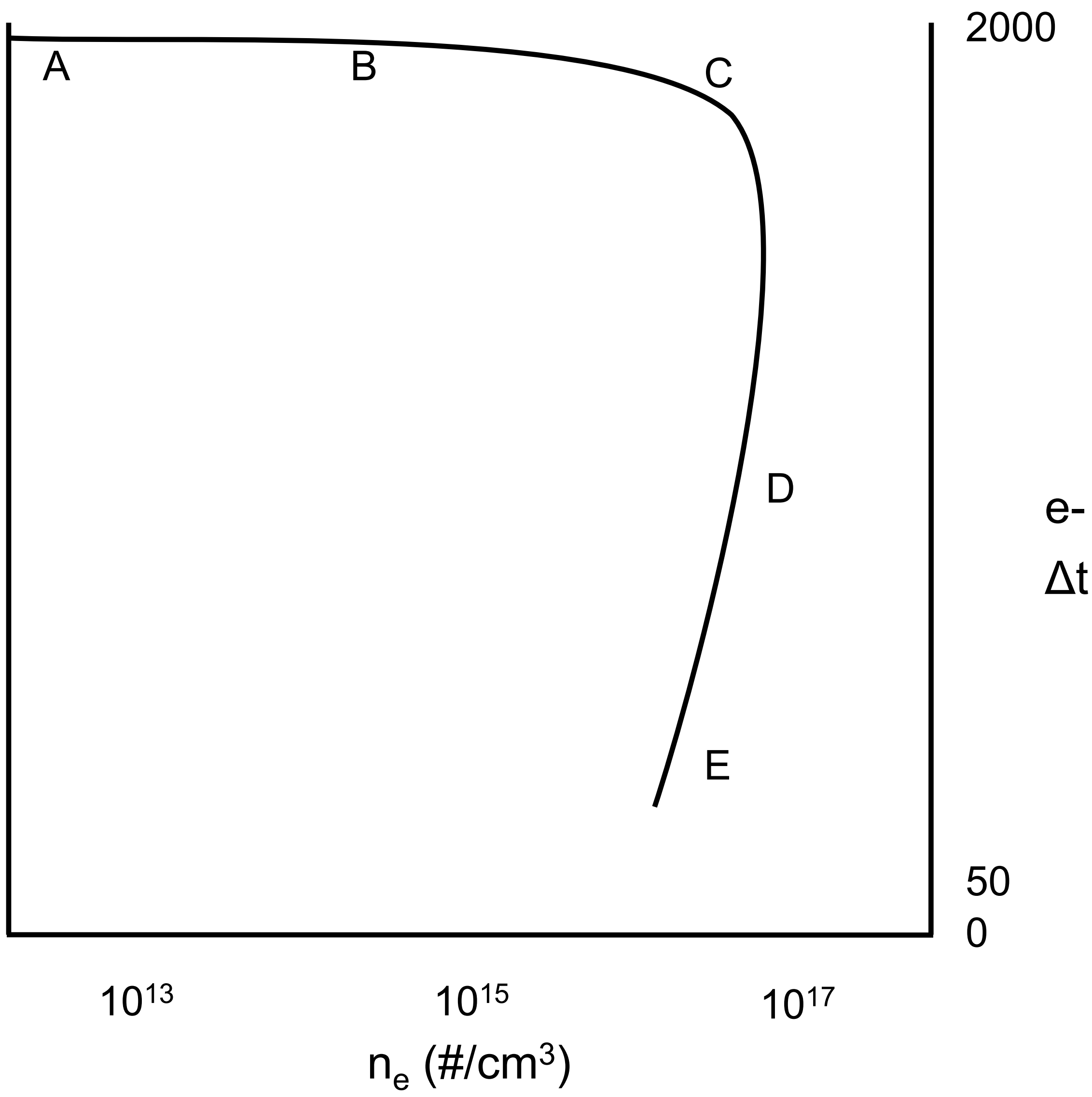
C: Breakdown

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

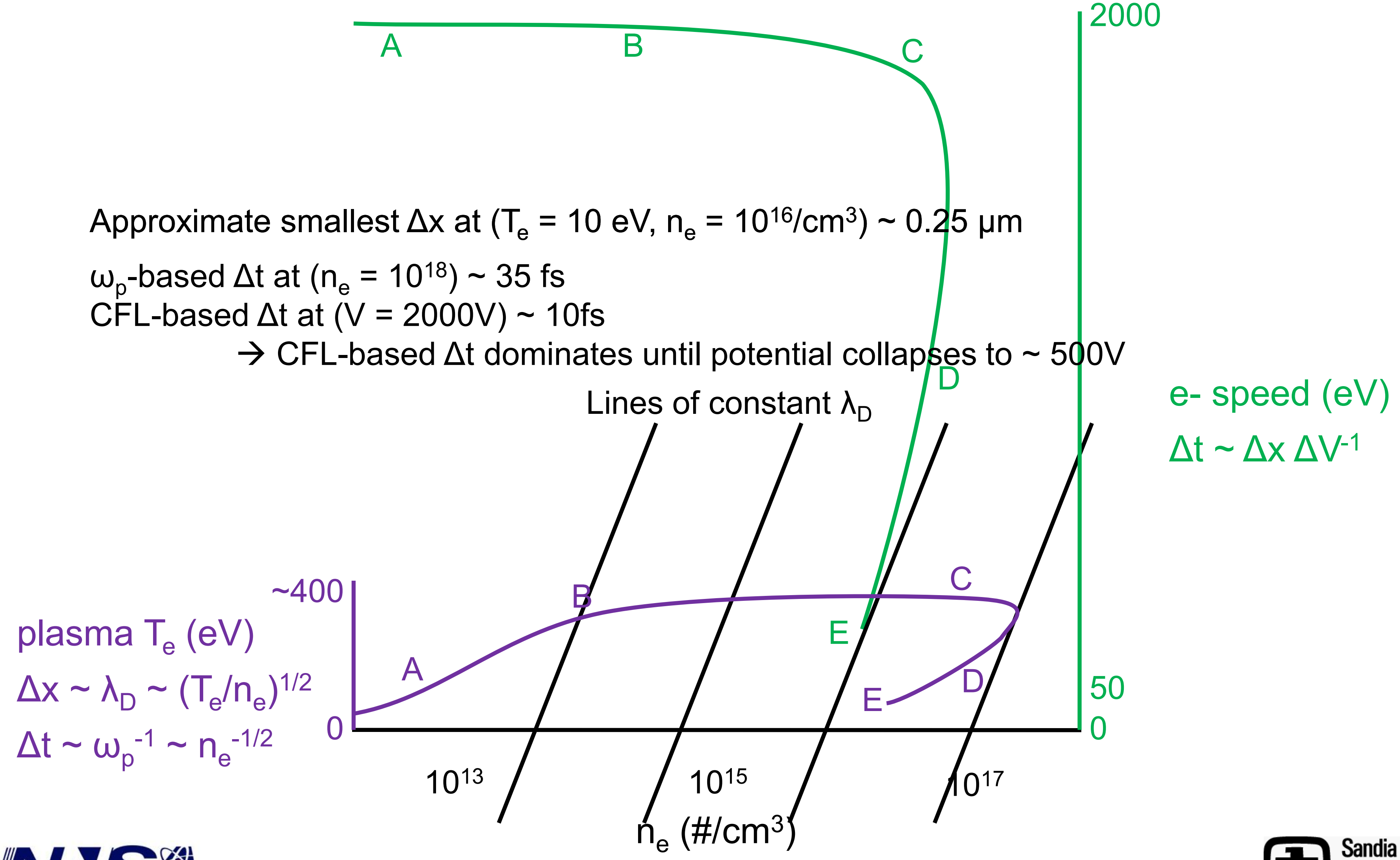
E: Steady operation (ΔV
~50V, I ~100A)

3D Model of Cu-Cu Arc System

- 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



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

3D Model of Cu-Cu Arc System

$4\ \text{mm} \times 1.5\ \text{mm} \times 2\ \text{mm} = 24\ \text{mm}^3$

\+ $\text{vol}_E = 0.1\ \mu\text{m}^3$

\+ ~ 5% of volume is at smallest Δx

~ 5B elements

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

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

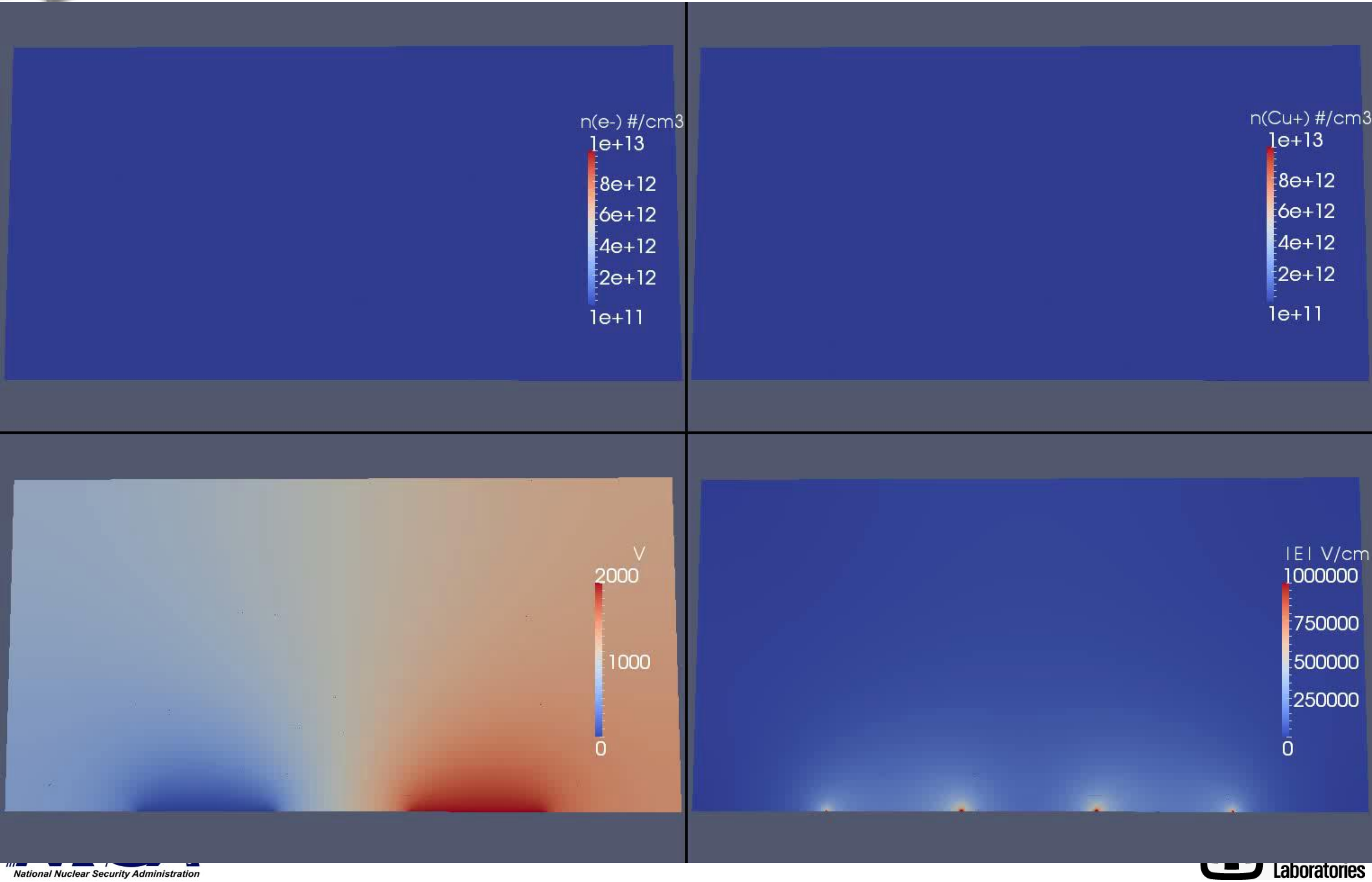
\+ ~ 5% of volume is at smallest Δx

2M timesteps

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

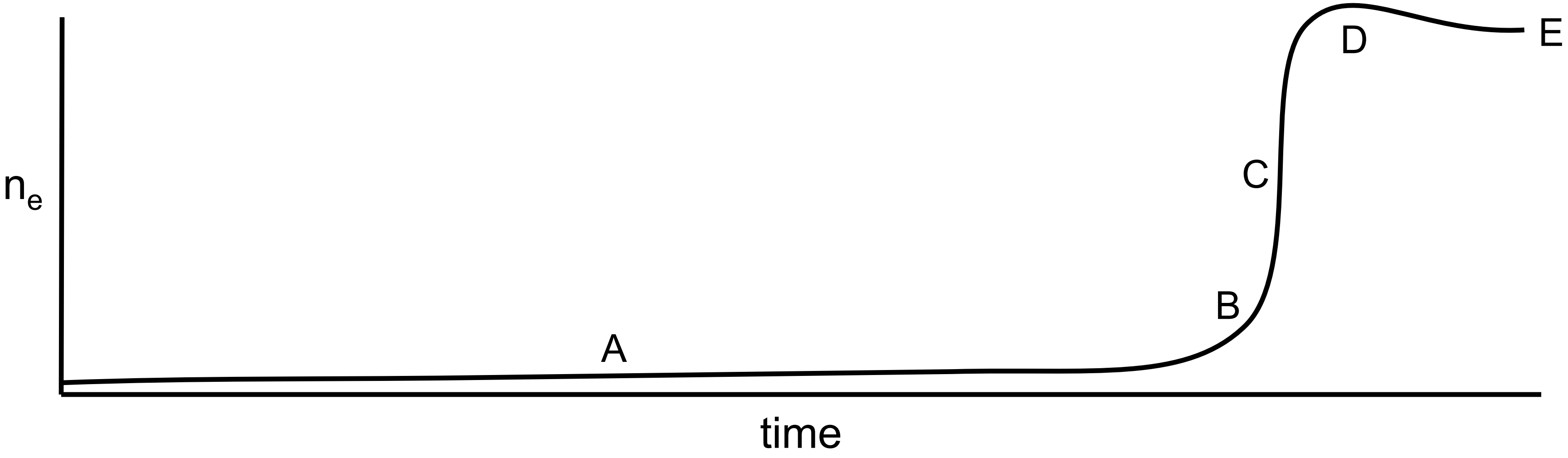
... not there, yet. The following results are 1/10th domain size, 2x Δx, 10^{18} background Cu ... on 256 cores ... awaiting better meshing capability ...

3D Model of Cu-Cu Arc System



3D Model of Cu-Cu Arc System

3D Model of Cu-Cu Arc System

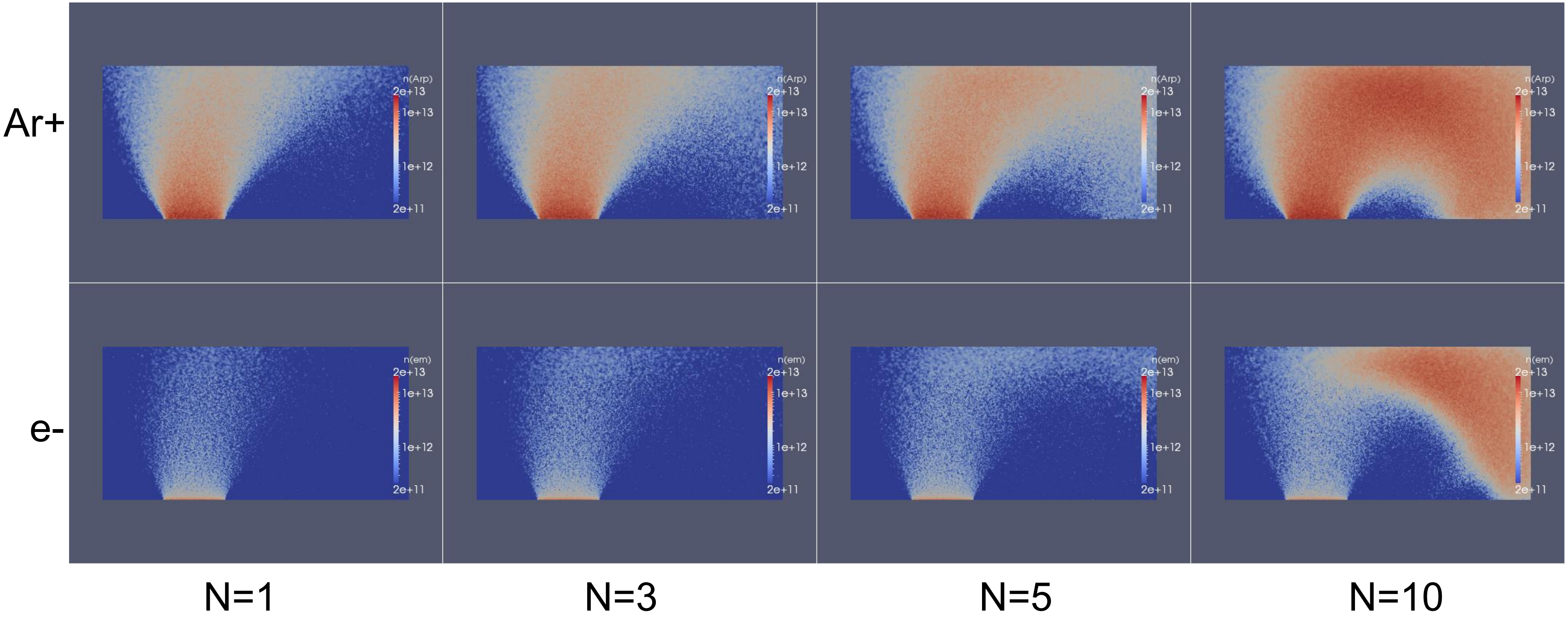


"Plan B" Develop a good initial condition for phase B:

- Why solve everything during stage A, especially at the e- time step?
- Solve a series of quasi-static stages until we approach B:
  - Evolve ions at $\Delta t_{ion} = N \times \Delta t_{e-}$.
  - Find quasi-static e- solution (10 steps at Δt_{e-} from last e- solution).
  - Ionize for Δt_{ion} timestep.
  - (Neutrals are evolved at $N \times \Delta t_{ion}$ but are uninteresting for now.)

  ... repeat until there are "significant" fields, i.e., plasma (stage B).

~~3D~~ 2D Model of Accelerated Cu-Cu Arc System



Snapshot time = 1.2 ns. Background of 1 torr 300K Ar. Δt_{e-} = 25 fs. Δx = 1 um (2.8×10^{13} #/cm^3 at T_e = 0.5 eV). Work savings = N. N = 10 is clearly too far.

Vacuum Arc Modeling Summary

- Good experience in 1D.
- EXPENSIVE in 3D (but we knew that).
- Gaining more experience with breakdown in 2D and 3D.
- Mesh sizes are now a big bottleneck.
- Currently scaling OK on 10K's of cores.
- Surface models (e.g., secondary yields) are necessary but not sufficient for real (ugly) physical systems.

Future Work

- Separate "collision mesh" according to different particle interactions. Is this always a patch of PIC cells?
- Smarter ways to identify when the plasma state (fields) has changed enough to terminate subcycling.
- Interested in hybrid approaches that are compatible with accurate vacuum simulation.
- Scale to 100K+ cores.

MeVArc 2012

3rd International Workshop on Mechanisms of Vacuum Arcs
Albuquerque, New Mexico, USA
October 2 – 4, 2012

http://www.regonline.com/MeVArc2012

Topics include:
- **High electric field gradient devices (e.g., accelerators)**
- **Effect of electrode material processing**
- **Material/electrode damage characterization**
- **Primary mechanisms for discharge**
- **Diagnostic methods for interrogating breakdown, surface structure, plasma constituents, etc.**
- **Modeling and simulation**

We welcome new areas of investigation in addition to the above. The multidisciplinary nature of vacuum arcs and vacuum devices provides a rich environment for finding physics of shared interest from multiple sources.

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International Balloon Fiesta

is the following week, beginning Friday 10/5

Thank You!

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:

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

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

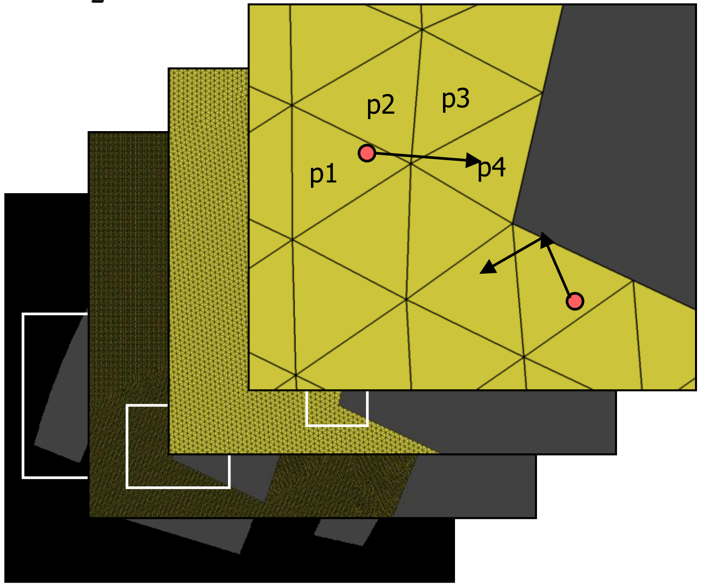
2. Compute intersections (non-trivial in parallel).
3. Transfer charges from particle mesh to static mesh.
4. Solve for $\mathbf{E}^{n+1}$,

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

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

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

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



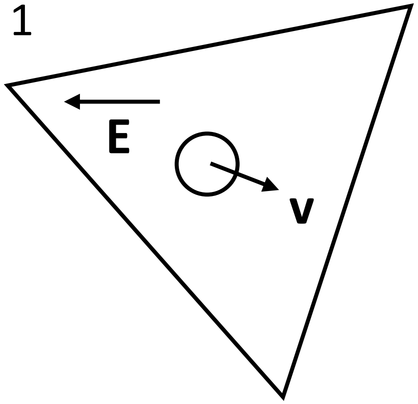
7. Perform DSMC collisions: sample pairs in element, determine cross section and probability of collision. Roll a digital die, and if they collide, re-distribute energy.
8. Perform chemistry: for each reaction, determine expected number of reactions. Sample particles of those types, perform reaction (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).

Cloning

1. Choose a high weight parent particle.
2. Generate a pair of random positions in the element, symmetric about the parent position.
3. Compute modified velocities at the new positions by accounting for displacement in the potential field.
4. If nonphysical velocities result, repeat 2-3.
5. Adjust weights for parent and new particles.

Repeat 1-5 until target number or limiter is met.

1



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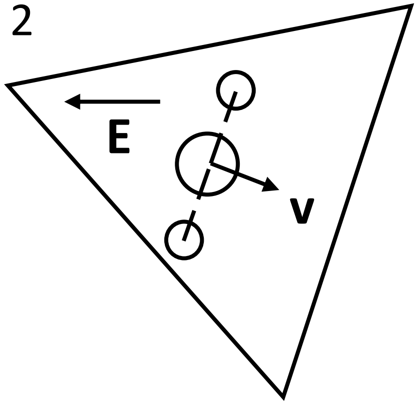

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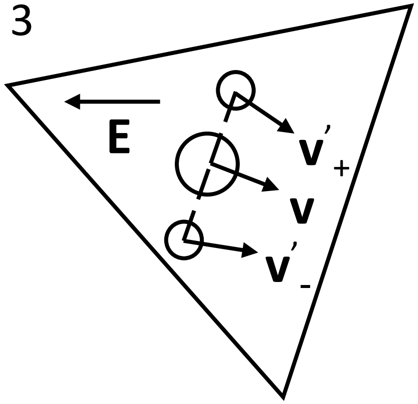

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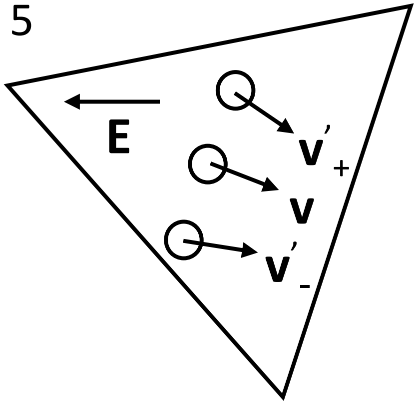
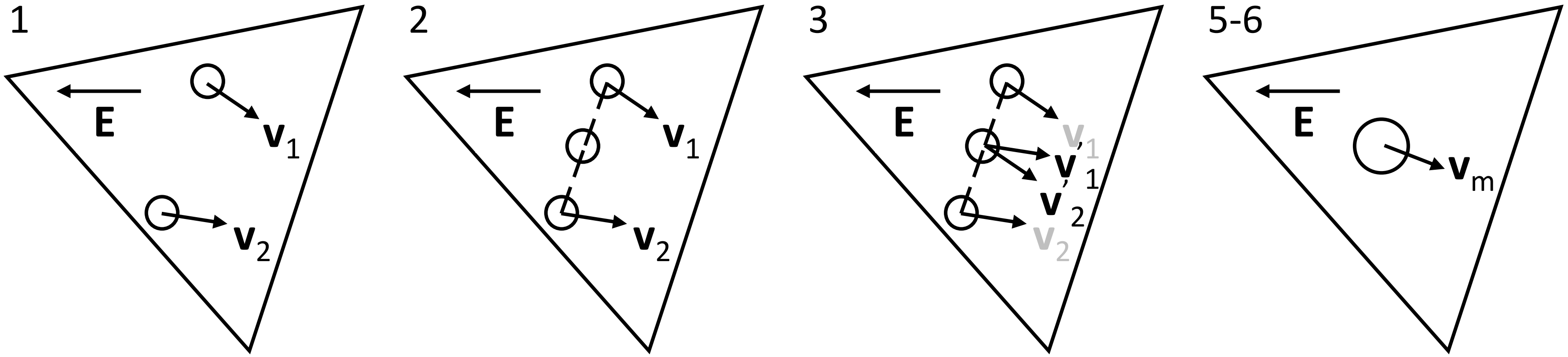


Merging

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.



Merging

What makes particles “too different” to merge?

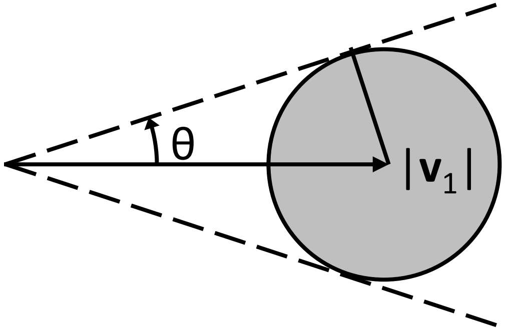
Only approve merge pairs that are close in both position and velocity – close in phase space.

The spatial bin is the element, approves any pair.

The velocity bin has many options. Can use MC sampling to select pairs randomly. (let $|\mathbf{v}_1| < |\mathbf{v}_2|$)

Velocity Sphere

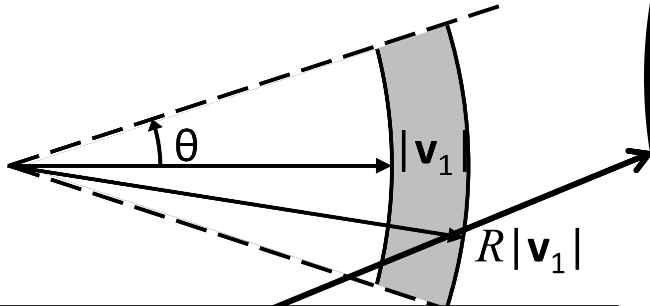
$$\left|\mathbf{v}_2 - \mathbf{v}_1\right| < \left|\mathbf{v}_1\right| \sin(\theta)$$



Velocity Proportion

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

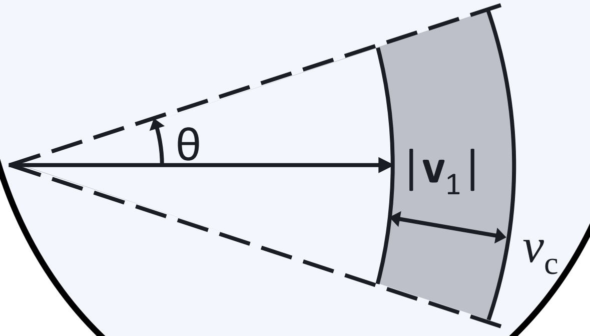
$$\left|\mathbf{v}_2\right| < R\left|\mathbf{v}_1\right|$$



Velocity Interval

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

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



We use this, plus sorting the S particles by energy in each cell to increase chances of finding merge partner.

Example: Growing Xe Sheaths

Injection

V = 5V

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

v_D = 3 cm/μs

T_e = 1eV

T_{Xe+} = 300K

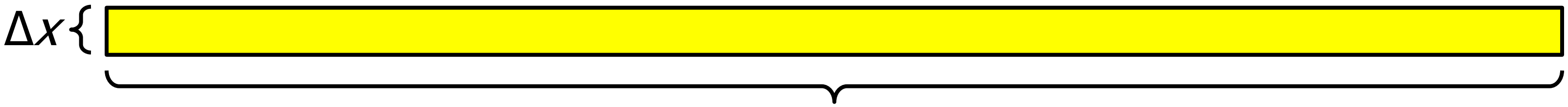
Side walls

$dV/dn = 0$

specular

Wall

V = 0V



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

Bulk plasma parameters

v_{Bohm} = 0.086 cm/μs

λ_D = 7.4 x 10^{-3} cm to 7.4 x 10^{-4} cm

Δx = 2.5 x 10^{-4} cm

Δt = 20 ps

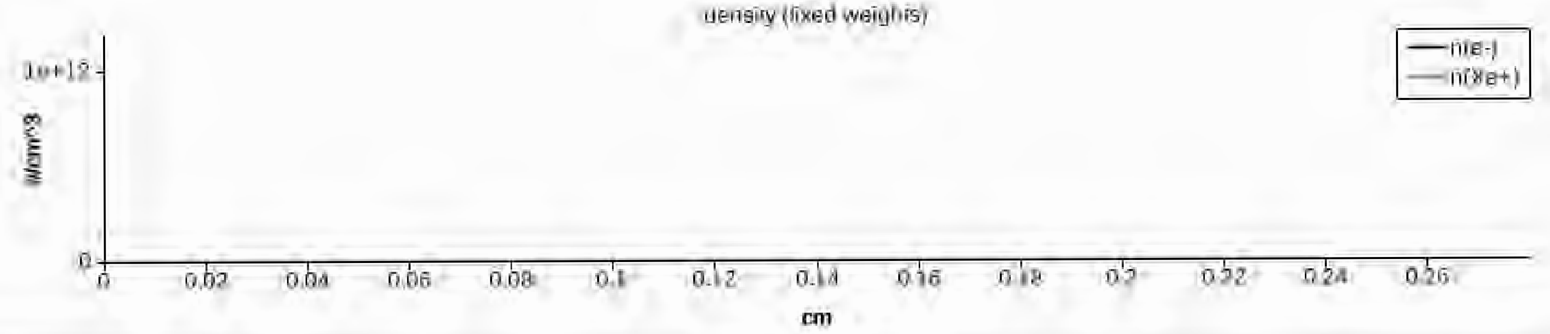
$\lambda_D / \Delta x$ = 30 to 3

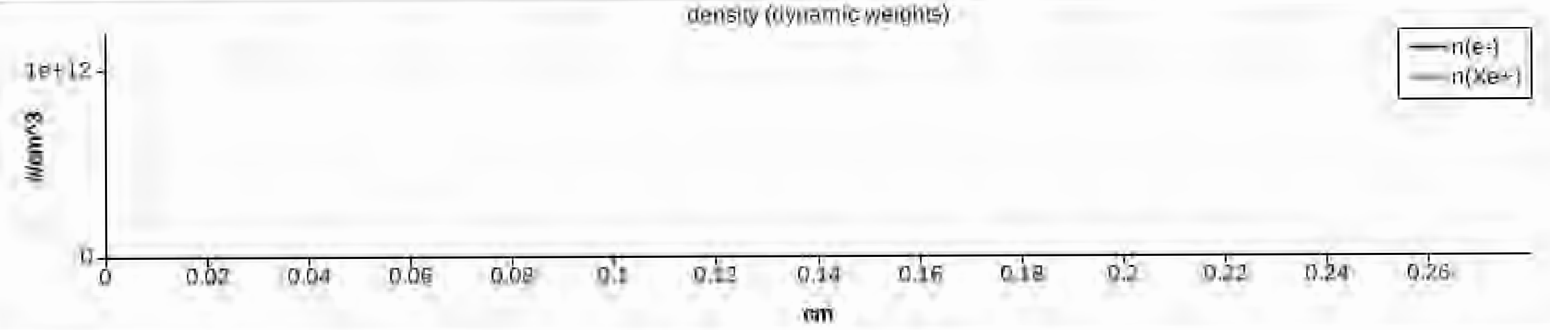
$\omega_p \Delta t$ = 0.11 to 1.1

Two solutions:

- Fixed particle weight
- Dynamic particle weight (Merge + Clone)

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


density (fixed weights)
1e+12
#/cm^3
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm
n(e-)
n(Xe+)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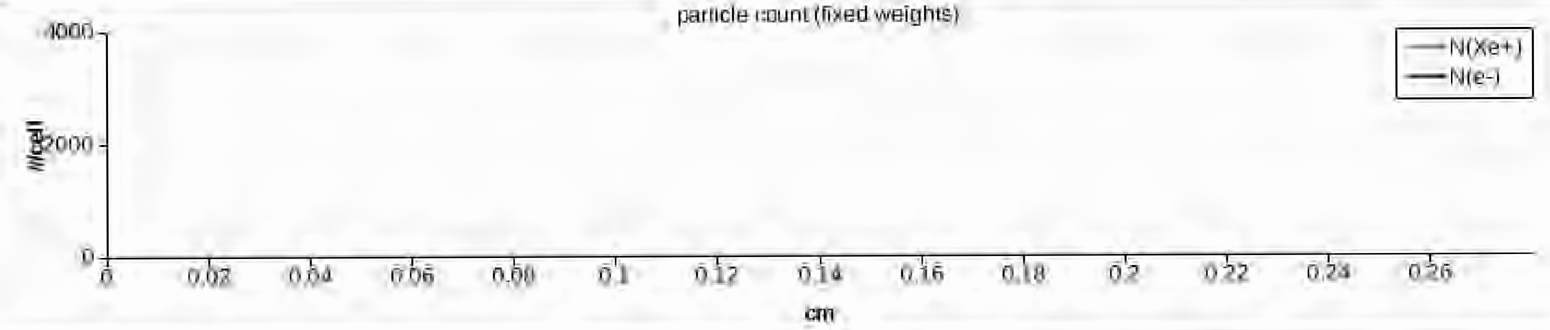
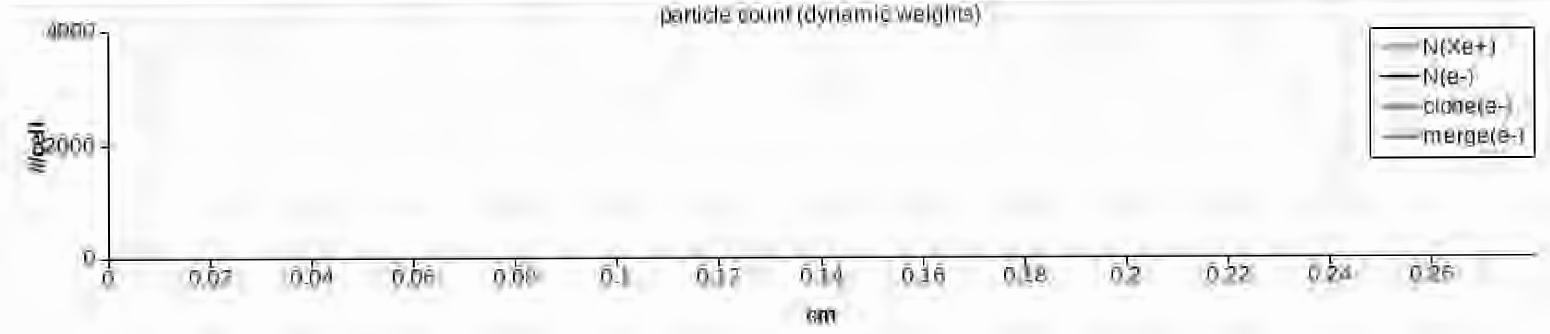
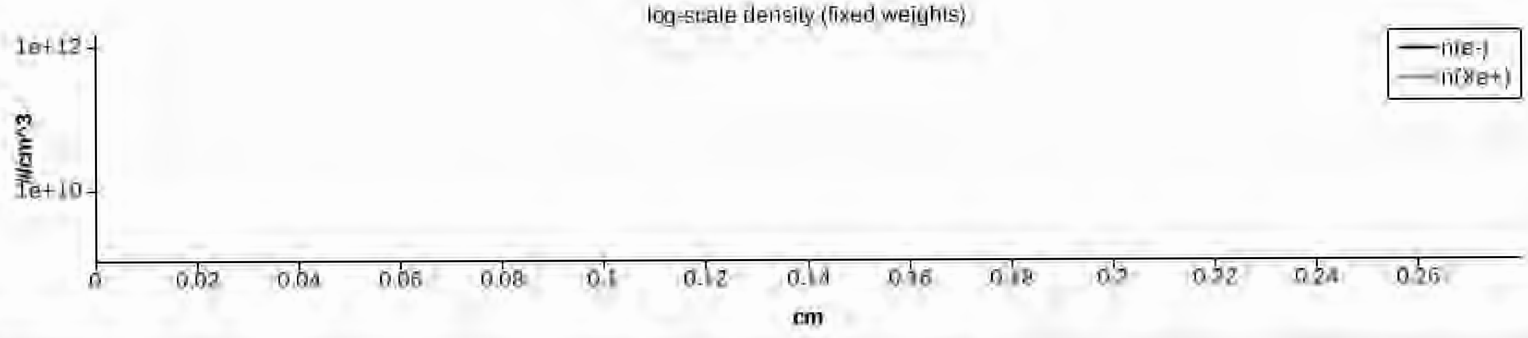
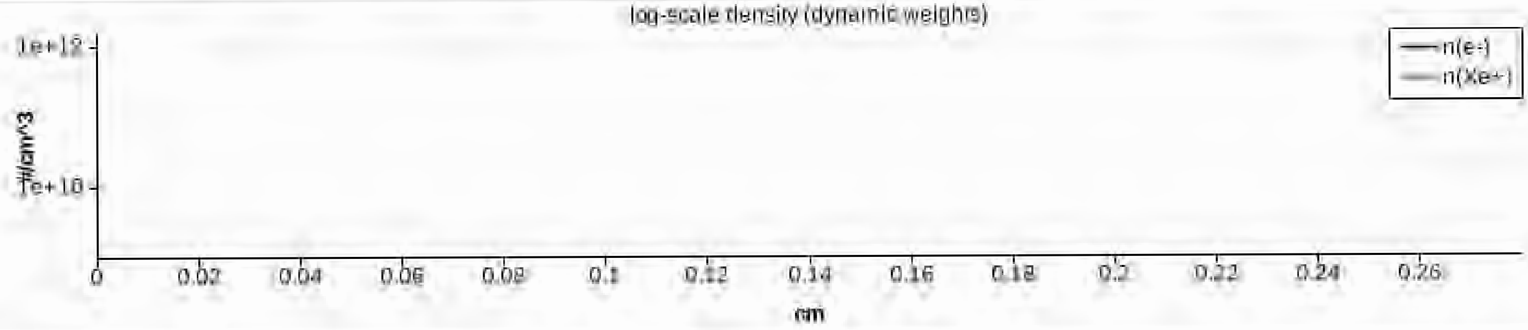
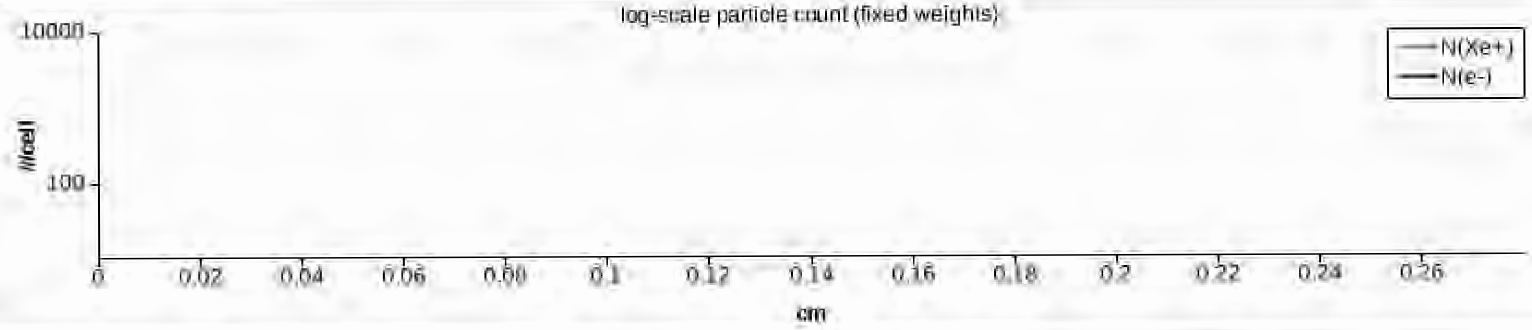
1e+12
#/cm^3
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm
n(e-)
n(Xe+)

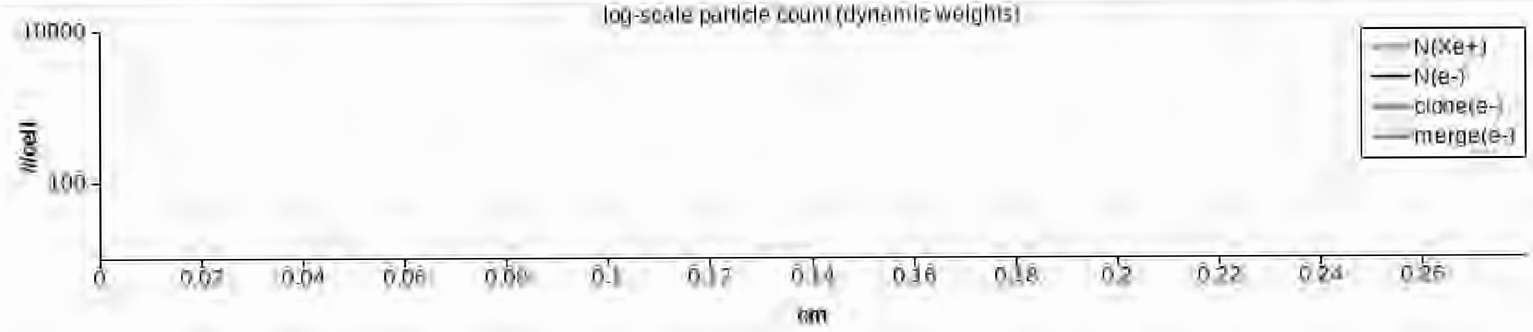

particle count (fixed weights)
4000
2000
#/cell
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm
N(Xe+)
N(e-)

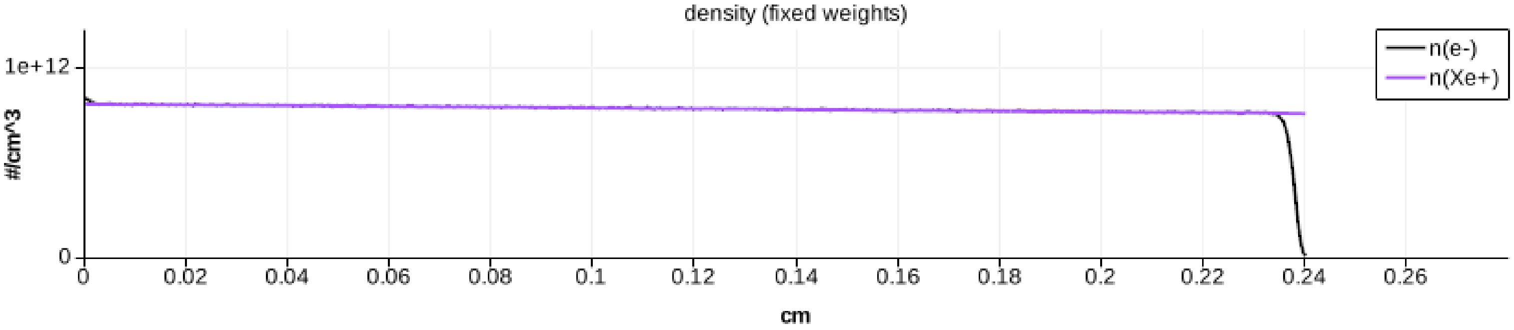

particle count (dynamic weights)
4000
2000
#/cell
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm
N(Xe+)
N(e-)
clone(e-)
merge(e-)


log-scale density (fixed weights)

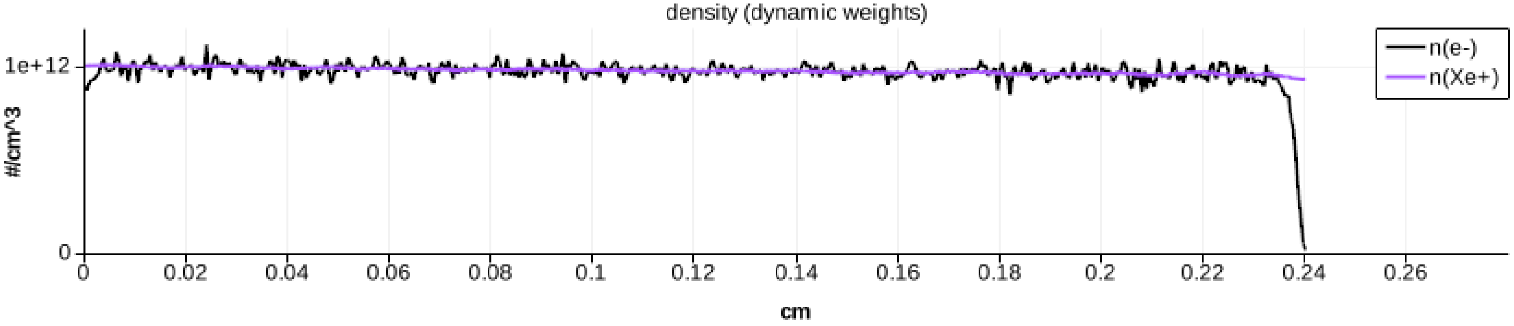

log-scale density (dynamic weights)


log-scale particle count (fixed weights)

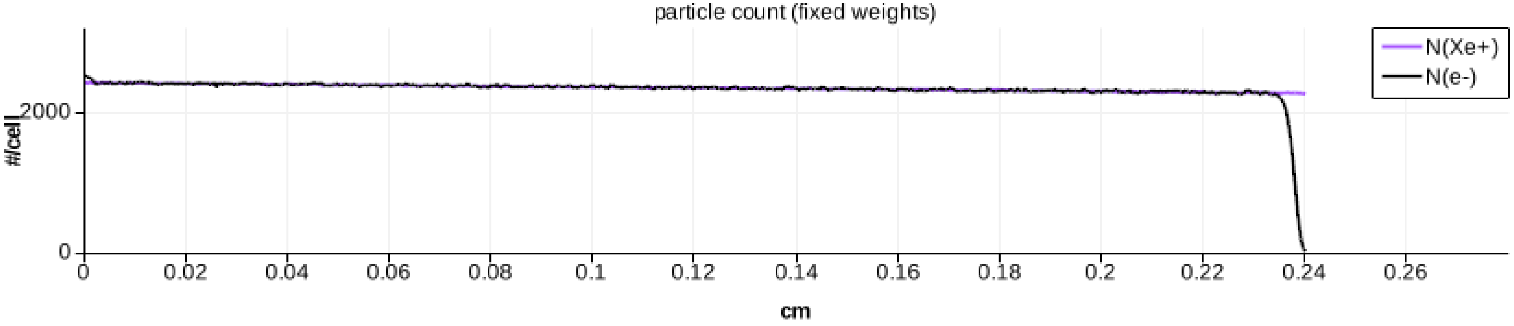

log-scale particle count (dynamic weights)

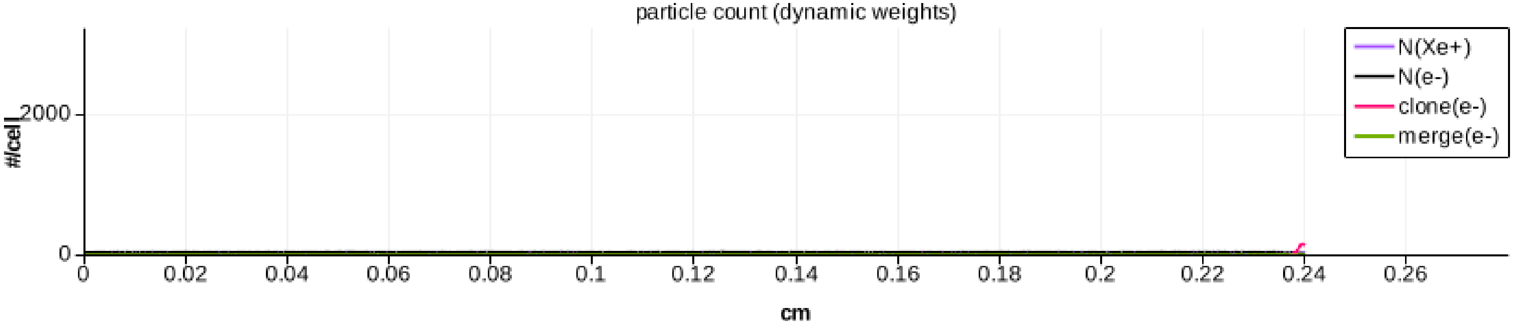

density (fixed weights)

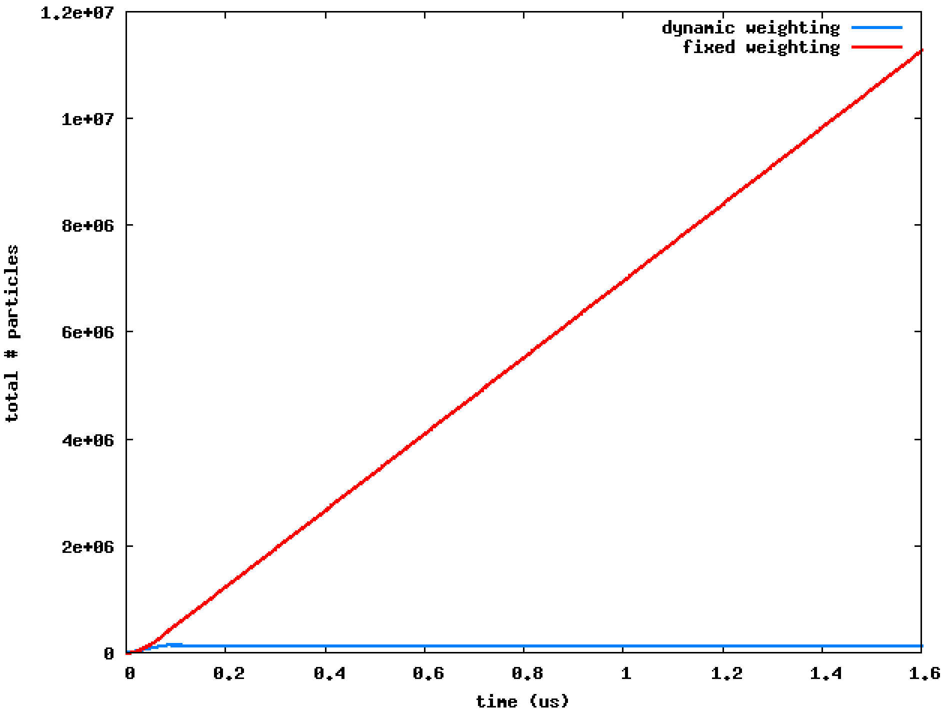
147371s,
= 11M

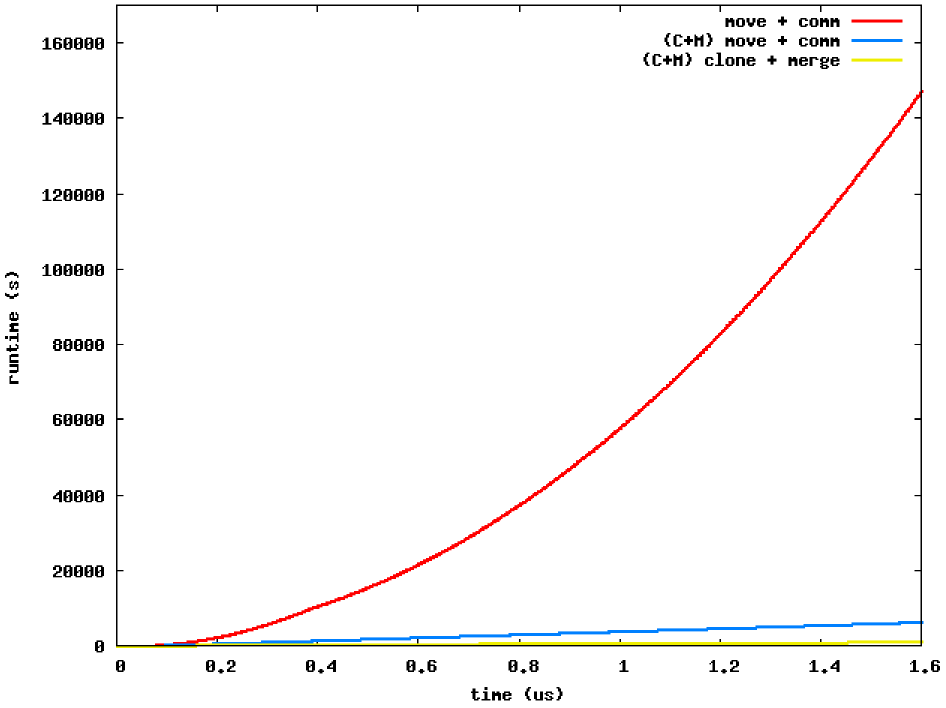

density (dynamic weights)

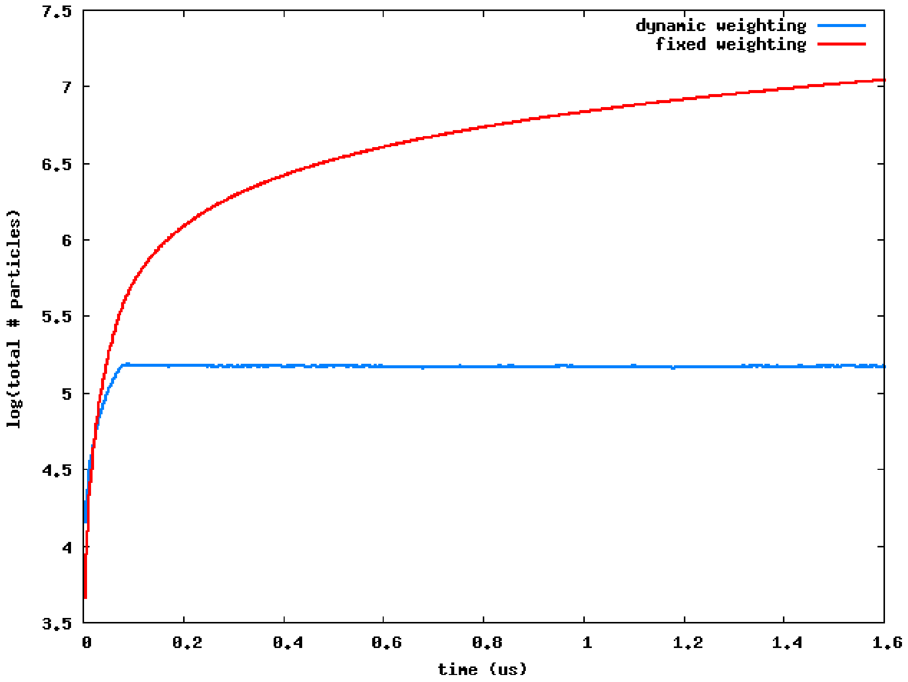
7435s,
= 150k


particle count (fixed weights)


particle count (dynamic weights)







95% reduction in runtime!

Example: 1D Cu Arcs

No reweighting

30138s total

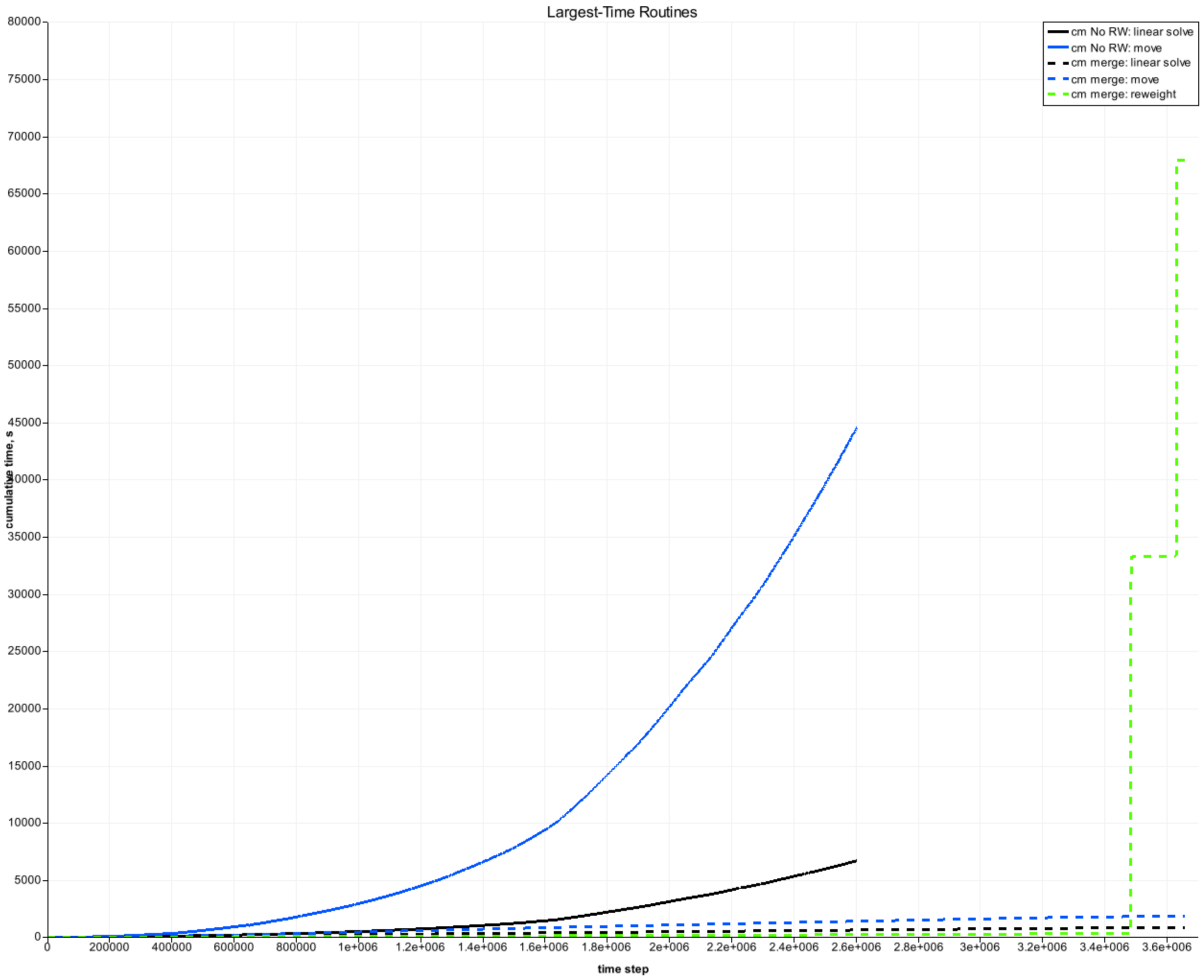
Reweighting all species

882s move

+ 148s reweighting

= 1030s total

97% reduction in runtime!



Dynamic Particle Weighting Summary

- Dynamic particle reweighting can provide very significant savings in runtime.
- As with every other model/algorithm, one size does *not* fit all!
- Good target: transient growing simulations where accuracy is required at all timescales.
- Bad target: simulations with essentially fixed densities.
- Current headache: varying element sizes.

Future Work

- Allow [N_{low}, N_{high}] to vary by location, time, element size, collisionality, other state parameters, ...
- Better ways to correct for energy discrepancies. Have considered creating the upper triangular N_S x N_S matrix of energy discrepancies to merge the optimum pairs. “Full pivot merge”
- Identify a good problem where cloning does more than just provide smooth output. E.g., reaction system based on trace species. Cloning will provide more particles of the trace species for less noise in the reaction rate.

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 capabili

SV: Solution the right solution

V: Validati ality. Ideally, tion verificat

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

SA: Sensitiv ermine which numerical/physical parameters impact the 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.