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Dynamic Particle Weighting and Velocity Distributions

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National Nuclear Security Administration

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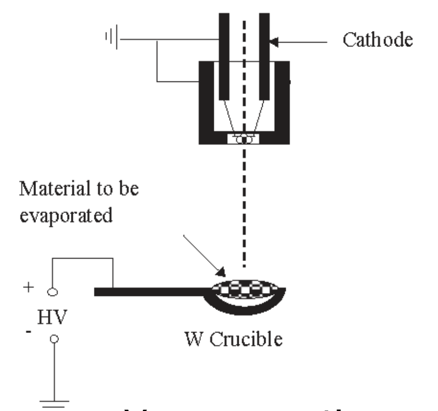
Modeling Needs and Challenges

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

- 2D or 3D Cartesian
- Hybrid PIC + DSMC
- Electrostatics
- Fixed B field
- Solid conduction
- Ambipolar approximation
- Dual mesh (Particle and Electrostatics/Output)
- Advanced surface (electrode) physics models
- Collisions, charge exchange, chemistry, excited states, ionization
- Advanced particle weighting methods
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for easily extending BCs, post-processed quantities, etc.
- Currently utilizing ~1000’s of processors (>30M elements, >1B particles)

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:

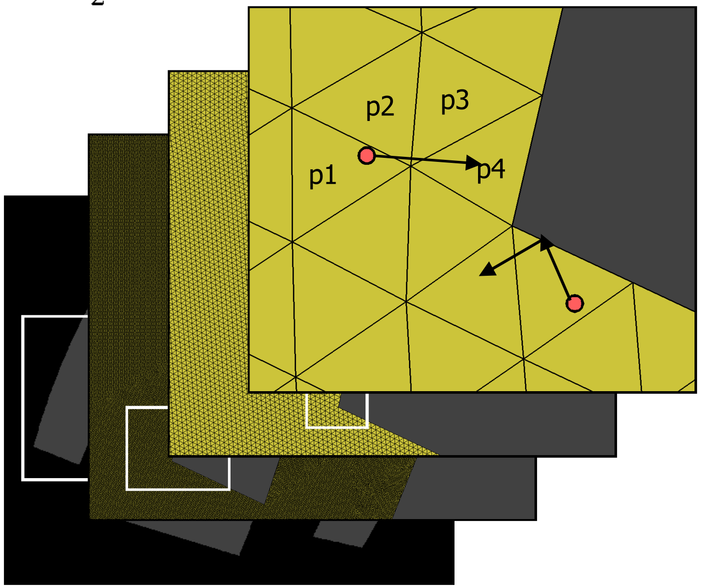
$$v_i^{n+1/2} = v_i^n + \frac{\Delta t}{2}\left(\frac{q_i}{m_i}\mathbf{E}^n\right)$$

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

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. Sometimes.
10. Compute post-processing and other quantities and write output.
11. Rebalance particle mesh if appropriate (variety of determination methods).

Dynamic Particle Reweighting

- Maintain velocity distribution function (vdf) to the extent possible (don't assume Maxwellian). Don't use grid-based methods – don't "resample" particle velocities.
- All other PIC/DSMC internals adapted to include variably weighted particles – every particle can have a different weight.
- Minimize energy discrepancy when it cannot be avoided.

Basic idea:

for each cell,

for each particle type *S*,

let N_s = # of particles of type *S*

if $N_s < N_{low}$

clone more *S* particles

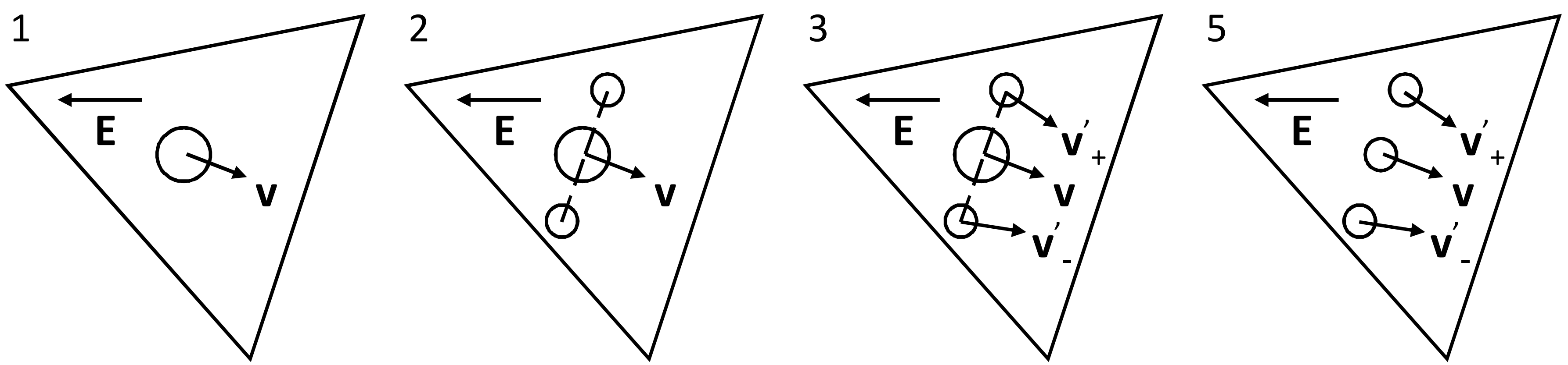
if $N_s > N_{high}$,

merge some *S* particles

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.

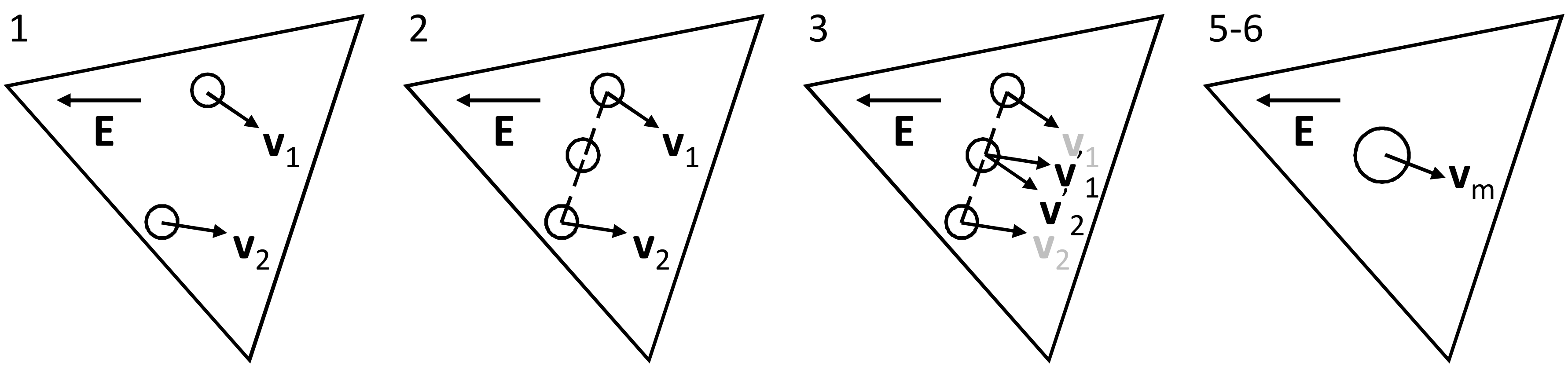
Repeat 1-5 until target number or limiter is met.



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 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?

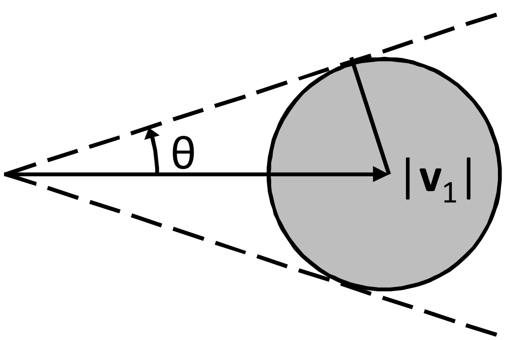
Only approve merge pairs that are close in both position and velocity – close in phase space.

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

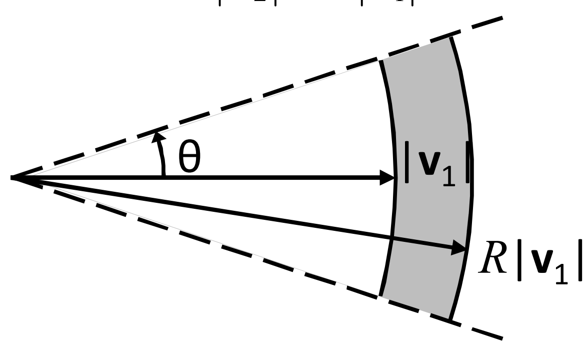
$$\left|\mathbf{v}_2 - \mathbf{v}_1\right| < \left|\mathbf{v}_1\right| \sin(\theta)$$



Velocity Proportion

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

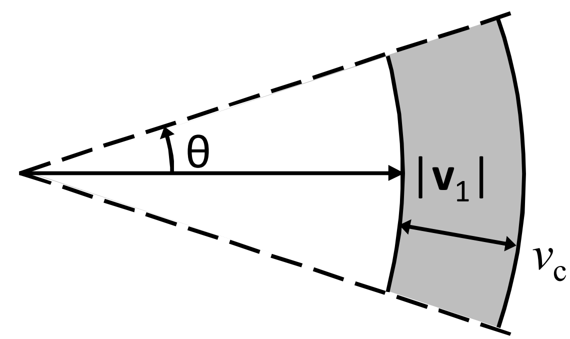
$$\left|\mathbf{v}_2\right| < R\left|\mathbf{v}_1\right|$$



Velocity Interval

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

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

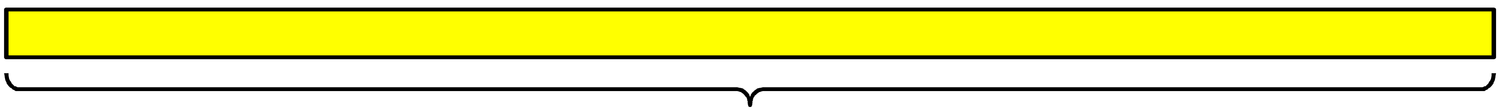


Example: Xe Sheaths

Injection
V = 5V
$n_{Xe+} = n_e = 10^{10}/cm^3$
v_D = 3 cm/μs
T_e = 1eV
T_{Xe+} = 300K

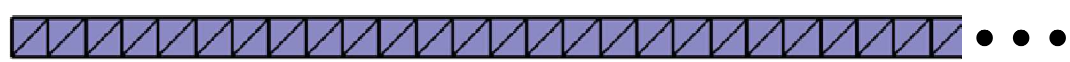
Side walls
$dV/dn = 0$
specular

Wall
V = 0V

Δx {


$10\lambda_D = 300\Delta x$

Bulk plasma parameters
v_{Bohm} = 0.086 cm/μs
$\lambda_D = 7.4 \times 10^{-3}$ cm
$\Delta x = 2.5 \times 10^{-4}$ cm
Δt = 20 ps
$\lambda_D / \Delta x = 30$
$\omega_p \Delta t = 0.11$

Left side of mesh


Two solutions:
- Fixed particle weight
- Dynamic particle weight (Merge + Clone)

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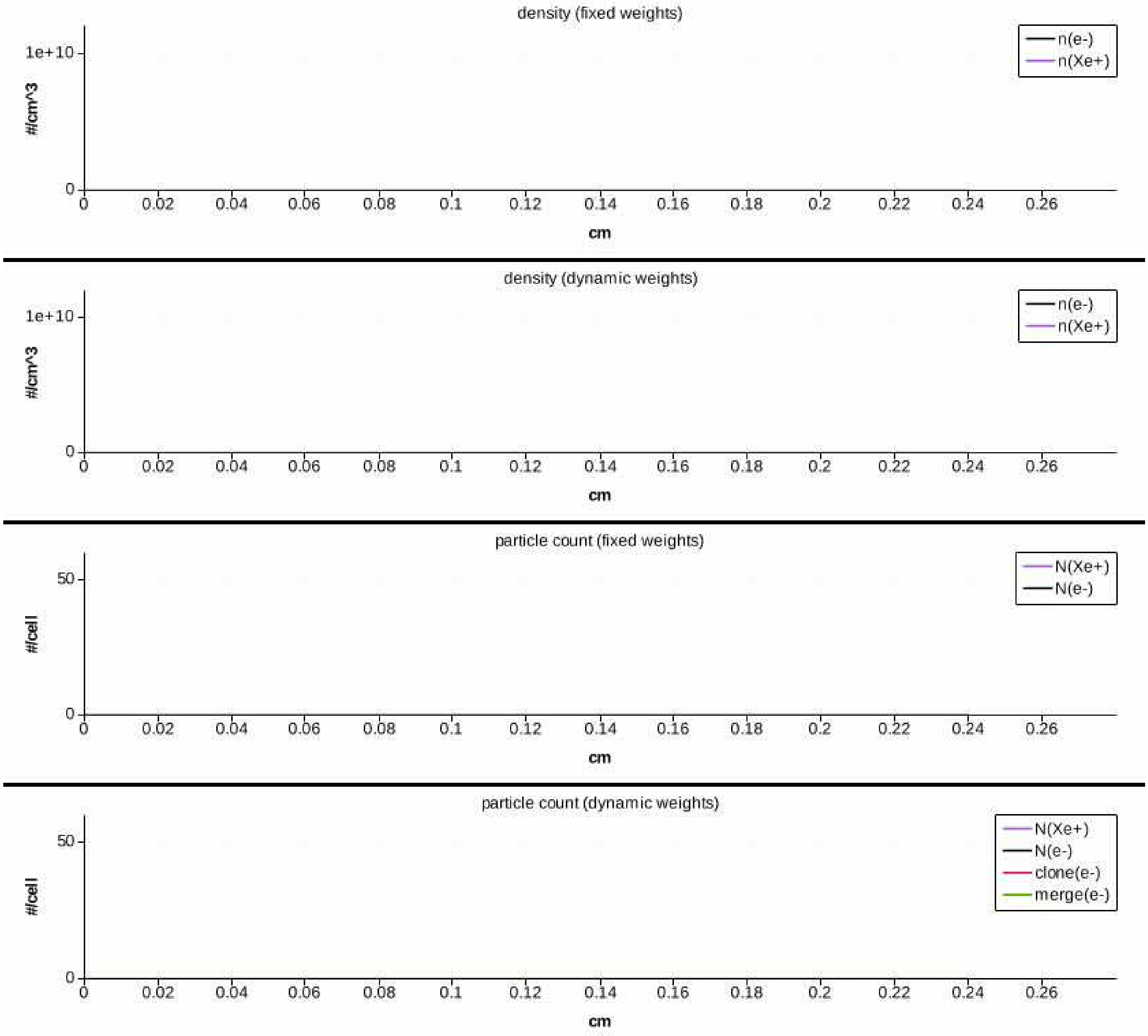
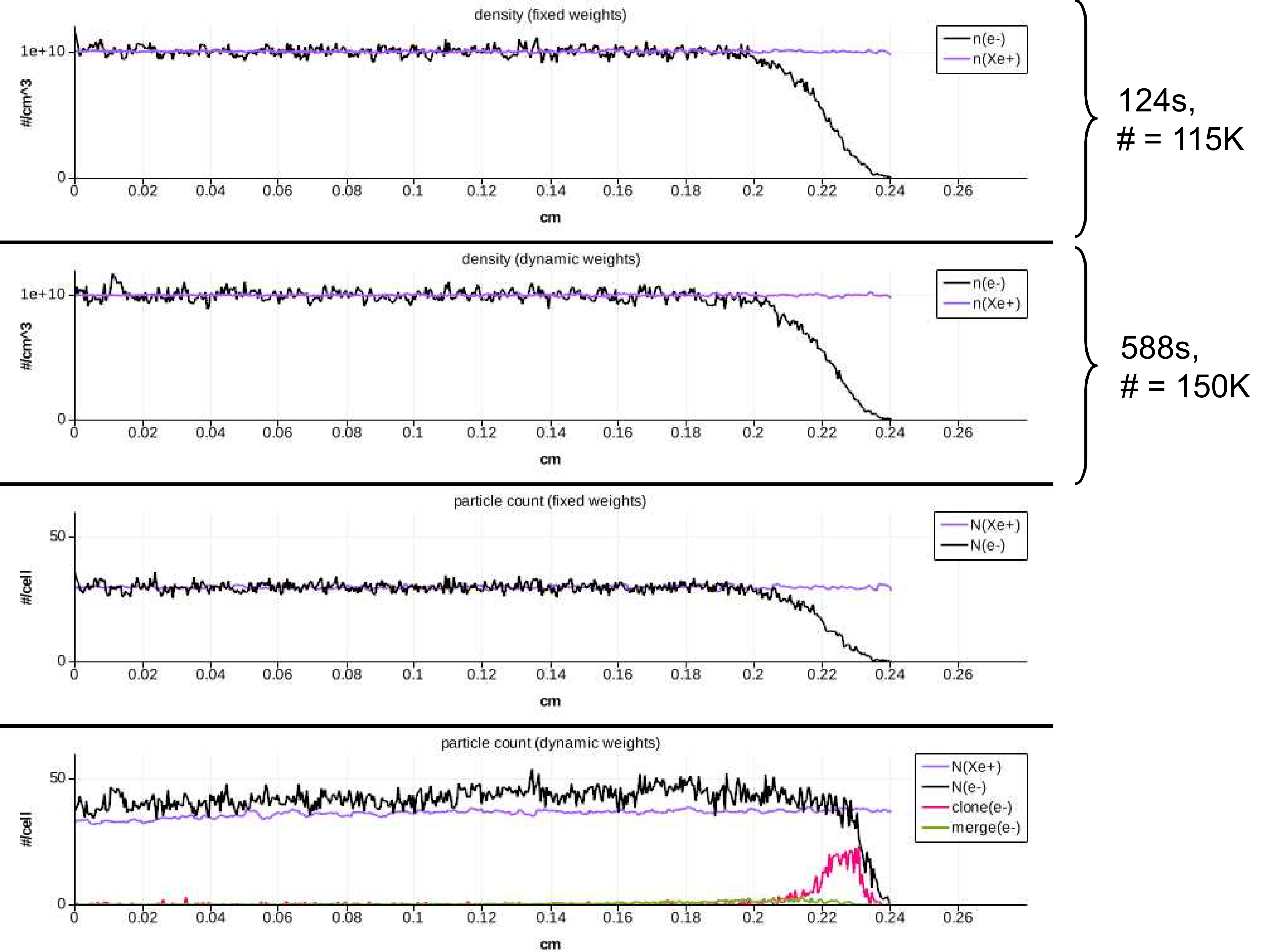

density (fixed weights)
1e+10
0
#/cm^3
0 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16 0.18 0.2 0.22 0.24 0.26
cm
n(e-)
n(Xe+)
density (dynamic weights)
1e+10
0
#/cm^3
0 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16 0.18 0.2 0.22 0.24 0.26
cm
n(e-)
n(Xe+)
particle count (fixed weights)
50
0
#/cell
0 0.02 0.04 0.06 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)
50
0
#/cell
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-)


density (fixed weights)
n(e-)
n(Xe+)
#/cm^3
cm
density (dynamic weights)
n(e-)
n(Xe+)
#/cm^3
cm
particle count (fixed weights)
N(Xe+)
N(e-)
#/cell
cm
particle count (dynamic weights)
N(Xe+)
N(e-)
clone(e-)
merge(e-)
#/cell
cm
124s,
= 115K
588s,
= 150K

Example: Growing Xe Sheaths

<u>Injection</u>

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

<u>Side walls</u>

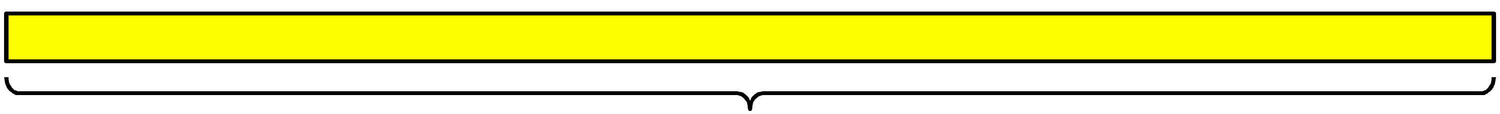
$dV/dn = 0$

specular

<u>Wall</u>

V = 0V

Δx {



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

<u>Bulk plasma parameters</u>

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

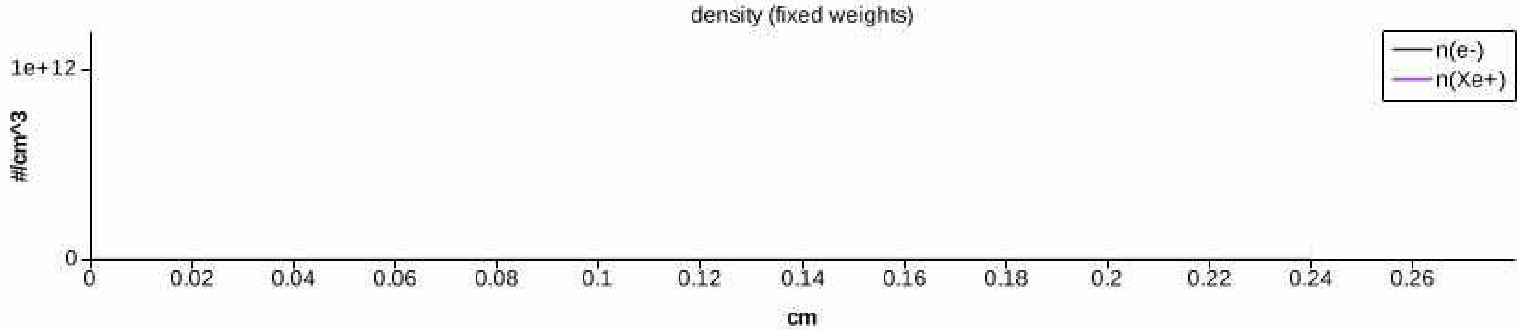
$\lambda_D / \Delta x$ = 30 to 3

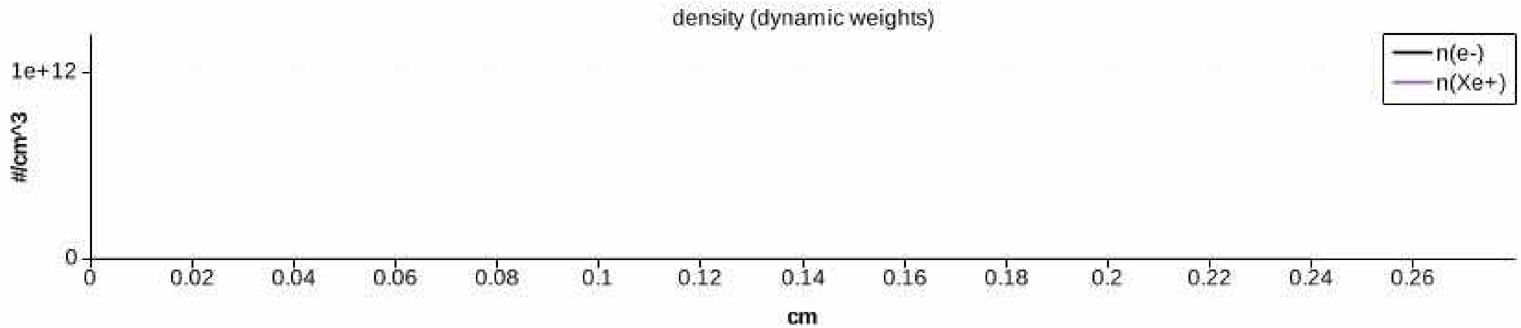
$\omega_p \Delta t$ = 0.11 to 1.1

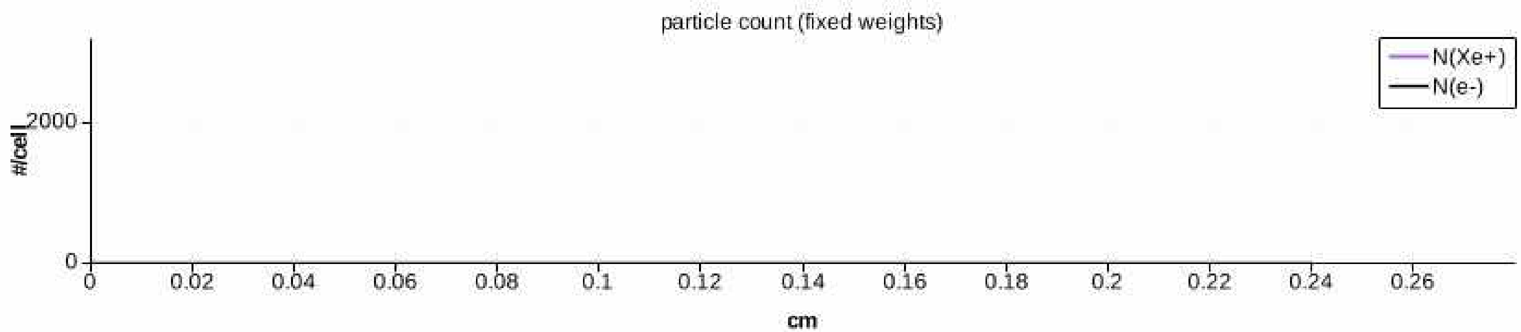
Two solutions:

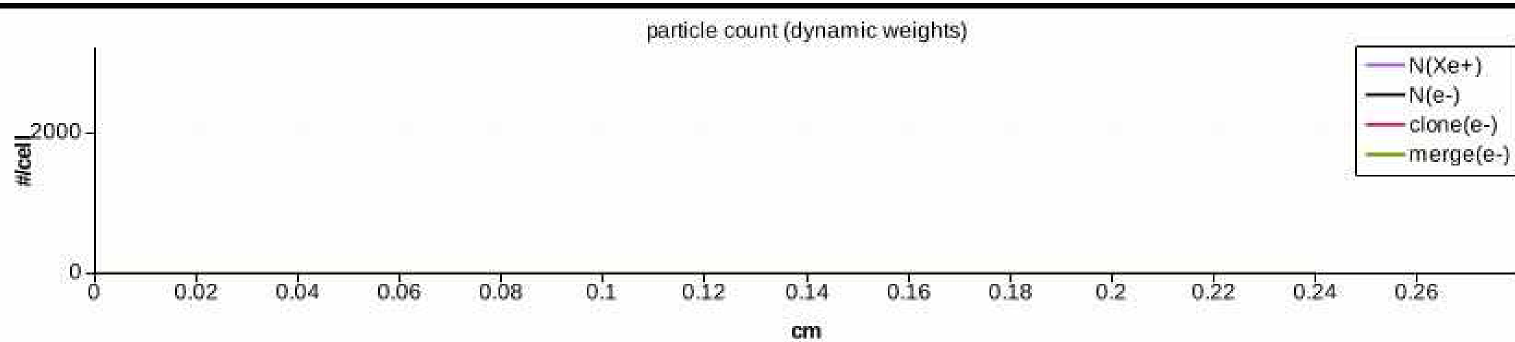
- Fixed particle weight
- Dynamic particle weight (Merge + Clone)

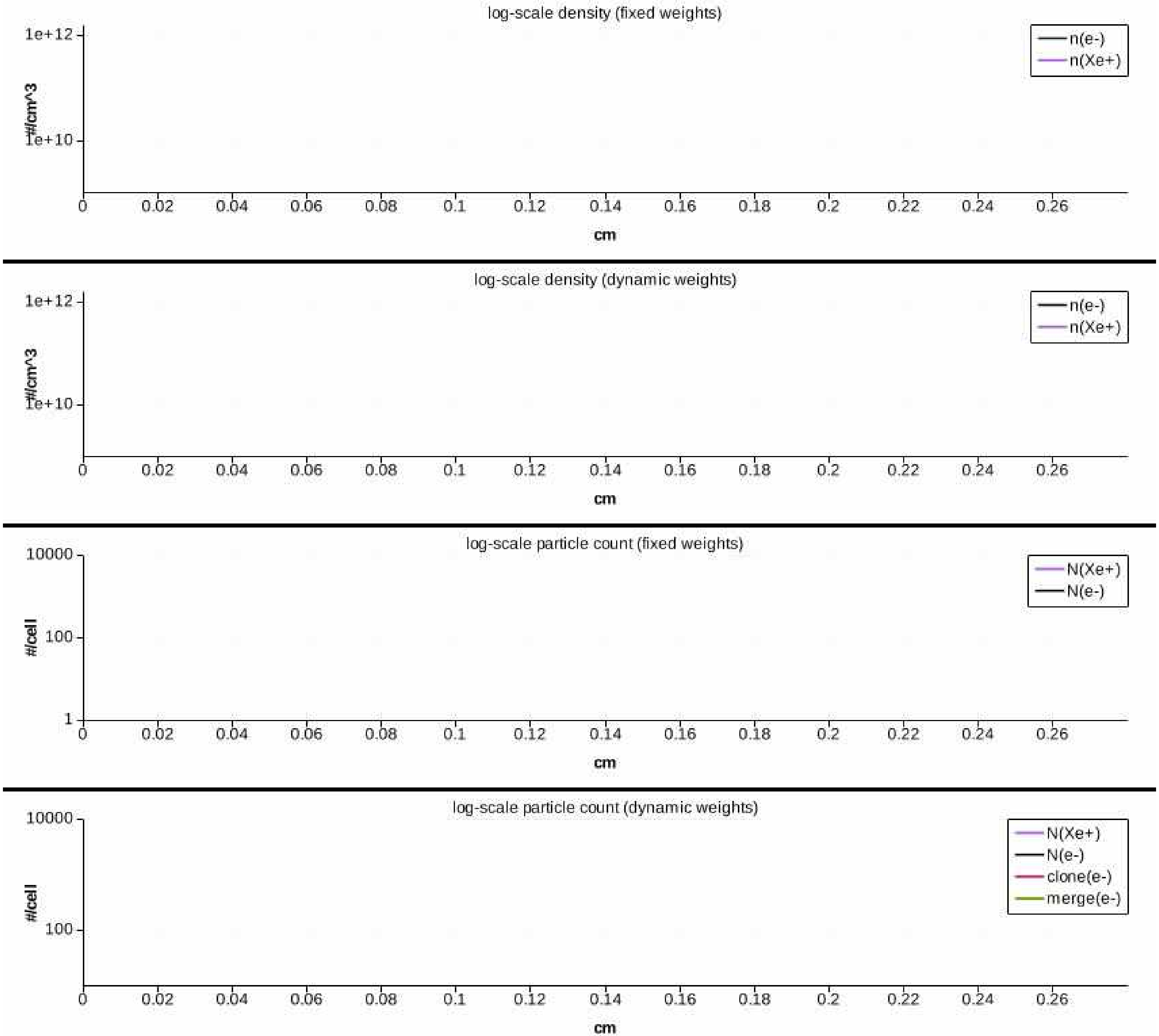
Small weight vs. large weight vs. requirements...

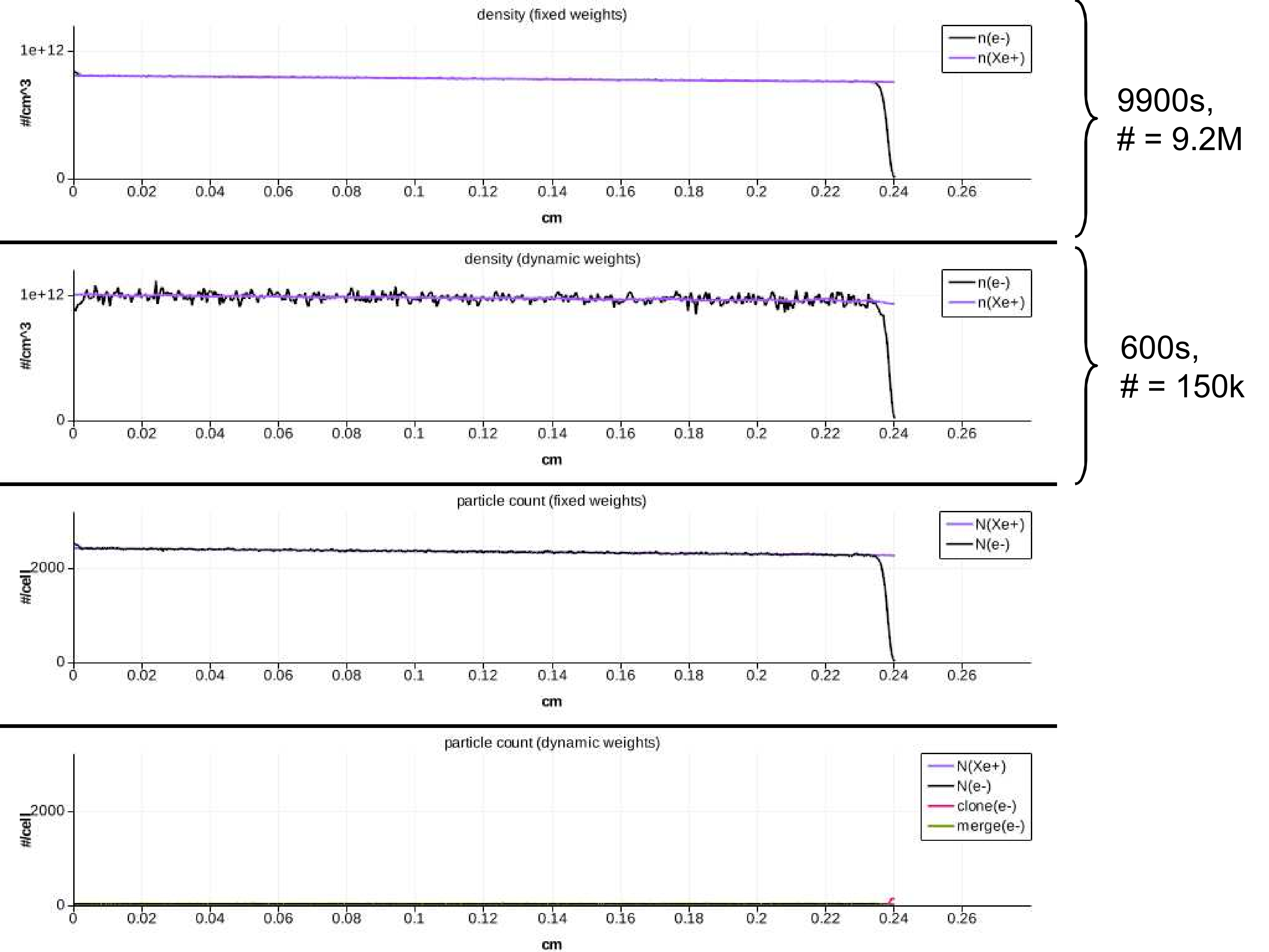

density (fixed weights)
n(e-)
n(Xe+)
1e+12
0
#/cm^3
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm

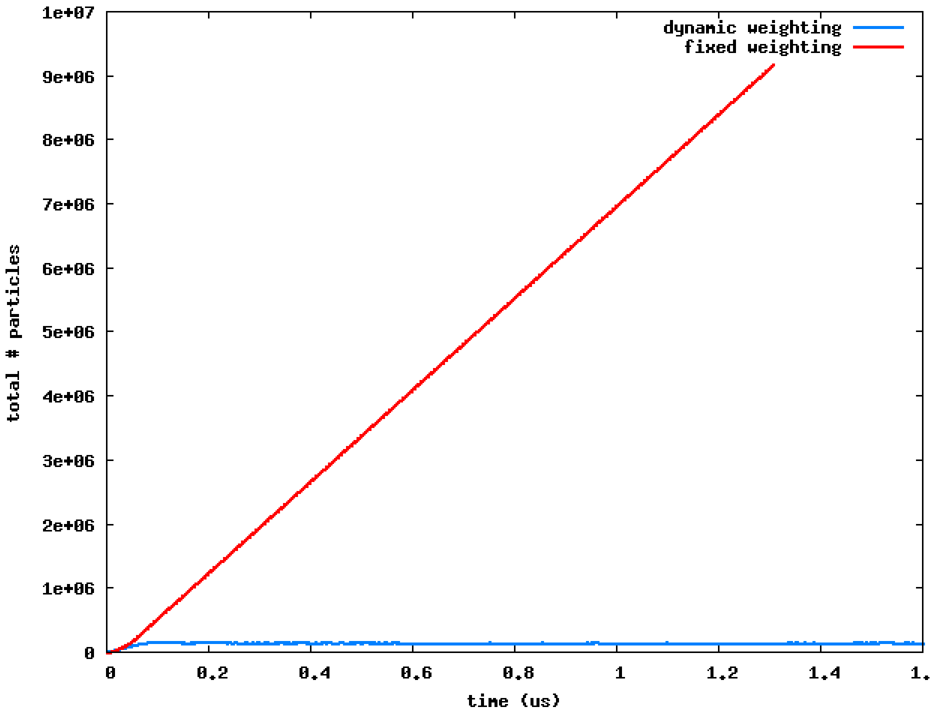

density (dynamic weights)
n(e-)
n(Xe+)
1e+12
0
#/cm^3
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm

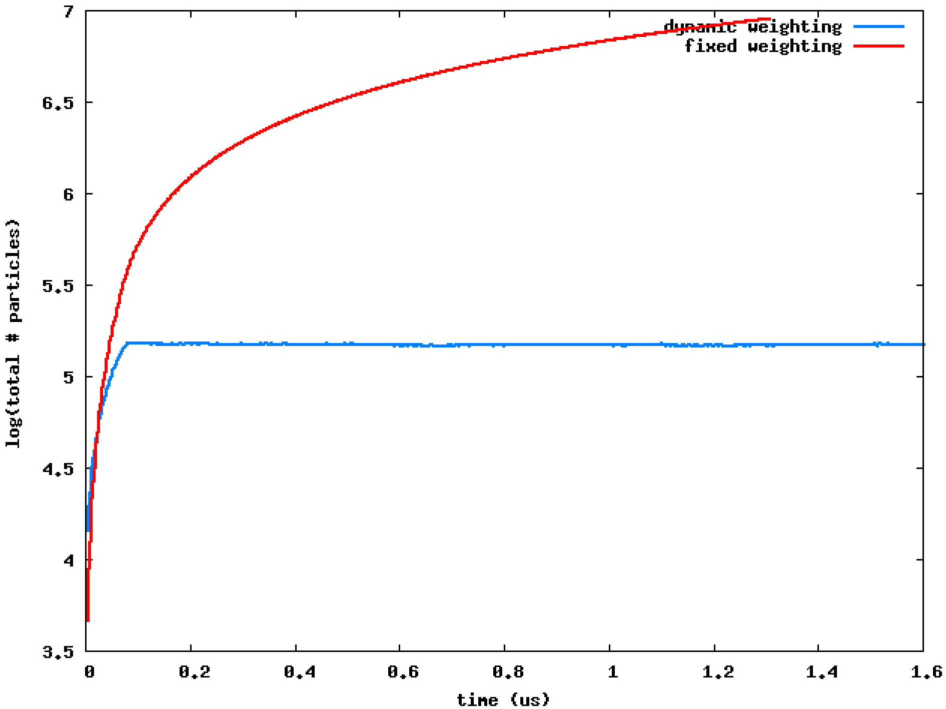

particle count (fixed weights)
N(Xe+)
N(e-)
2000
0
#/cell
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm

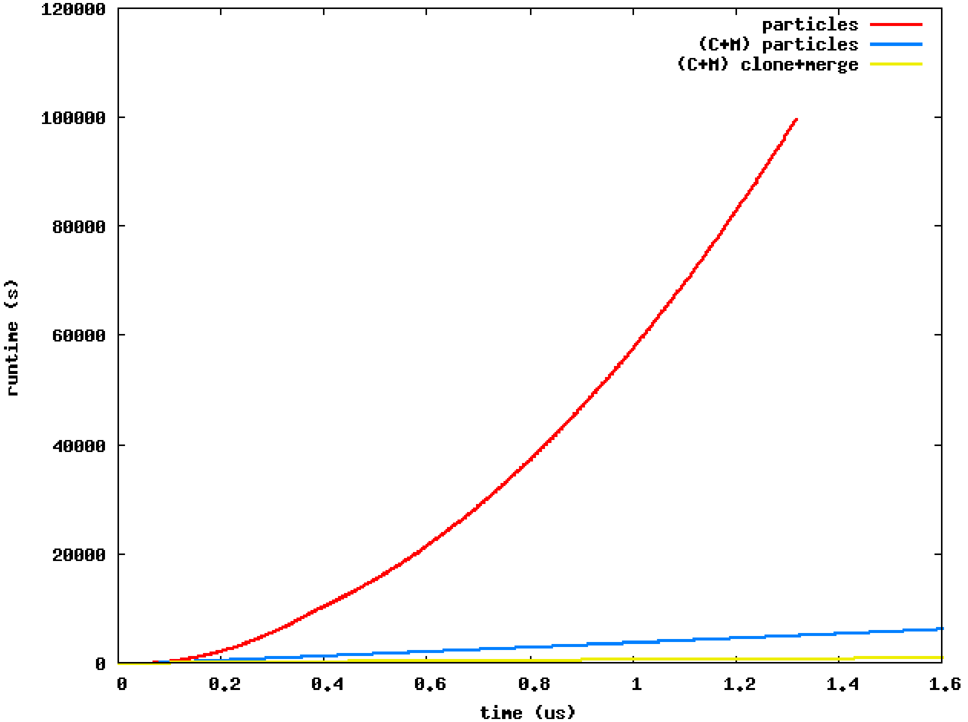

particle count (dynamic weights)
N(Xe+)
N(e-)
clone(e-)
merge(e-)
2000
0
#/cell
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
0.22
0.24
0.26
cm


log-scale density (fixed weights)
1e+12
1e+10
#/cm^3
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+)
log-scale density (dynamic weights)
1e+12
1e+10
#/cm^3
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+)
log-scale particle count (fixed weights)
10000
100
1
#/cell
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-)
log-scale particle count (dynamic weights)
10000
100
#/cell
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-)


density (fixed weights)
n(e-)
n(Xe+)
#/cm^3
1e+12
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
9900s,
= 9.2M
density (dynamic weights)
n(e-)
n(Xe+)
#/cm^3
1e+12
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
600s,
= 150k
particle count (fixed weights)
N(Xe+)
N(e-)
#/cell
2000
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
particle count (dynamic weights)
N(Xe+)
N(e-)
clone(e-)
merge(e-)
#/cell
2000
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







94% reduction in runtime!

Example: 1D Cu Arcs

Injection "cathode"

f_{Cu} = 10^{22}/cm^2/s

f_e = 10^{24}/cm^2/s

$v_{Cu} = v_e$ = 0m/s

T_e = 2.9 x 10^3K

T_{Cu} = 2.9 x $10^6 K$

V = 0V

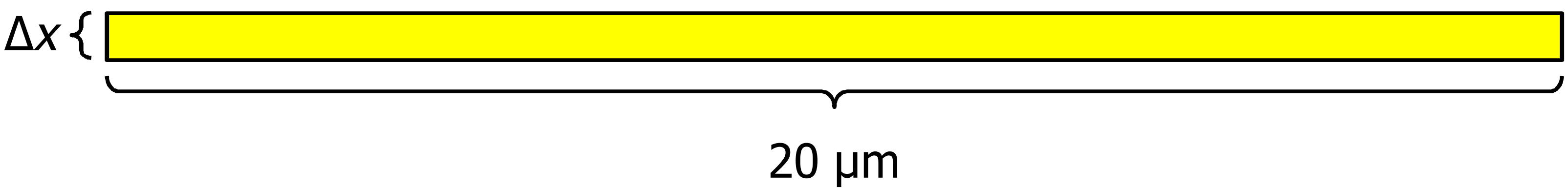
Side walls

dV/dn = 0

specular

Wall "anode"

V = 10kV



Both "electrode" surfaces sputter

e- → Cu (2.9 x 10^6K) at 1% yield

Cu → Cu+ (2.9 x 10^6K) at 100% yield

Cu is also reflected specularly

Simulation parameters

Δx = 2.5 x 10^{-4} cm

Δt = 1 fs

One bulk reaction

e- + Cu → e- + Cu+ + e-

Two solutions:

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

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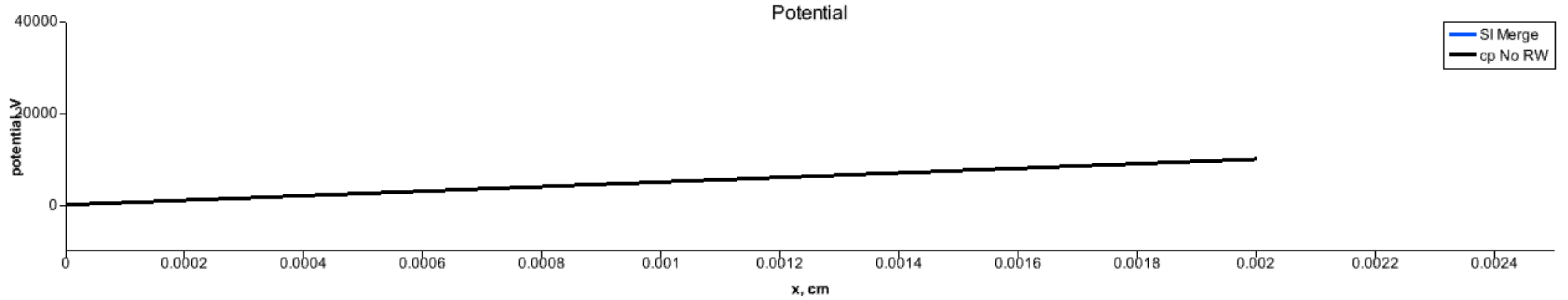
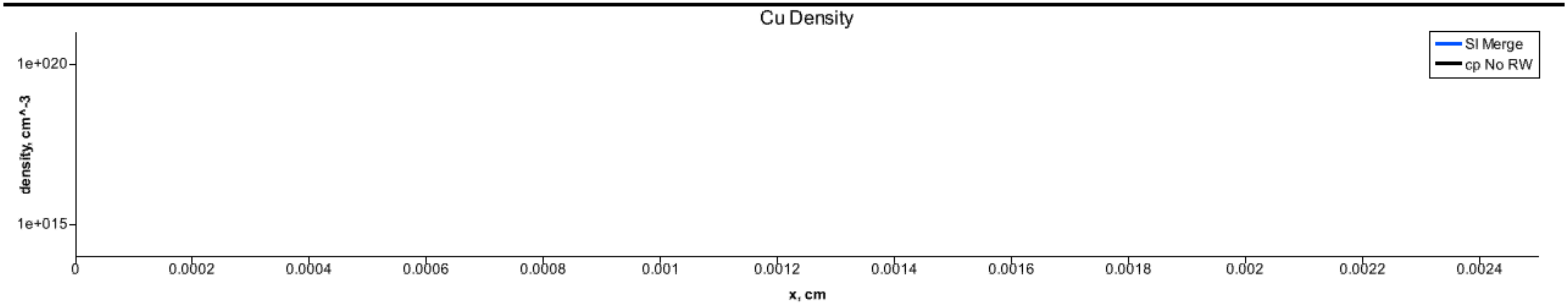
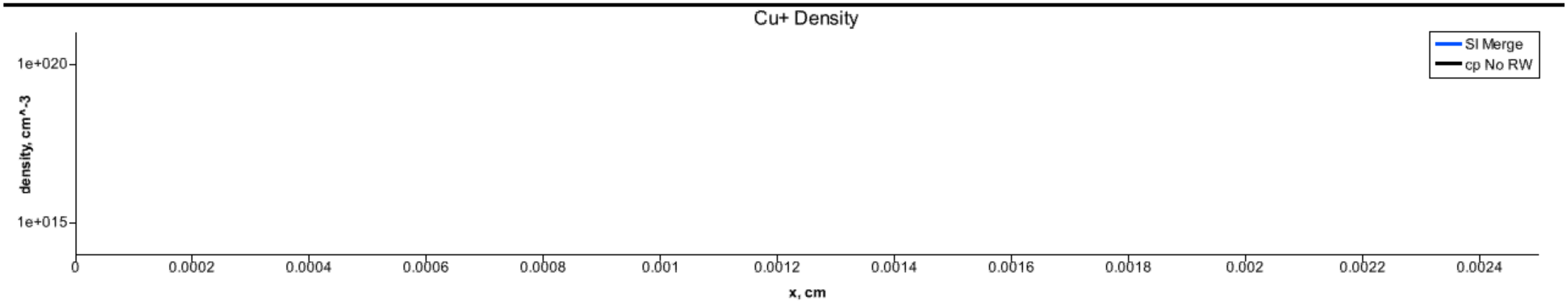
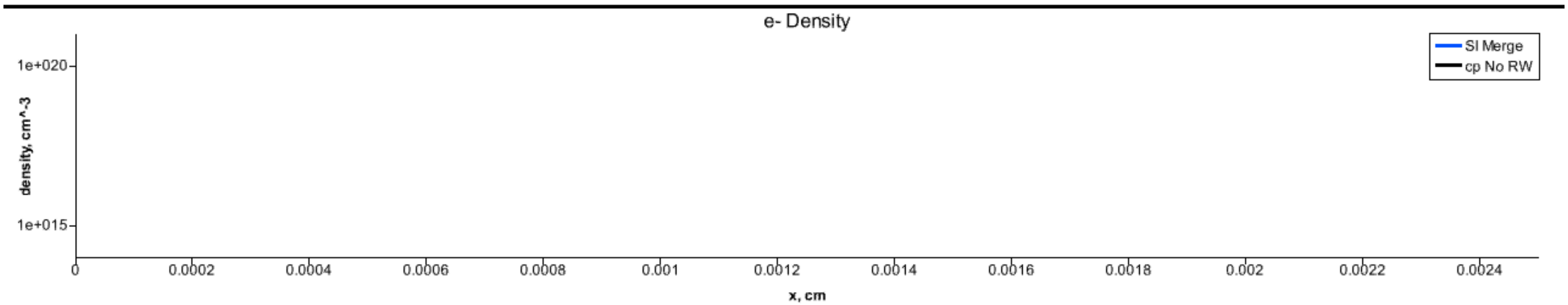

Potential
SI Merge
cp No RW
potential, V
40000
20000
0
0
0.0002
0.0004
0.0006
0.0008
0.001
0.0012
0.0014
0.0016
0.0018
0.002
0.0022
0.0024
x, cm


Cu Density
SI Merge
cp No RW
density, cm^-3
1e+020
1e+015
0
0.0002
0.0004
0.0006
0.0008
0.001
0.0012
0.0014
0.0016
0.0018
0.002
0.0022
0.0024
x, cm


Cu+ Density
SI Merge
cp No RW
density, cm^-3
1e+020
1e+015
0
0.0002
0.0004
0.0006
0.0008
0.001
0.0012
0.0014
0.0016
0.0018
0.002
0.0022
0.0024
x, cm


e- Density
SI Merge
cp No RW
density, cm^-3
1e+020
1e+015
0
0.0002
0.0004
0.0006
0.0008
0.001
0.0012
0.0014
0.0016
0.0018
0.002
0.0022
0.0024
x, cm

Example: 1D Cu Arcs

No reweighting

30138s total

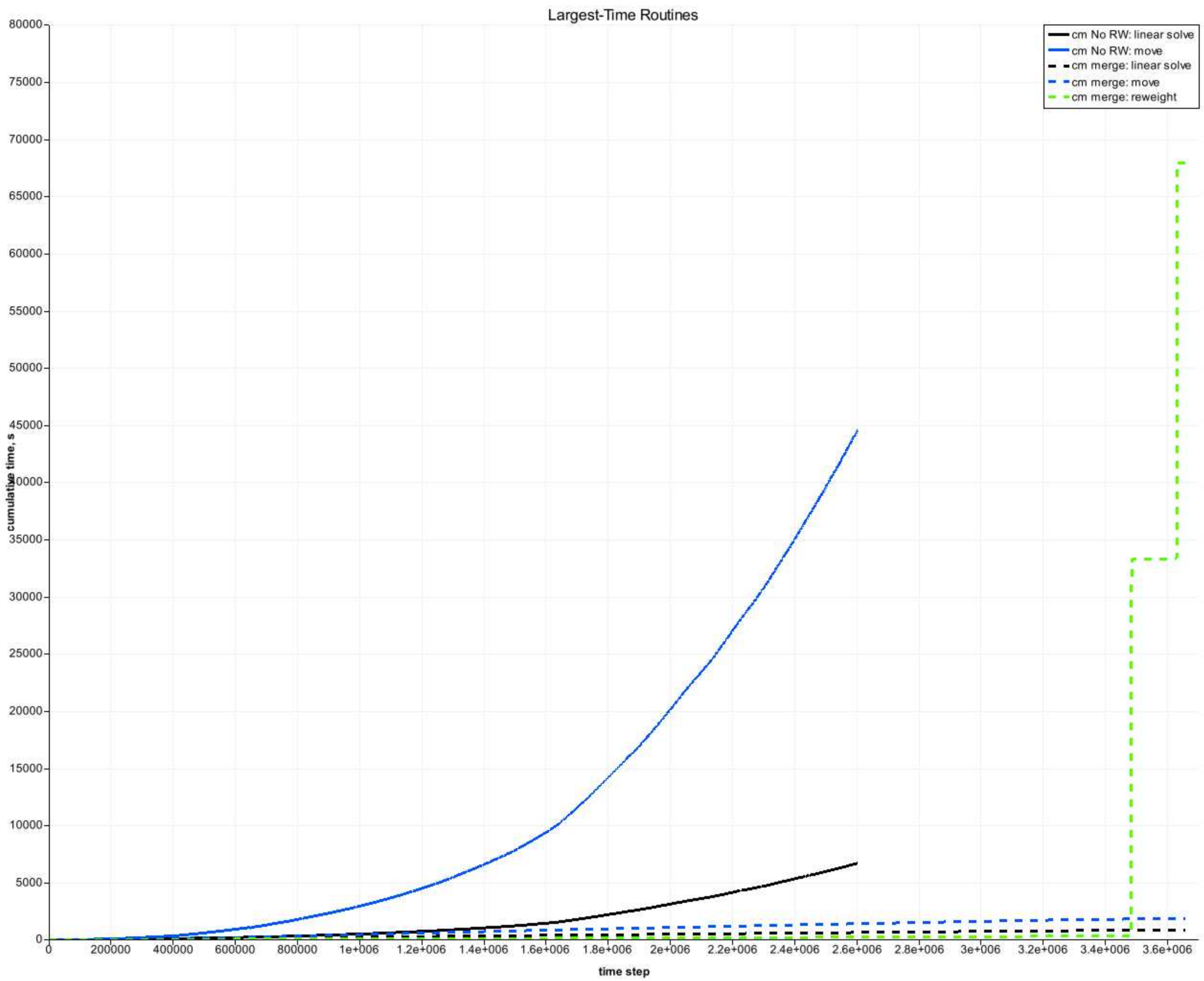
Reweighting all species

882s move

+ 148s reweighting

= 1030s total

97% reduction in runtime!



Conclusions

- 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.

Future Work

- Allow [N_{low}, N_{high}] to vary by species, location, time, 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.

Thank You!