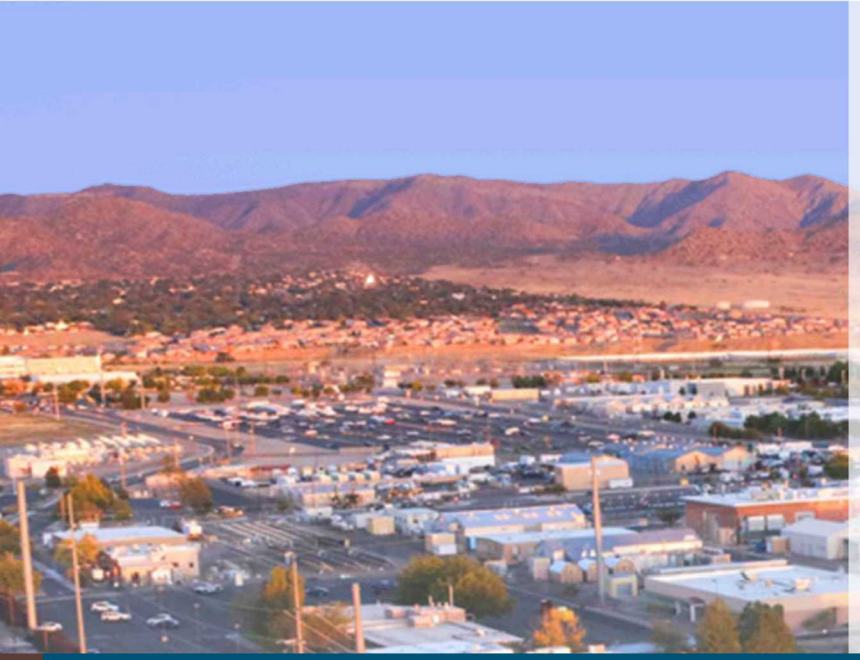


SAND2019-3147PE

Collisional e-Beam Modeling

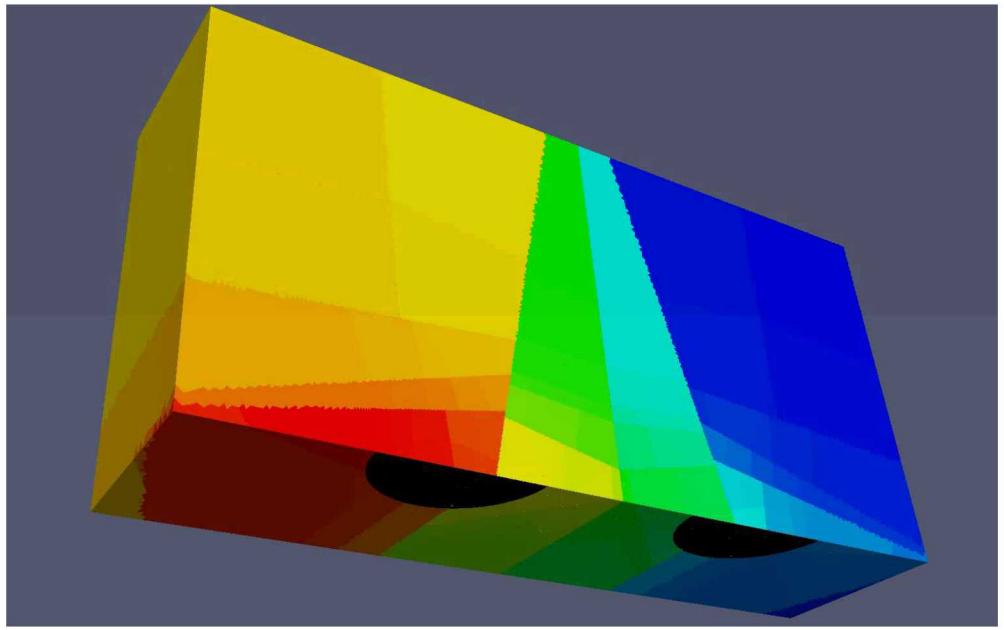
Presented by Matthew M. Hopkins

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Goals

- Use existing capability (Aleph) to answer some questions, EMPIRE will take over.
- Develop high fidelity model for comparison to benchtop experiments (from Ben Yee).
- Understand the importance of more vs. less detailed plasma chemistry models.
- Assess differences from cross section extension models.
- Experience with 0D vs. 1D modeling approaches.
- Stepping stone to full 3D EM-PIC-DSMC simulations.

Aleph Simulation Tool



- 1, 2, or 3D Cartesian
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Hybrid PIC + DSMC (PIC-MCC)
- Electrostatics
- Fixed B field
- Solid conduction
- Advanced surface (electrode) models
- e- approximations (quasi-neutral ambipolar, Boltzmann)
- Collisions, charge exchange, chemistry, excited states, ionization
- Photon transport, photoemission, photoionization
- Advanced particle weighting methods
- Dual mesh (Particle and Electrostatics/Output)
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for extending BCs, post-processed quantities, etc.
- Currently utilizing up to 64K processors (>1B elements, >1B particles)

Aleph Simulation Tool

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:

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

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

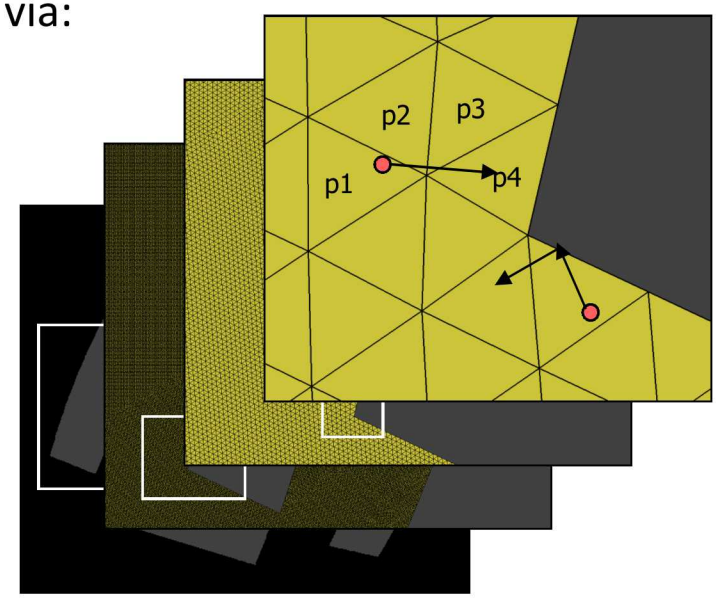
2. Compute intersections (non-trivial in parallel).
3. Transfer charges from particle mesh to static mesh.
4. Solve for $\mathbf{E}^{n+1}$,

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

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

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

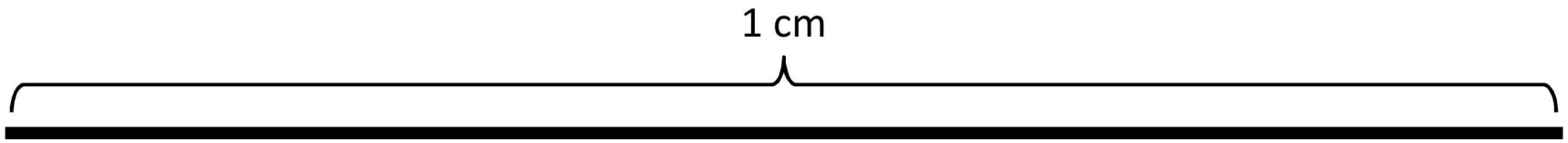
$$v_i^{n+1} - v_i^{n+1/2} + \frac{\Delta t}{2}\left(\frac{q_i}{m_i}\mathbf{E}^{n-1}\right)$$



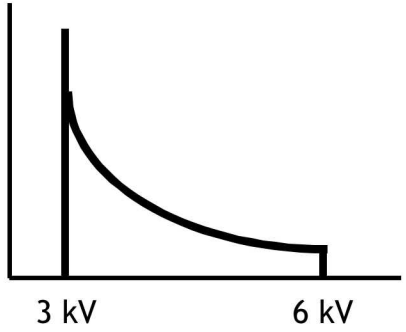
7. Perform DSMC collisions: sample pairs in element, determine cross section and probability of collision. Roll a digital die, and if they collide, re-distribute energy.
8. Perform chemistry: for each reaction, determine expected number of reactions. Sample particles of those types, perform reaction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

1D Model Setup

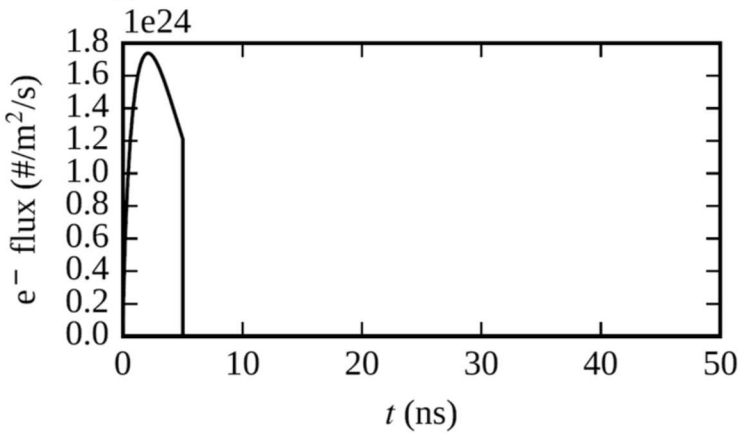
gap filled with 100 mtorr argon gas, 300 K

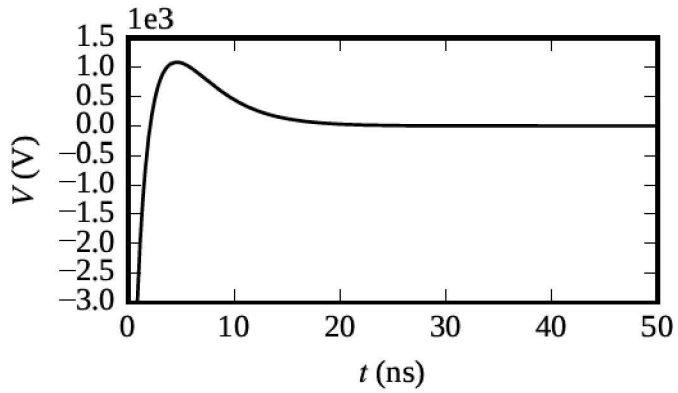


e- injection surface
- $V = 0$
- Energy distribution
- Flux informed by vacuum current measurements
- Injection time ~15 ns



target surface
- V informed by pressurized current measurements, then $V = L\, dI/dt$ (L = 2 nH)





Fullest Argon Chemistry Model

IST-Lisbon argon cross sections retrieved from LXCat (includes contributions from multiple sources):

- e- + Ar elastic scattering
- e- + Ar → e- + Ar+ + e- ionization
- e- + Ar → e- + Ar(x eV) excitation for:

Ar(3P2)	Ar(4p[5/2]3)	Ar(4p'[3/2]1)	Ar(3d[7/2]4)	Ar(5p[5/2]3)	Ar(5p'[3/2]1)	Ar(6s)
Ar(3P1)	Ar(4p[5/2]2)	Ar(4p'[3/2]2)	Ar(3d[7/2]3)	Ar(5p[5/2]2)	Ar(5p'[1/2]1)	Ar(4d')
Ar(3P0)	Ar(4p[3/2]1)	Ar(4p'[1/2]1)	Ar(3d[3/2]1)	Ar(5p[3/2]1)	Ar(5p'[3/2]2)	
Ar(1P1)	Ar(4p[3/2]2)	Ar(4p'[1/2]0)	Ar(3d'[5/2]2)	Ar(5p[3/2]2)	Ar(5p'[1/2]0)	
Ar(4p[1/2]1)	Ar(4p[1/2]0)	Ar(3d[3/2]2)	Ar(5p[1/2]1)	Ar(5p[1/2]0)	Ar(4d)	

Grouped states: Ar(3d[1/2]0+3d[1/2]1, Ar(3d[5/2]2+5s[3/2]2), Ar(3d[5/2]3+5s[3/2]1), and Ar(3d'[5/2or3/2]3or2+5s'[1/2]0or1)

- These are represented in Aleph according to their excitation energy (from IST-Lisbon), e.g.,
  - species Ar(3P2) maps to Aleph species Ar(11.5480)
  - species Ar(3P1) maps to Aleph species Ar(11.6230)
  - species Ar(3d'[5/2or3/2]3or2+5s'[1/2]0or1) maps to Aleph species Ar(14.2300)
  - species Ar(4d') maps to Aleph species Ar(14.9670)

Fullest Argon Chemistry Model (there's more!)

In addition to this we track all the transitions amongst all excited states and the ground state with their Einstein A coefficients,

- Ar(11.5480) -/-> (metastable)
- Ar(11.6230) -> Ar(0), 1.320e+08
- Ar(11.7230) -/-> (metastable)
- Ar(11.8280) -> Ar(0), 5.32e+08
- Ar(12.9070) -> Ar(11.5480), 1.89e+07
- Ar(12.9070) -> Ar(11.6230), 5.4e+06

Some grouped states have their rates split and averaged (better ideas?):

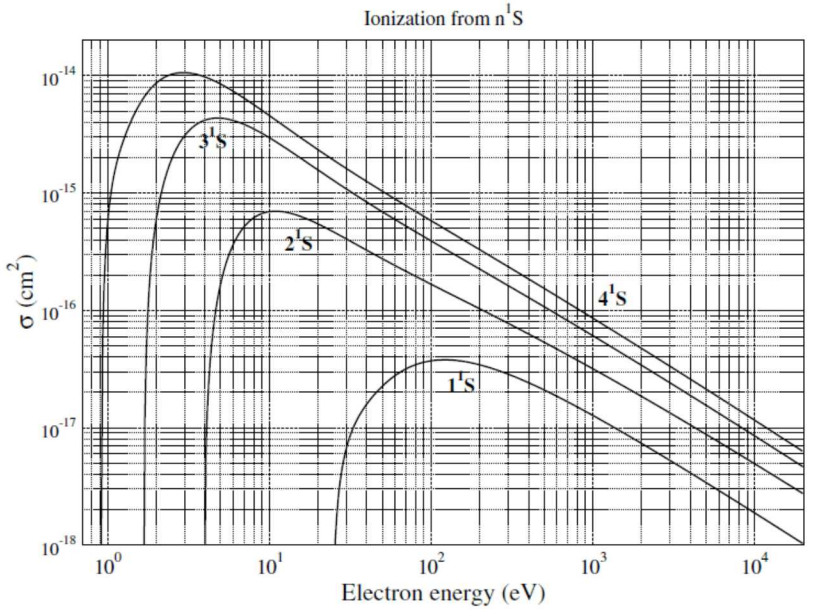
- Ar(14.0900) -> Ar(13.0760), 0.5 * 3.1e+06
- Ar(14.0900) -> Ar(13.0950), 0.5 * (2.0e+06 + 8.9e+06)
- Ar(14.2300) -> Ar(13.1530), 0.25 * (3.69e+05 + 2.22e+06 + 2.8e+05)

A total of 149 transitions.

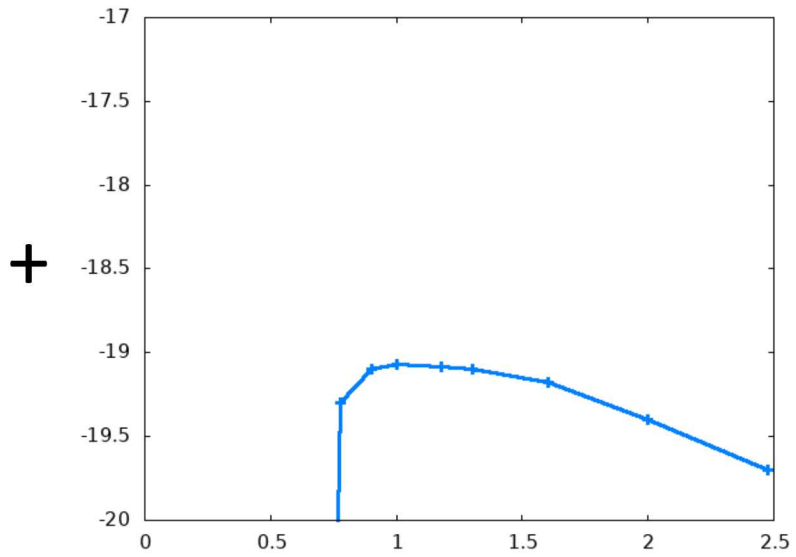
Fullest Argon Chemistry Model (there's still more!)

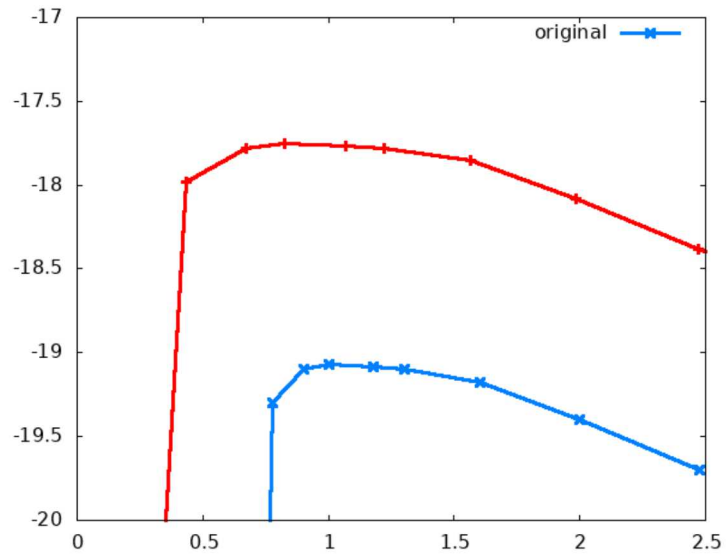
To account for multistep ionization we construct an ionization cross section for every excited state. Most of these do not exist so these are artificially derived.

- Shift cross section excitation threshold to ionization energy for excited state.
- Multiply entire cross section by factor derived from Ralchenko helium work.



Graph 41. Recommended electron-impact ionization cross sections from atomic terms of He I with $n \leqslant 4$.





Fullest Argon Chemistry Model (last stop)

Finally, because cross sections don't typically go to the energies we want, we have options on how to extend them:

- "don't", just let the last value extend to ∞ as a constant.
- Linearly interpolate in log-log space,

$$\log\left(\sigma(E_1)\right) = \log\left(\sigma(E_0)\right) + m\frac{\log(E_1)-\log(E_0)}{E_1-E_0},$$

  where m is computed from the last 2 data points.
- Bethe model as related in [Kip 1992],

$$\hat{E} = E/E_{\text{ionization}},$$

$$\sigma(E) = \frac{A\log(\hat{E})+B+C/\hat{E}}{\hat{E}+D},$$

  where the 4 coefficients must be fit to data. We usually employ :

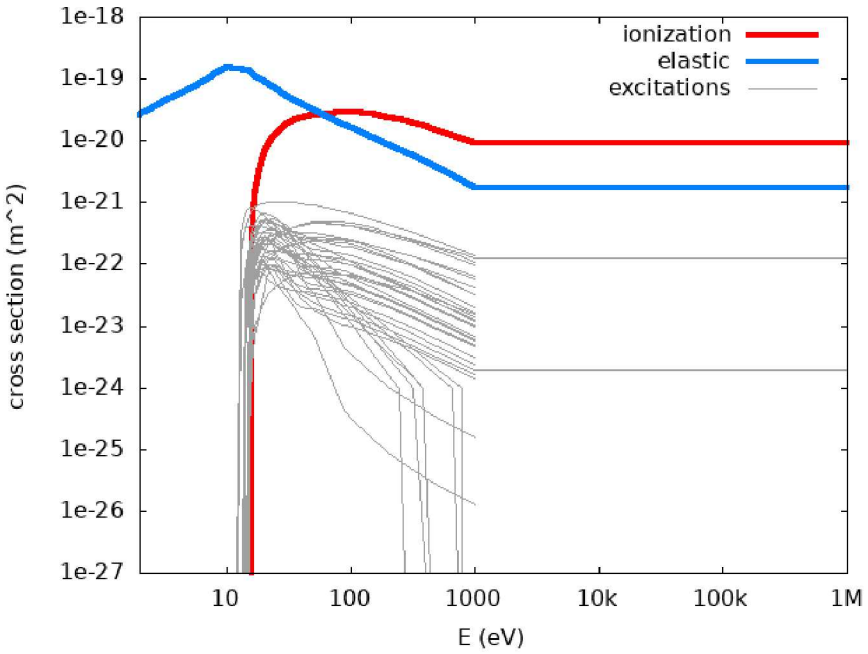
- Modified Bethe, accounting for only part of the full model,

$$\sigma(E) = A\frac{\log(\hat{E})}{\hat{E}},$$

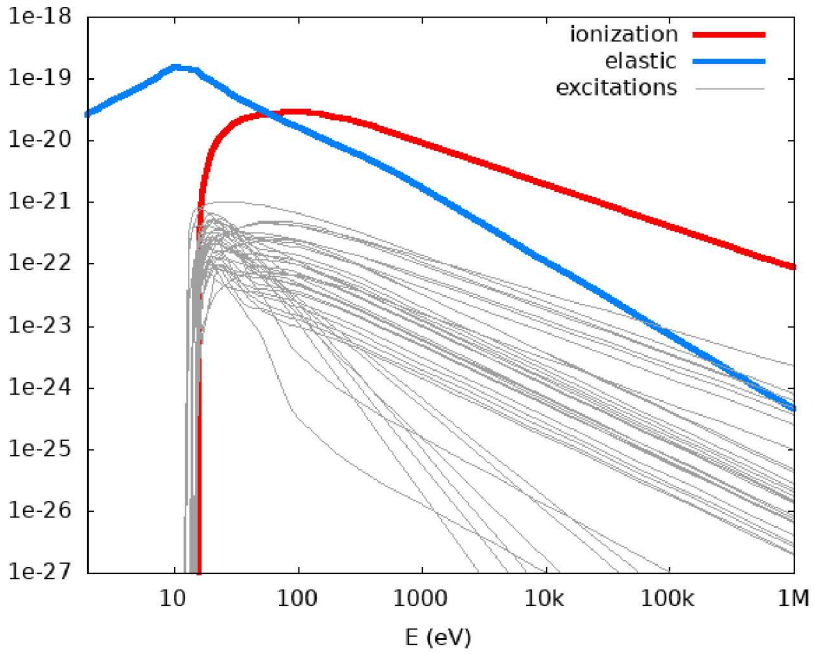
  where A is fit to the last data point.

Fullest Argon Chemistry Model (last stop)

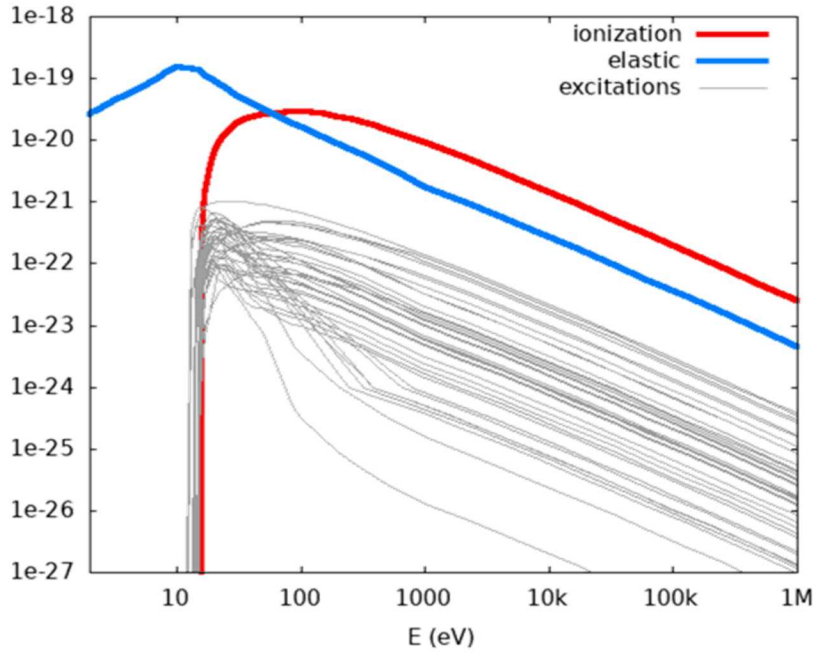
constant extension



log-log extension



modified Bethe extension

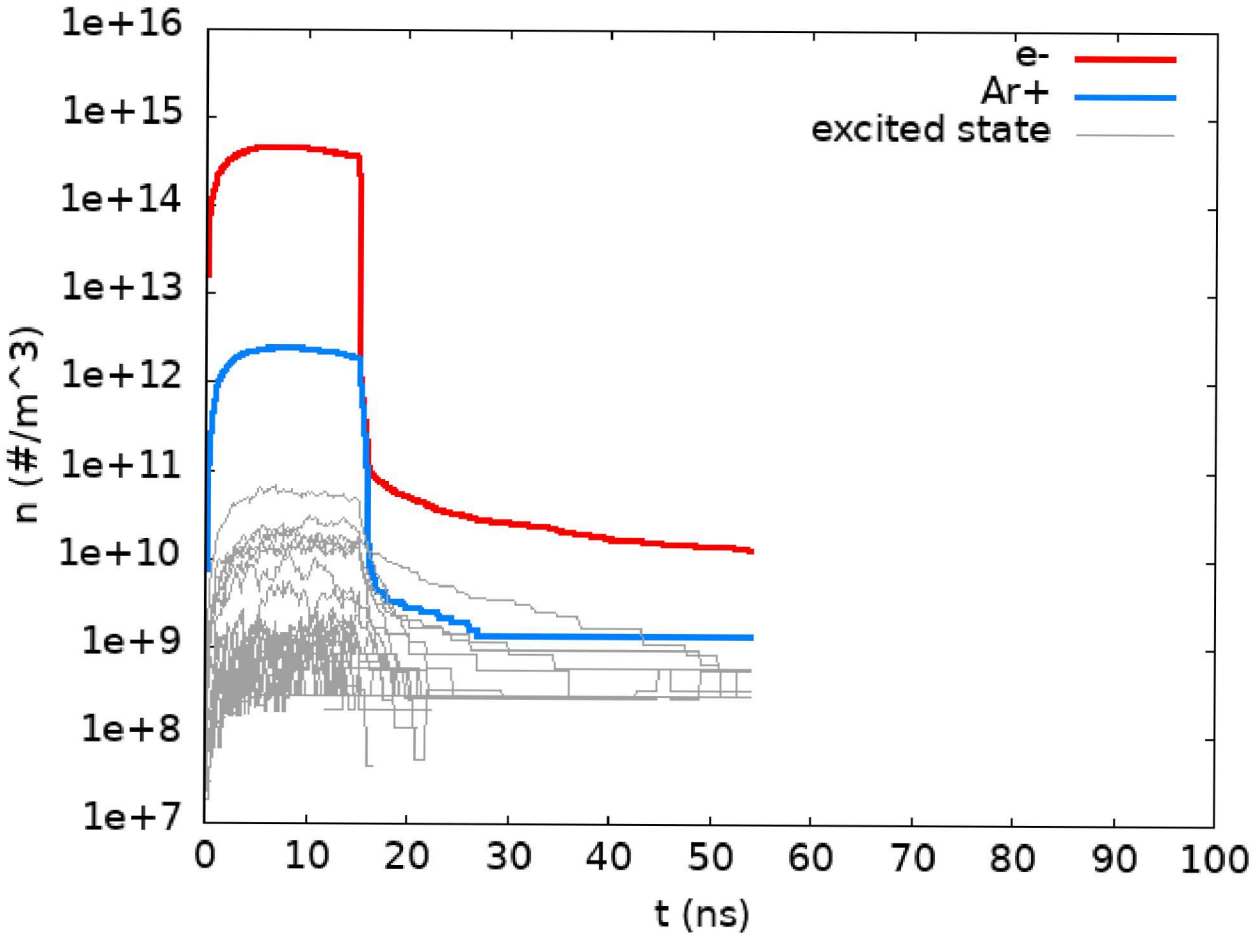


Simulation Constraints

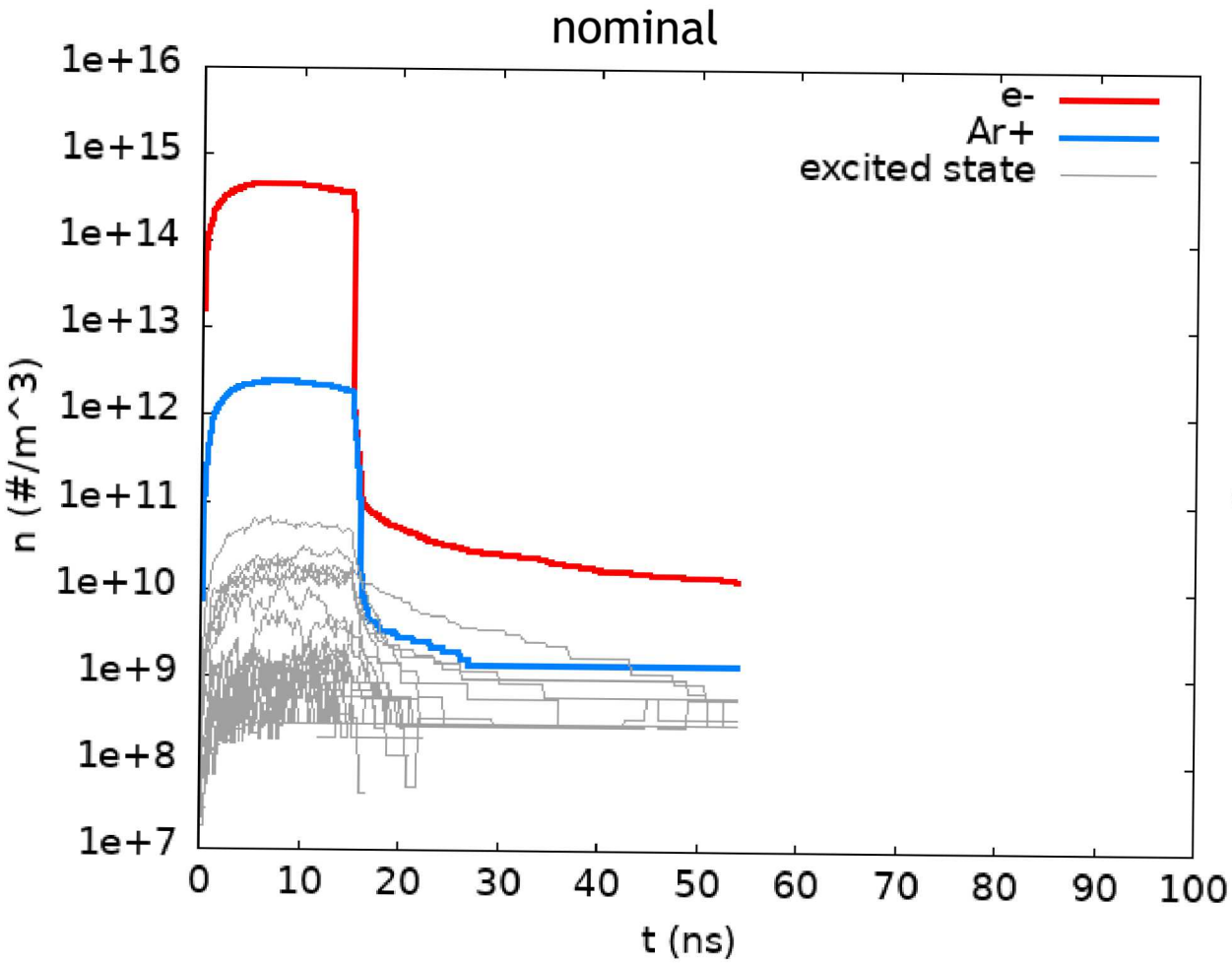
Constraint	Requirement
Debye length	$\Delta x < \lambda_D = \sqrt{\frac{k_B T_e \varepsilon_0}{n_e q_e^2}}$
Collision mfp	$\Delta x < \lambda_c = \frac{1}{n_{bg}\sigma_{max}}$
Particle CFL	$\Delta t < \frac{v_{max}}{\Delta x}$
Plasma frequency	$\Delta t < 2/\omega_p = 2\sqrt{\frac{\varepsilon_0 m_e}{n_e q_e^2}}$
Collision frequency	$\Delta t < 1/\omega_c = \frac{1}{n_{bg}\sigma_{max} v_{max}}$

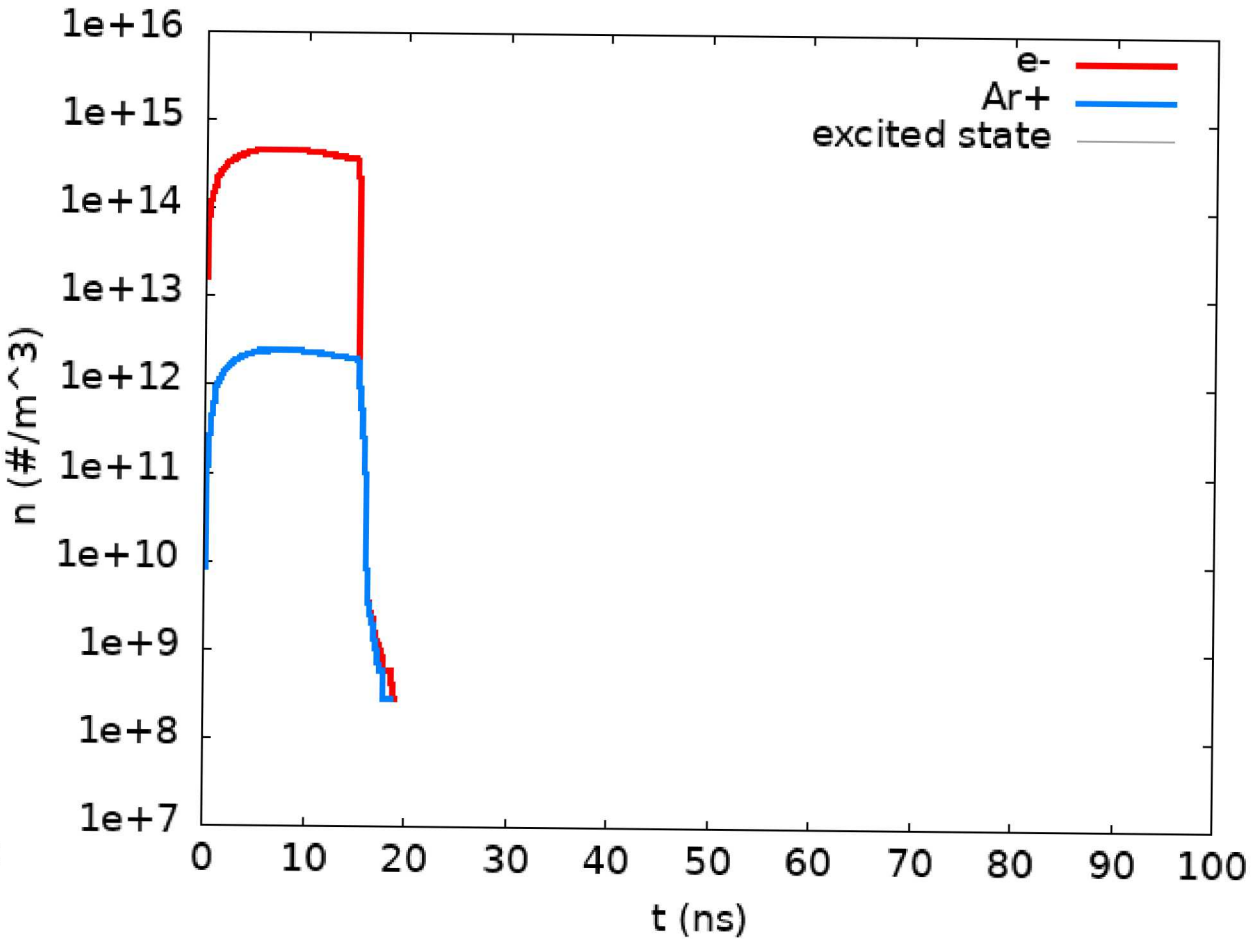
At T_e = 2 eV, n_e = 10^{19} m^{-3}, σ_{max} = 2 x 10^{-19} m^2, and n_{bg} = 9.7 x 10^{21} m^{-3}, v_{max} = 4.2 x 10^7 m/s,
λ_D = 3.2 um, λ_c = 500 um → Δx = 3 um
$v_{max}/\Delta x$ = 40 fs, $2/\omega_p$ = 11 ps, $1/\omega_c$ = 12 ps → Δt = 80 fs

Result: Different Chemistry: Fullest

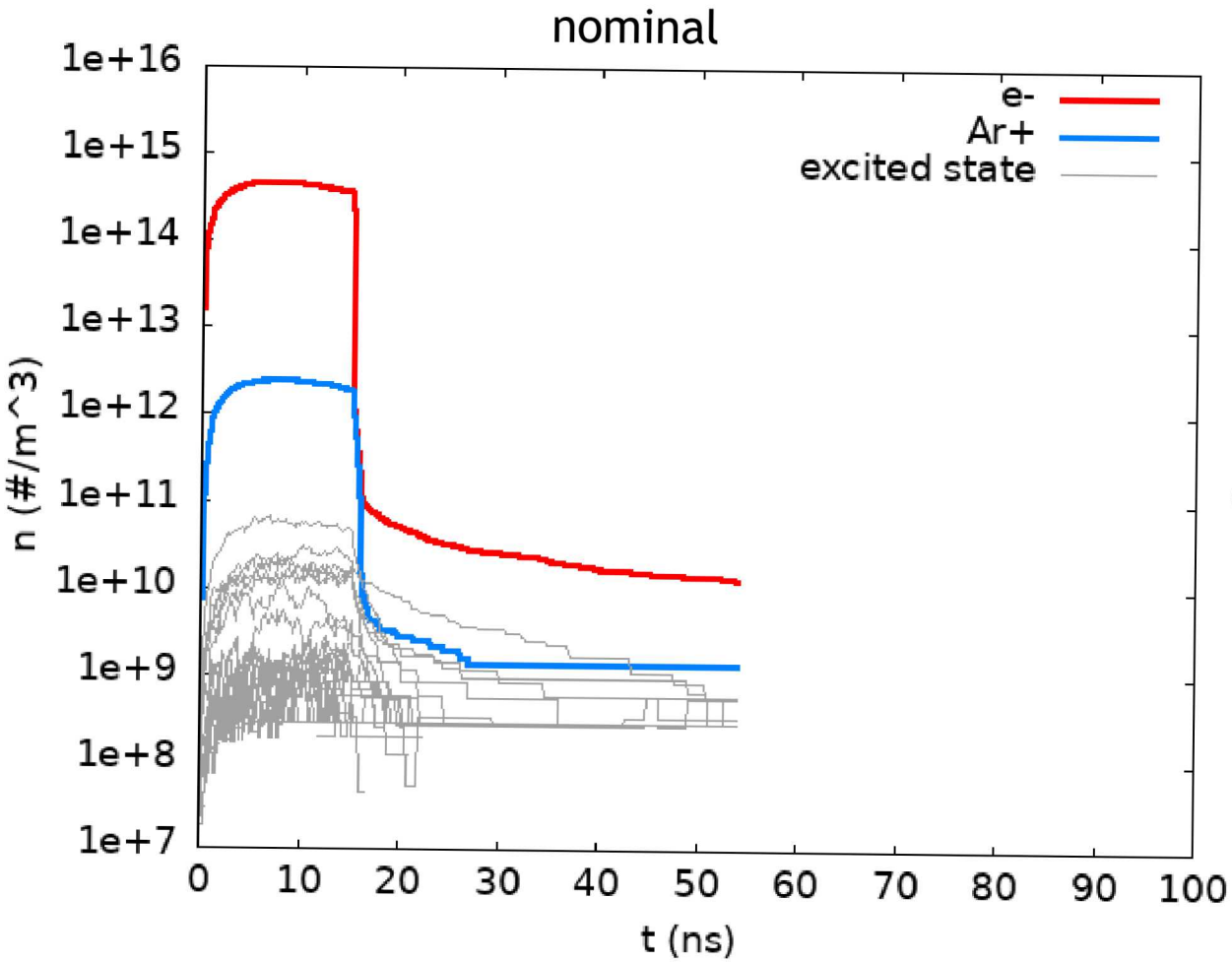


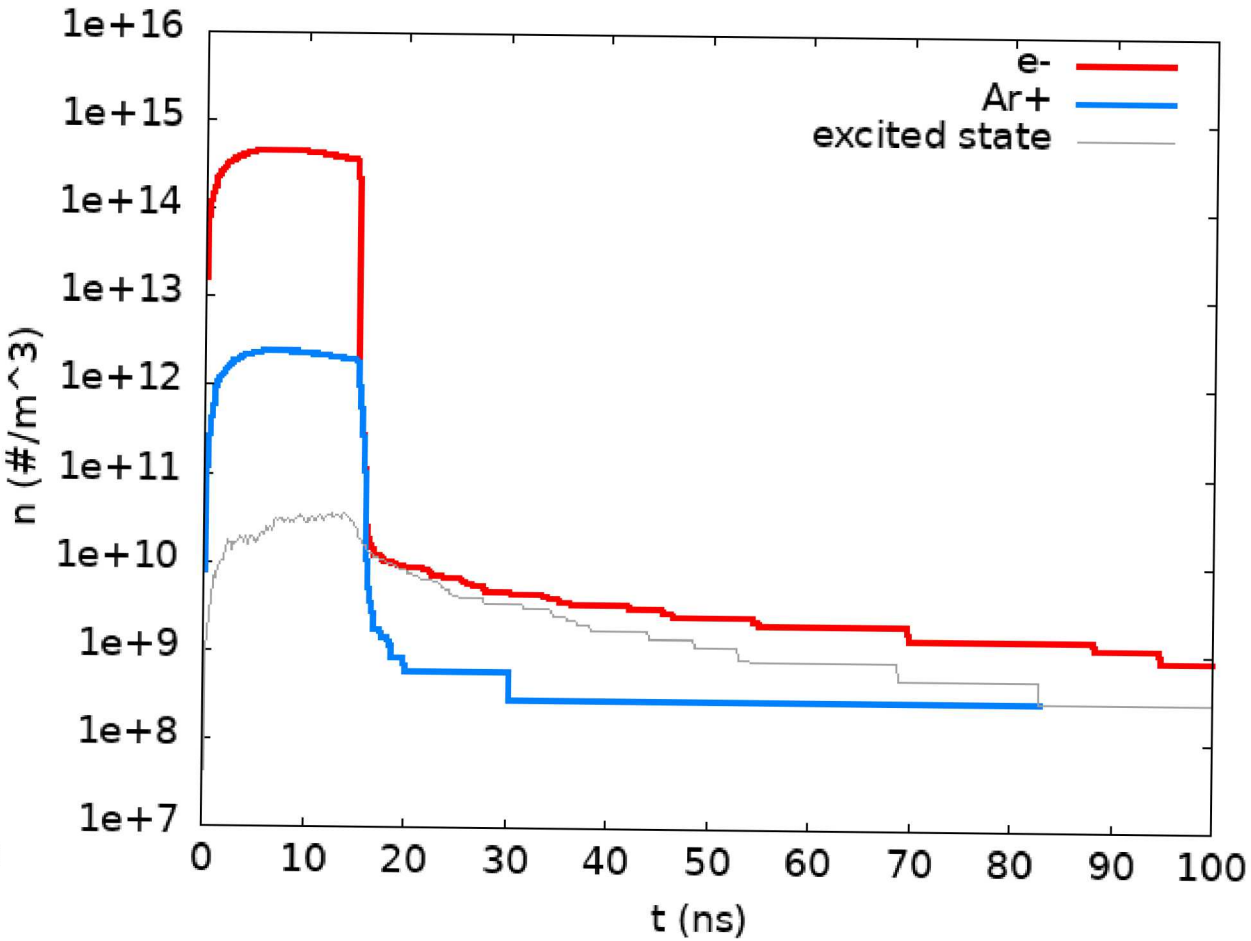
Result: Different Chemistry: Simplest



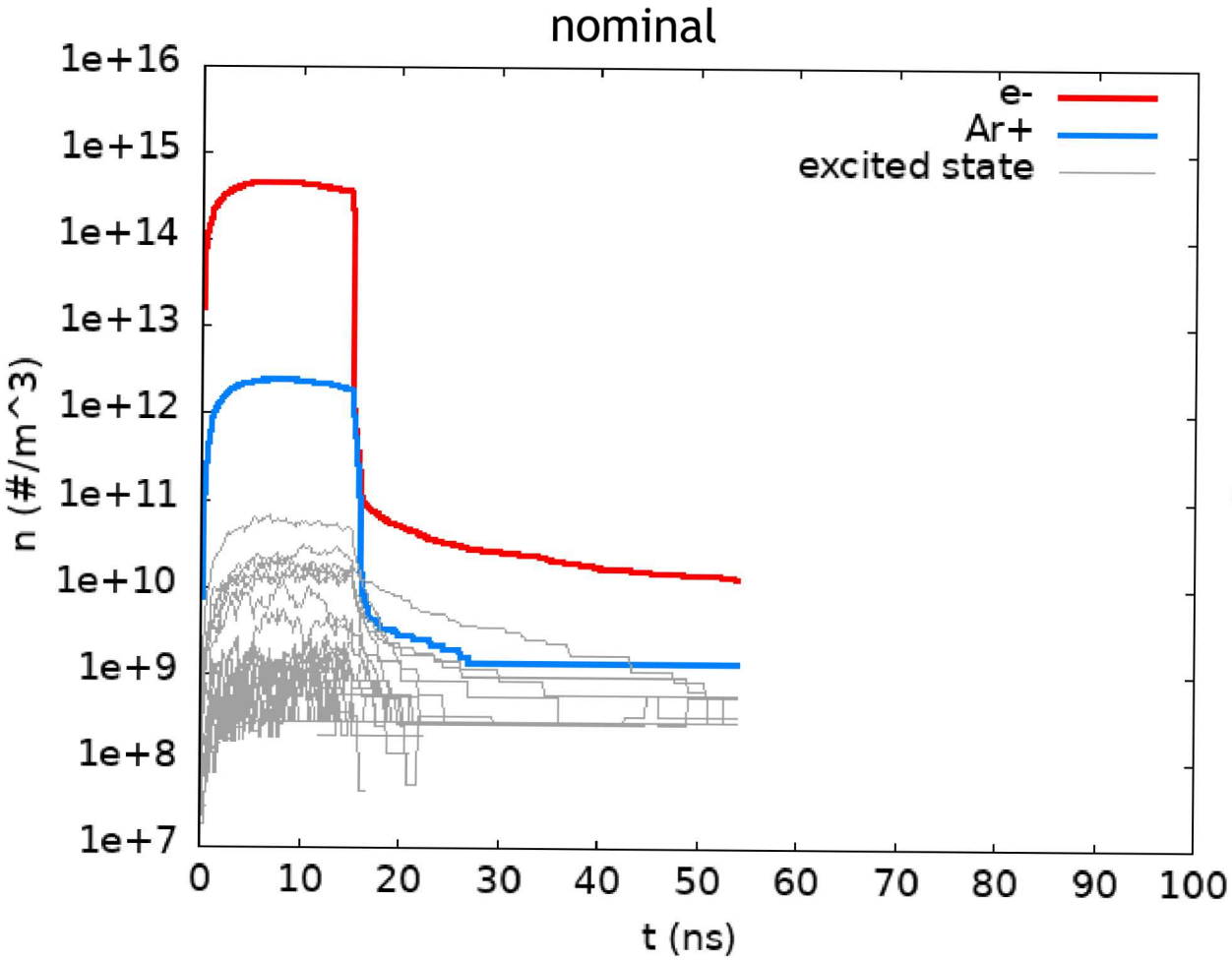


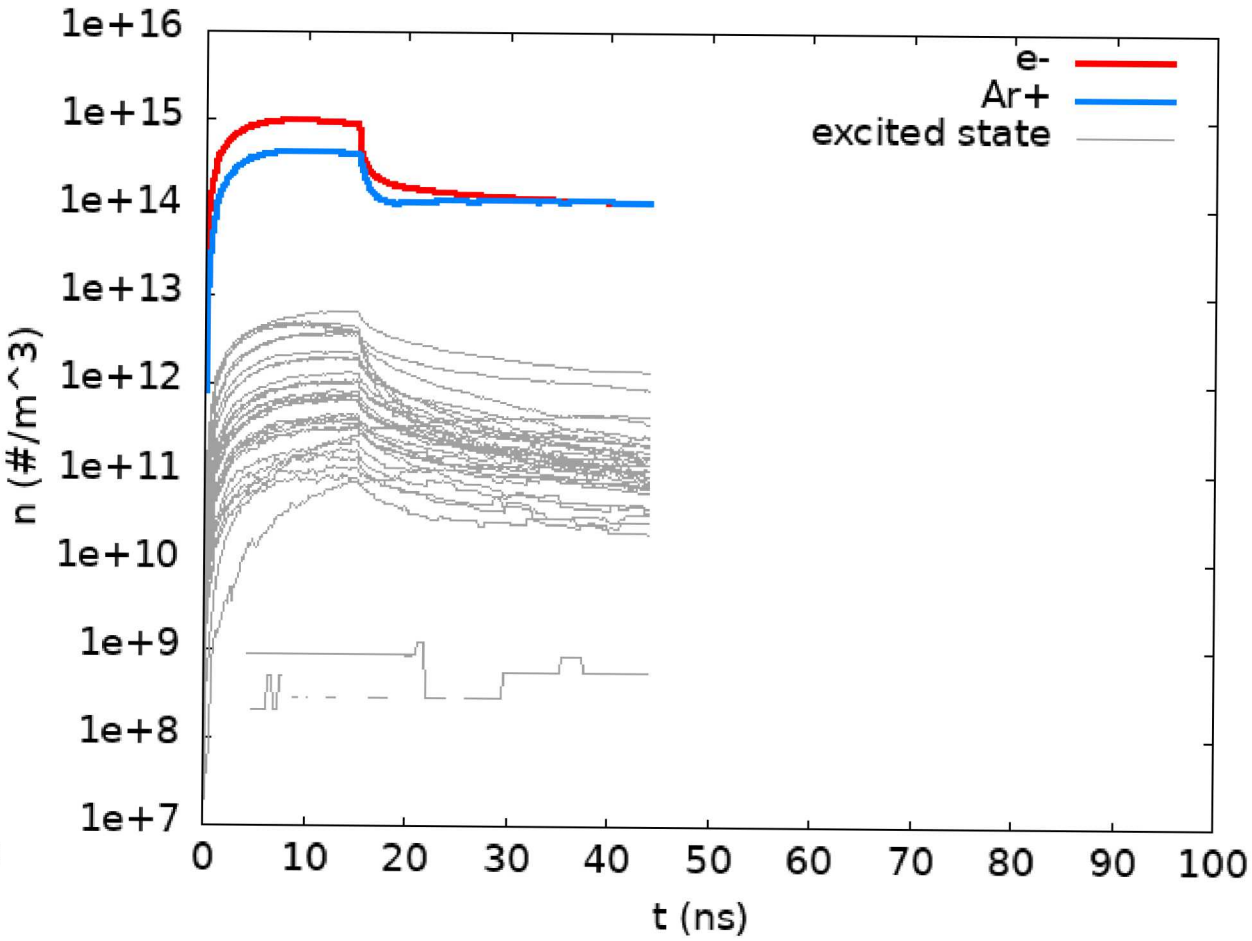
Result: Different Chemistry: Middle



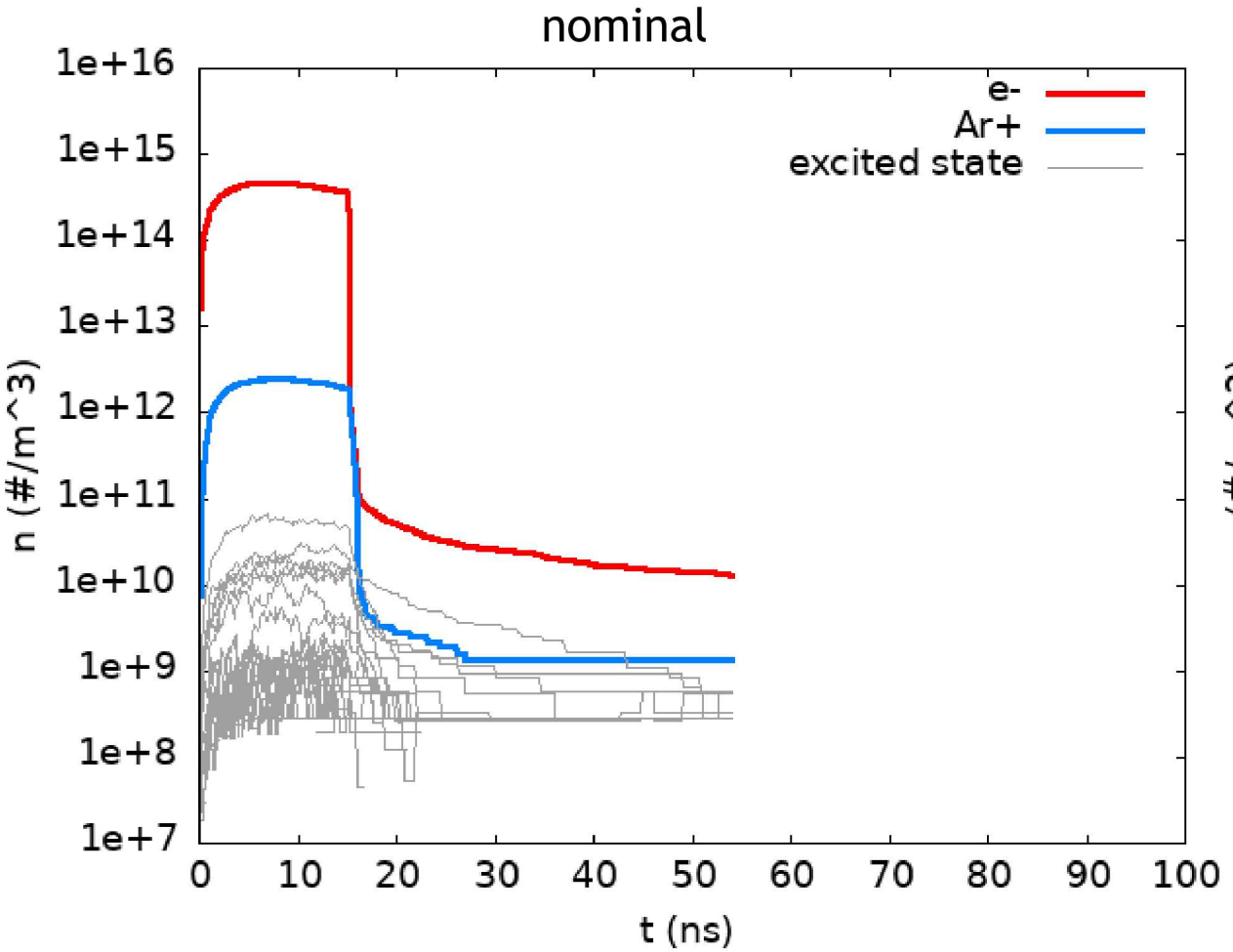


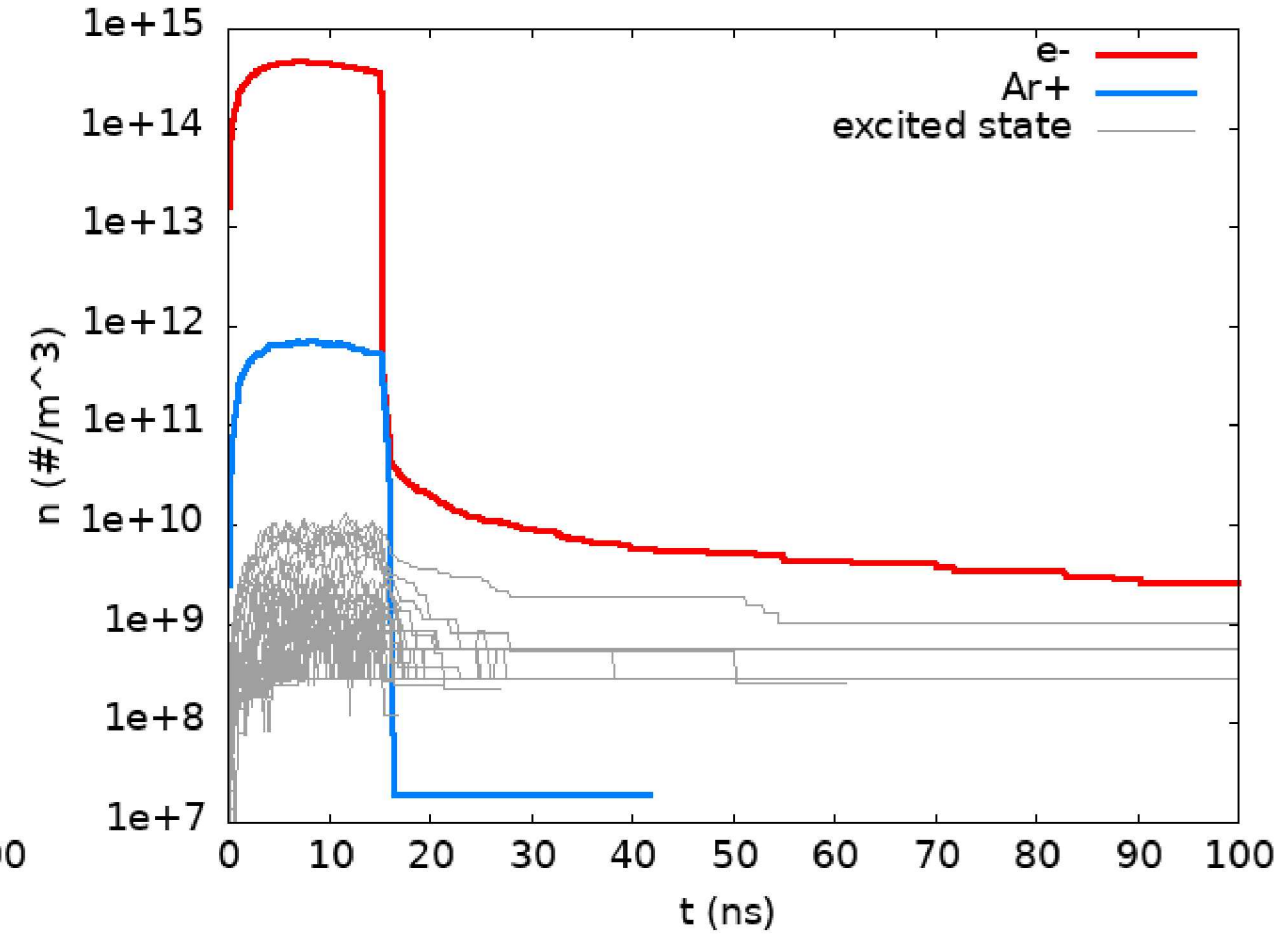
Result: Different Cross Section Extension: Constant





Result: Different Cross Section Extension: Modified Bethe





Observations

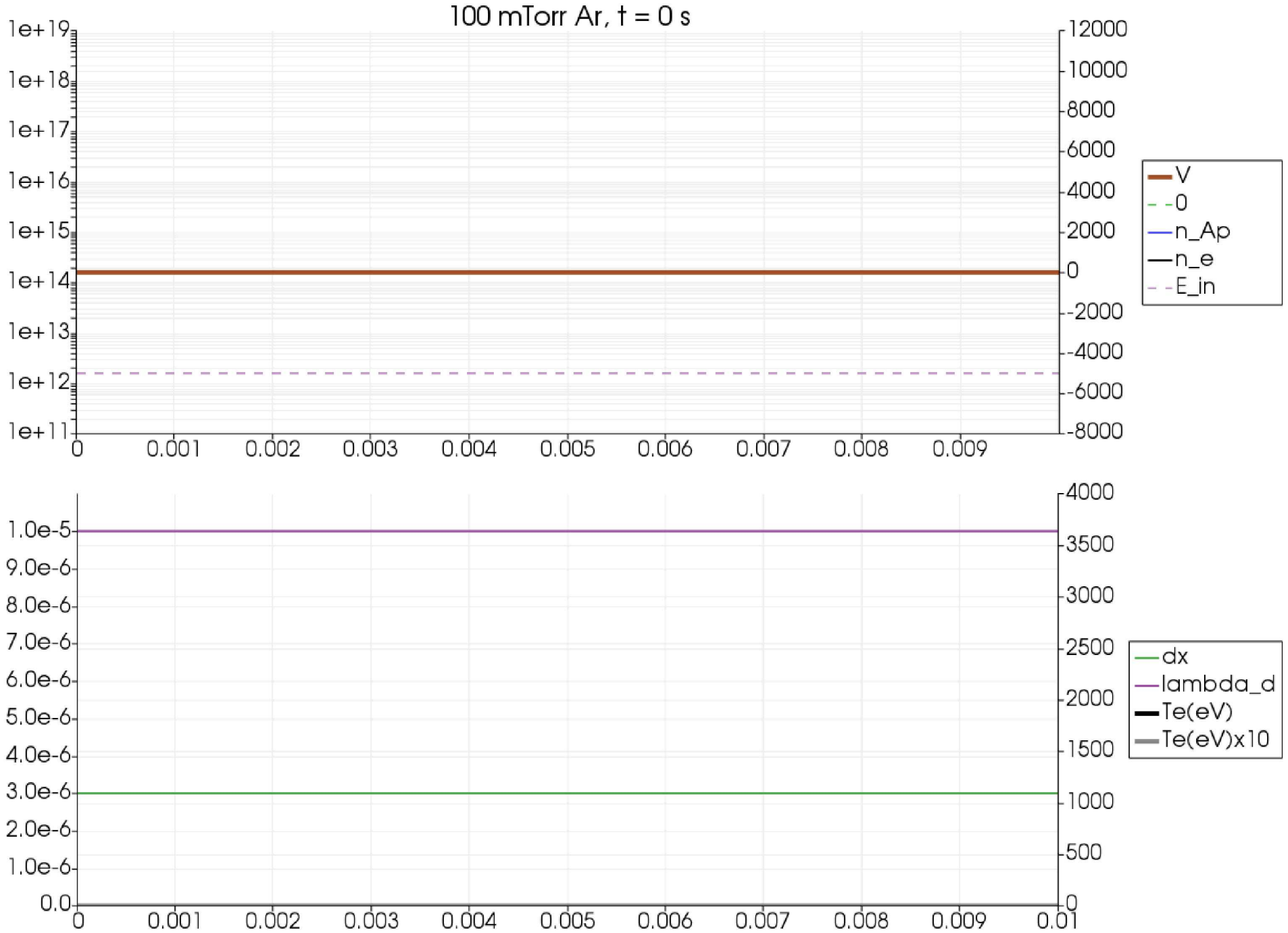
- If $n_e n_{bg} \sigma(E)$ is too small, no significant plasma is generated
  - Reduce E via negative space charge buildup (see animation next slide)
  - Increase n_e with more injected e-
  - Increase n_{bg} with higher pressure

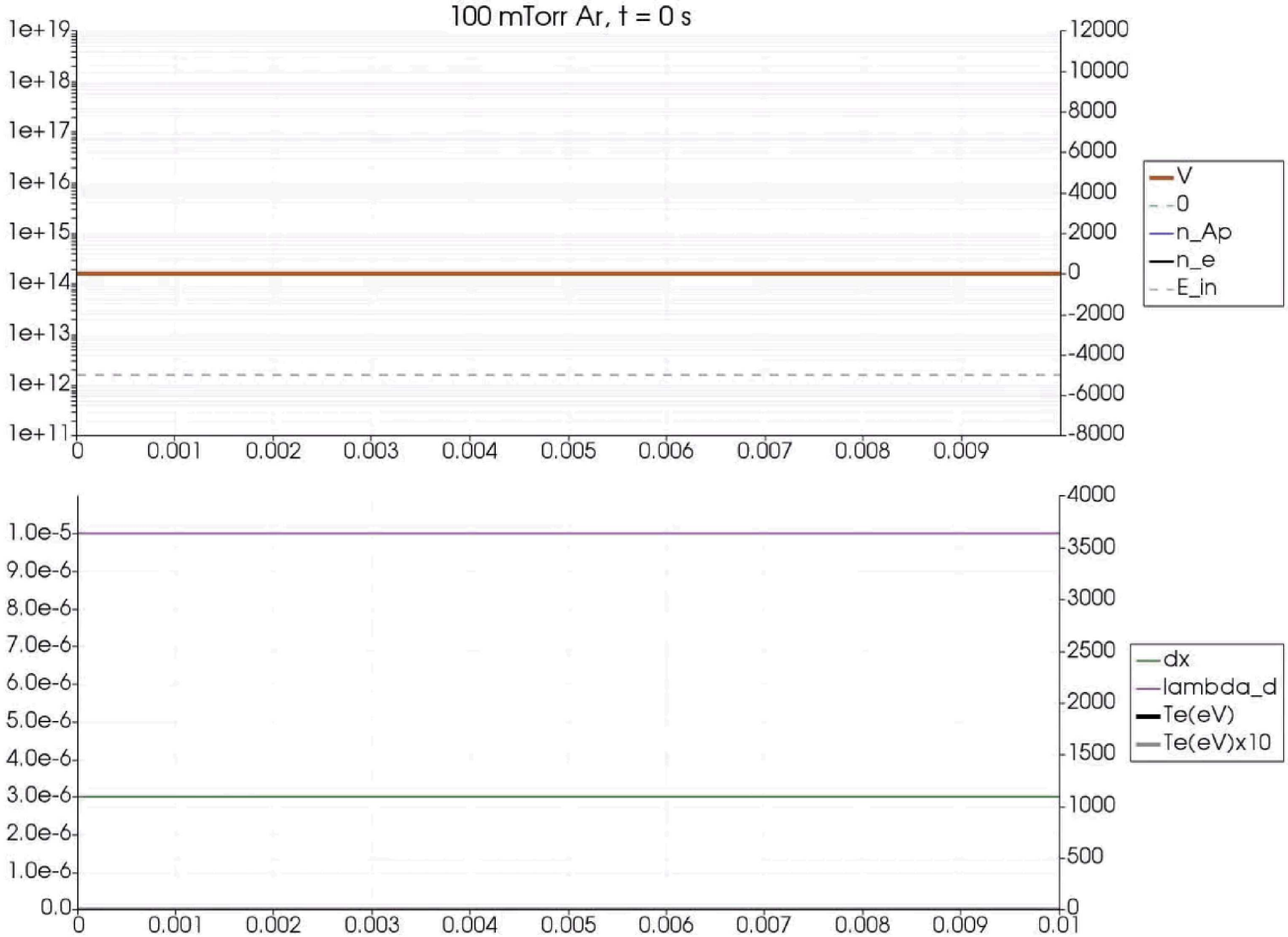
- Nbg = 100 mtorr, E = 5 kV, nbg*s = 48.3/m v = 4.2e7 ionization rate ~ 4e8/s; ne ~ 1e10 -> 4e19/s -> 4e10/ns; For E ~ 100 kV, ionization rate = 5e7/s.

- Pulse length for e is at least as important for generating *smaller* fields as for generating primary e-

- Generating regions of lower E is likely an extremely important contributor for generating plasma, however that happens (longer gap -> more negative space charge -> lower E). Trickle current experiment was uninteresting.

- Question: are there “zero energy” electrons that come from the foil, in the chamber, on gunk, on geometric features? Those would hit the low energies (higher collisionality) much better than the beam electrons.


100 mTorr Ar, t = 0 s
1e+19
1e+18
1e+17
1e+16
1e+15
1e+14
1e+13
1e+12
1e+11
12000
10000
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
V
0
n_Ap
n_e
E_in
1.0e-5
9.0e-6
8.0e-6
7.0e-6
6.0e-6
5.0e-6
4.0e-6
3.0e-6
2.0e-6
1.0e-6
0.0
4000
3500
3000
2500
2000
1500
1000
500
0
0.01
dx
lambda_d
Te(eV)
Te(eV)x10


100 mTorr Ar, t = 0 s
1e+19
1e+18
1e+17
1e+16
1e+15
1e+14
1e+13
1e+12
1e+11
12000
10000
8000
6000
4000
2000
0
-2000
-4000
-6000
-8000
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
V
0
n_Ap
n_e
E_in
1.0e-5
9.0e-6
8.0e-6
7.0e-6
6.0e-6
5.0e-6
4.0e-6
3.0e-6
2.0e-6
1.0e-6
0.0
4000
3500
3000
2500
2000
1500
1000
500
0
0.01
dx
lambda_d
Te(eV)
Te(eV)x10

Next Steps

Old:

- Improve models for voltage BC's. At least use an RLC BC.
- More accurate excited state chemistry. Remove "notional" excited state.
- Use nitrogen chemistry if comparing to full system experiments. Argon is still right for the bench scale comparisons.
- Include photons?
- Higher dimensions. 0D is too much. 1D may be too little. 2D (certainly 3D) should be "just right".

Next Steps

Old:

- ~~Improve models for voltage BC's. At least use an RLC BC.~~ *Real comparison demands EM treatment.*
- ~~More accurate excited state chemistry. Remove "notional" excited state.~~
- Use nitrogen chemistry if comparing to full system experiments. Argon is still right for the bench scale comparisons.
- Include photons?
- Higher dimensions. 0D is too much. 1D may be too little. 2D (certainly 3D) should be "just right". *Still the case – related to requiring EM.*

New:

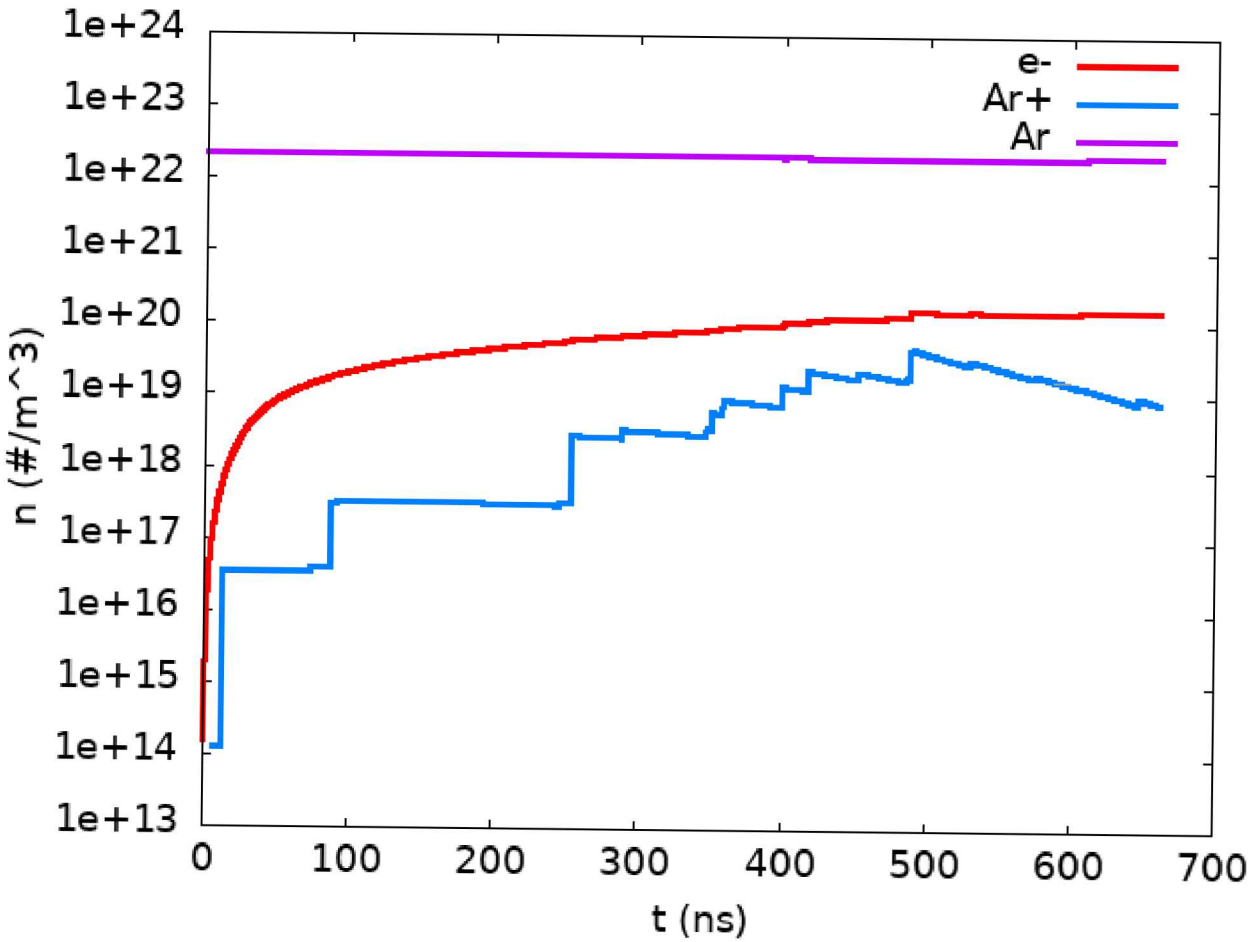
- How much effort to put into more realistic 1D ES simulations? (Maybe for lab scale.)
- More detailed comparison of chemistry in regime where it matters (lower energies). Those smaller energy regions must occur in full scale systems, otherwise there would be no plasma formed!
- Separate primary and secondary generation processes, also multistep.

0D and 0D CESAR Simulations

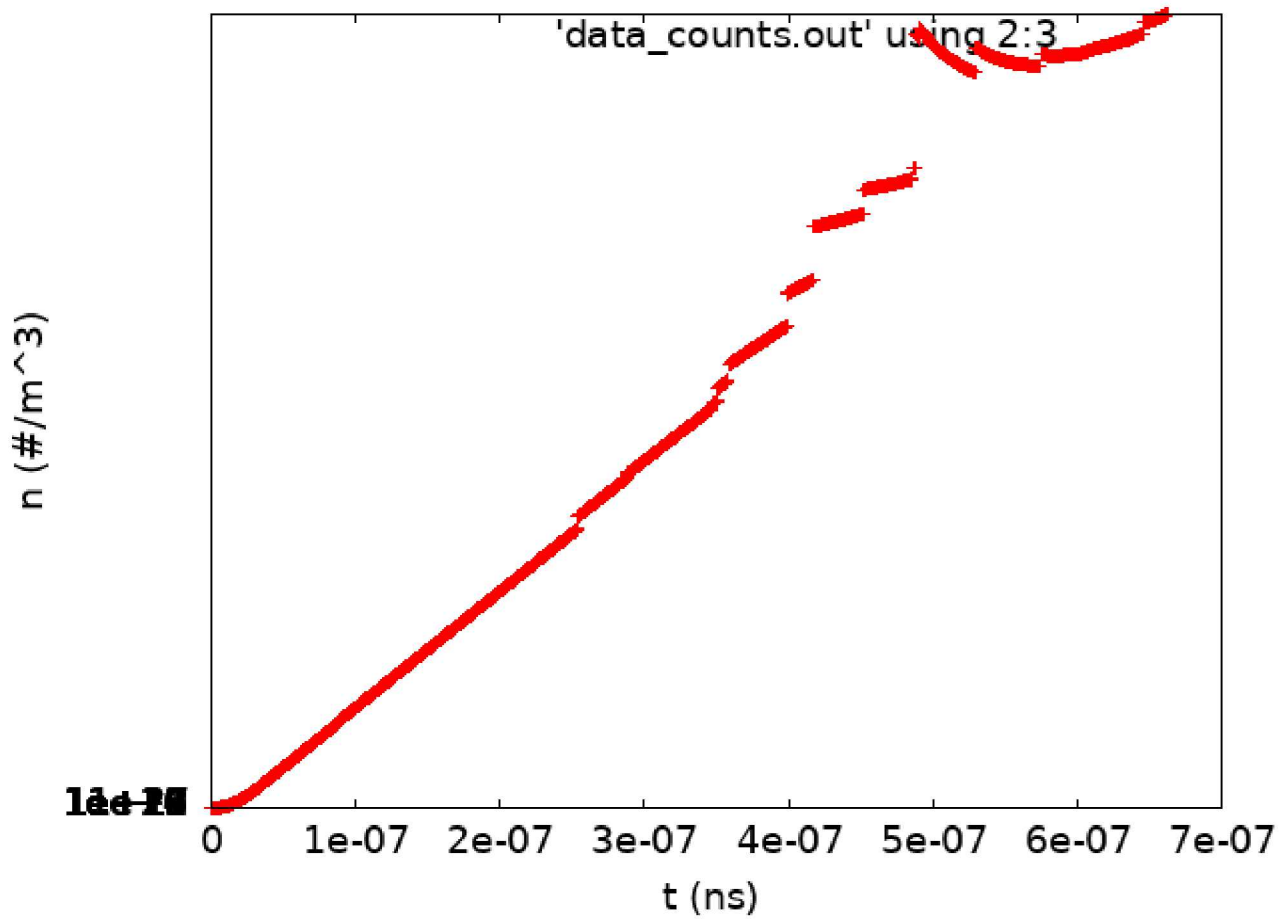
- V(t) = V0 = 800 kV
- I(t) = I0 * t/tau if t<tau
- I(t) = I0 if t>tau (I0 = 300 kA, tau = 30 ns)
- The beam and transport chamber diameters should be equal to 5 cm (woops, used 10cm)
- 1 mbar Ar 300K background

- e- injected into 0D domain at flux to give specified current density (at d = 10cm)

0D and 0D CESAR Simulations



0D and 0D CESAR Simulations



0D (not CESAR)

- Similar settings to SNL 1D simulations.

Observations About 0D

Bad:

- Entire domain is under a field – no way to develop sheaths, virtual cathodes, etc.
- “Injection” means no way to develop space charge limited emission.
- Electrons don’t leave. Do they just get pushed to runaway speeds?
- Repeat question about zero energy electrons on foil, etc.

Useful?

- Get all mechanisms working.
- Compare codes.