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Why do code-to-code comparisons: a vacuum arc discharge simulation case study

Helga Timko[a,b], Paul S. Crozier[c], Matthew M. Hopkins[d], Konstantin Matyash[e], Ralf Schneider[f]

[a]CERN, Genève 23, CH-1211, Switzerland
[b]Helsinki Institute of Physics and Department of Physics, P. O. Box 43, FIN-00014 University of Helsinki, Finland
[c]Scalable Algorithms, Sandia National Laboratories, P.O. Box 5800, MS 1322 Albuquerque, NM 87185, U.S.A.
[d]Nanoscale and Reactive Processes, Sandia National Laboratories, P.O. Box 5800, MS 0836 Albuquerque, NM 87185, U.S.A.
[e]Max-Planck-Institut für Plasmaphysik, EURATOM Association, Wendelsteinstr. 1, D-17491 Greifswald, Germany
[f]Institut für Physik, Ernst-Moritz-Arndt-Universität, Felix-Hausdorff Str. 6, D-17489 Greifswald, Germany

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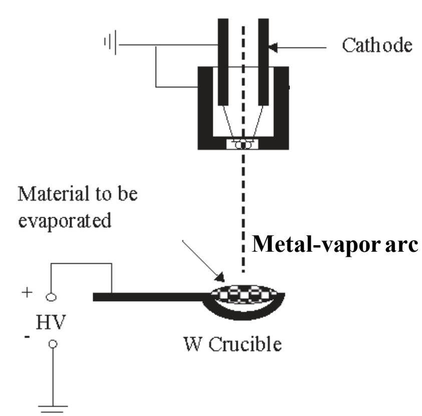
Motivation

- "Arcs" are high-current density, low voltage discharges in partially-ionized gases

- Of interest for
  - gas switches
  - ion sources
  - vacuum coatings (Thermionic Vacuum Arc: TVA)

- In TVA, evaporating anode generates arc plasma



Overall research goal

Perform PIC/DSMC simulation of vacuum arc formation

- Start with vacuum gap between two electrodes
- Can be 1-D, or quasi-1D
- Simulate emission of electrons, ions, and/or neutrals from electrodes
- Include important ionization processes
- Rapid rise in gap current
- Current avalanche --- breakdown
- Simple circuit in series with arc
- Simulate beyond breakdown

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Previous state-of-the-art in arc modeling

Brief literature survey summary of prior arc modeling efforts:

- Continuum models, no particles
- Ionization events not explicitly modeled
- Simplistic electrodes
- Conservation of energy, momentum, mass

Other particle simulation effort: group at CERN doing 1D particle model of vacuum arc breakdown

http://www.ipp.mpg.de/~knm/CERN/spark.html

Summary of simple 1D arc model

Simulation description:

- 1D PIC simulations
- 21 micron gap, 10kV potential drop
- Cu electrodes
- Assume constant emission of electrons and Cu neutrals from the cathode.
- “Sputtering” model: particles hitting electrodes knock off more Cu neutrals.
- Include elastic collisions and ionization collisions.
- 80 cells, 3.5 fs timesteps

Results:

- Cu neutrals build up in the gap
- Ionization occurs, creating plasma in the gap
- Breakdown occurs once the ionization mean free path < gap distance, which happens when the Cu neutral density surpasses 10^{24} m^{-3}
- Space charge starts to affect fields when the electron density surpasses 10^{21} m^{-3}

Simple vacuum discharge input parameters used for the code-to-code comparison

Parameter	Value
Scaling (general) parameters	
Grid size Δx	0.26283 μm
System length L_{sys}	21.026 μm (80 cells)
Real particle to superparticle ratio per unit volume	2.5×10^{19} /m^3
Time step	3.5 fs
Injection from the cathode	
Electron injection flux Φ_{e^-}	1.483×10^{29} /m^2/s
Neutral injection flux Φ_{Cu}	1.483×10^{27} /m^2/s
Electron injection temperature T_{e^-}	0.3 eV
Neutral injection temperature T_{Cu}	300 eV
Boundary collisions at the electrodes	
Cathode voltage	0 V
Anode voltage	10,000 V
Cu	is reflected back
Cu^+	sputters Cu with 100% probability
e^-	sputters Cu with 1% probability

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Collisions and reactions

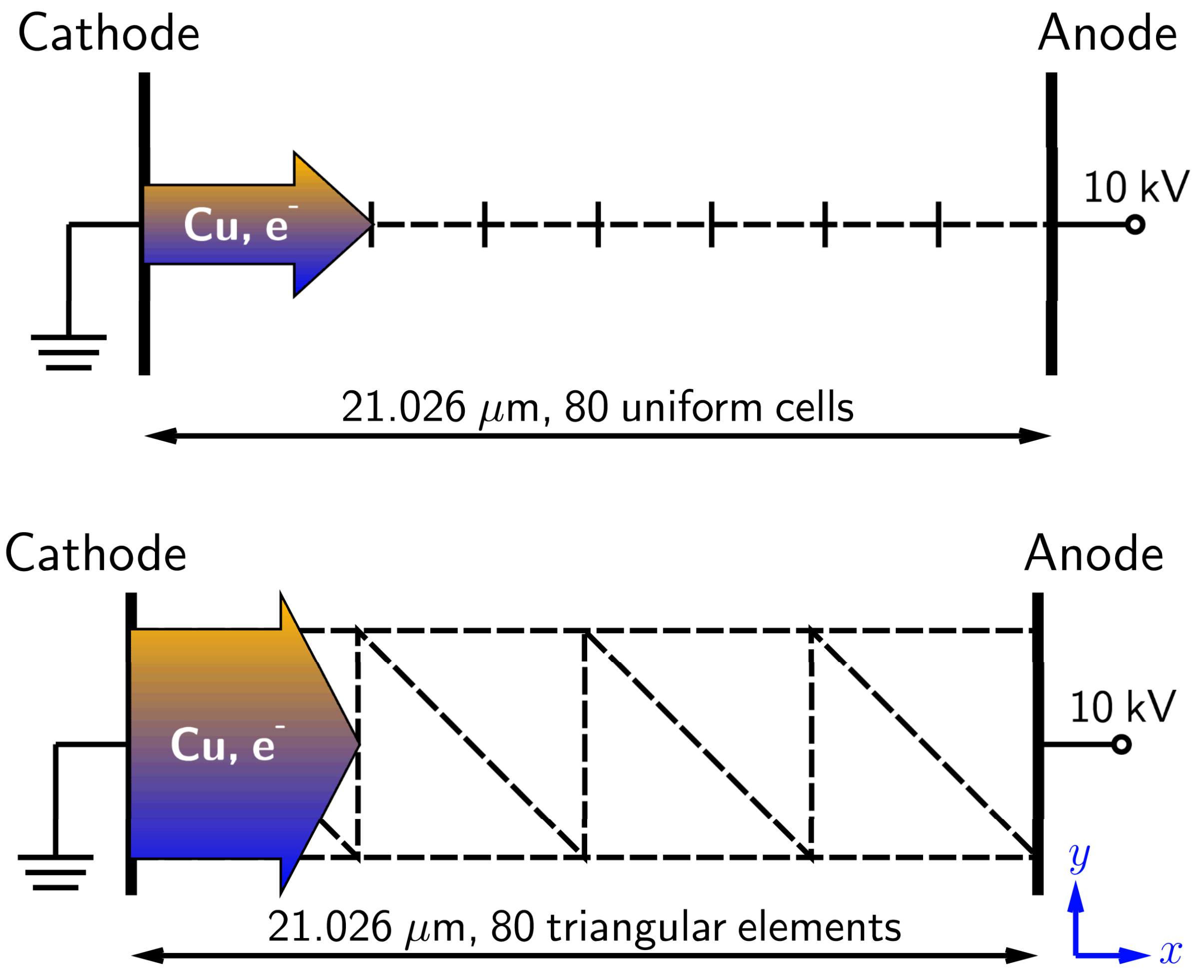
Coulomb collisions between the pairs (e^-, e^-), (Cu^+, Cu^+), (e^-, Cu^+)

Elastic collisions between the pairs (e^- + Cu), (Cu + Cu)

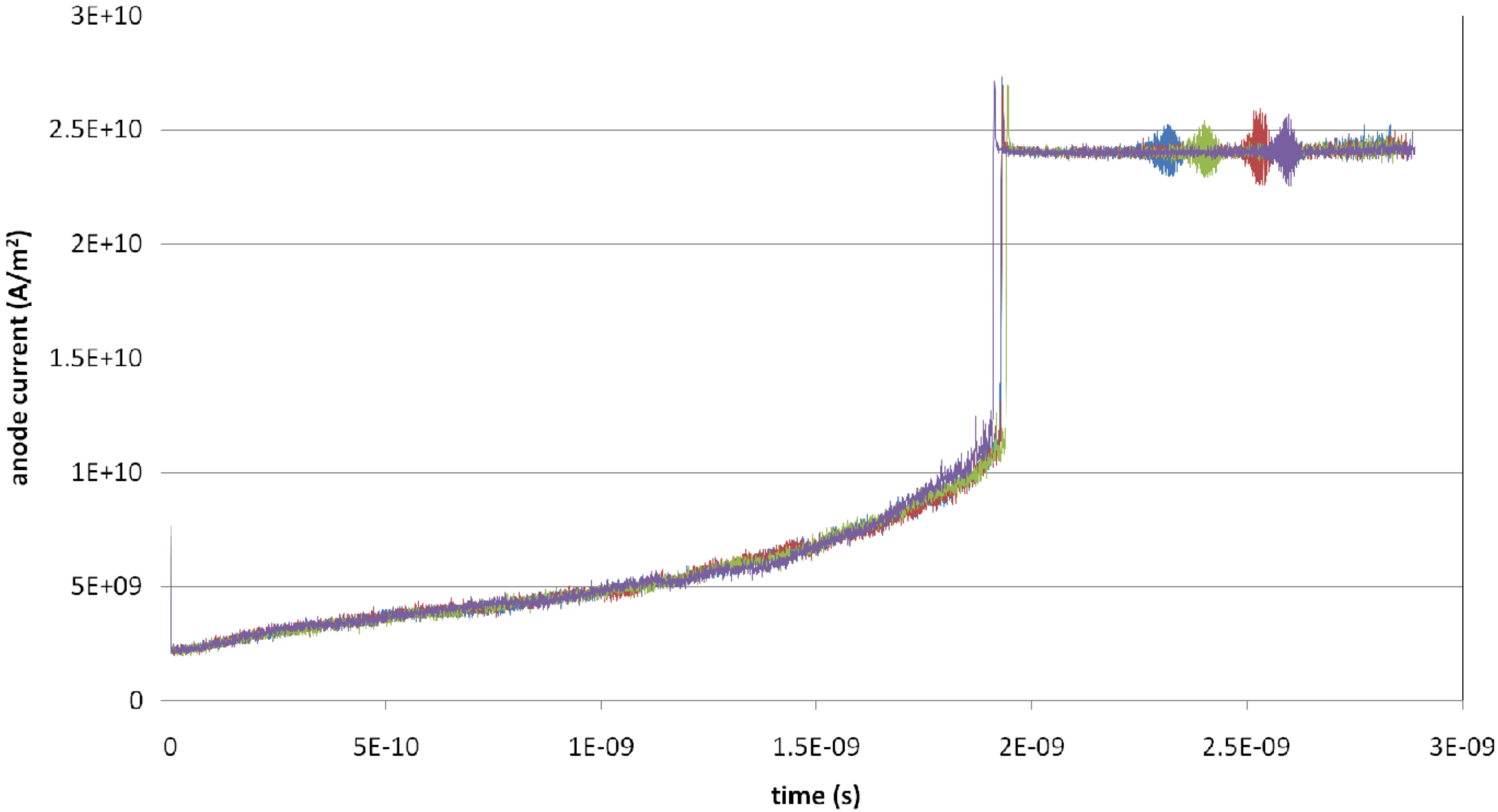
Impact ionization: $e^- + Cu \longrightarrow 2\,e^- + Cu^+$

Charge exchange and momentum transfer: $Cu^+ + Cu \longrightarrow Cu + Cu^+$

Geometries used in the comparison



Vacuum arc breakdown simulation results using Aleph
(presented May 7, 2010 at Breakdown Physics Workshop @ CERN)



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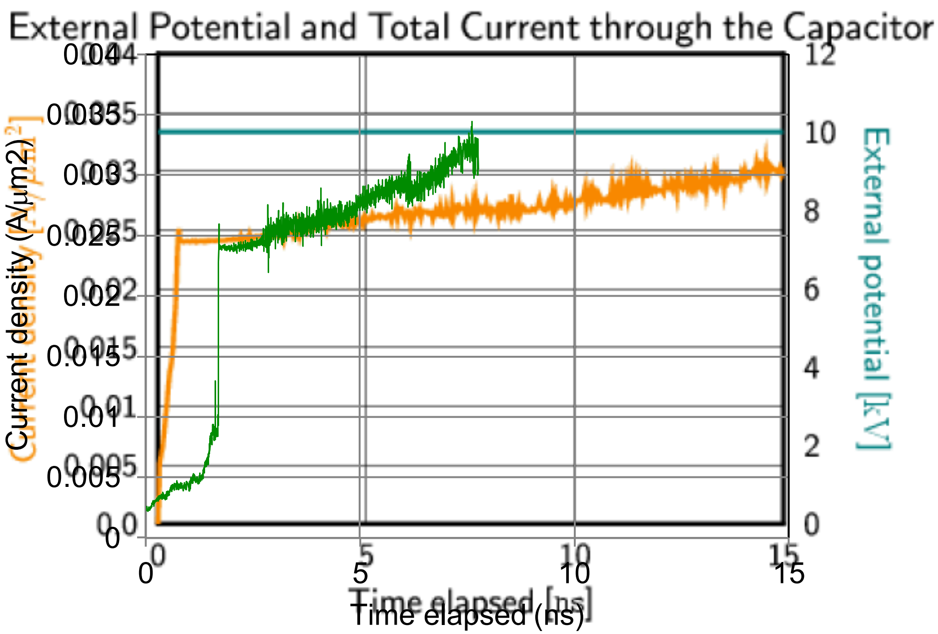
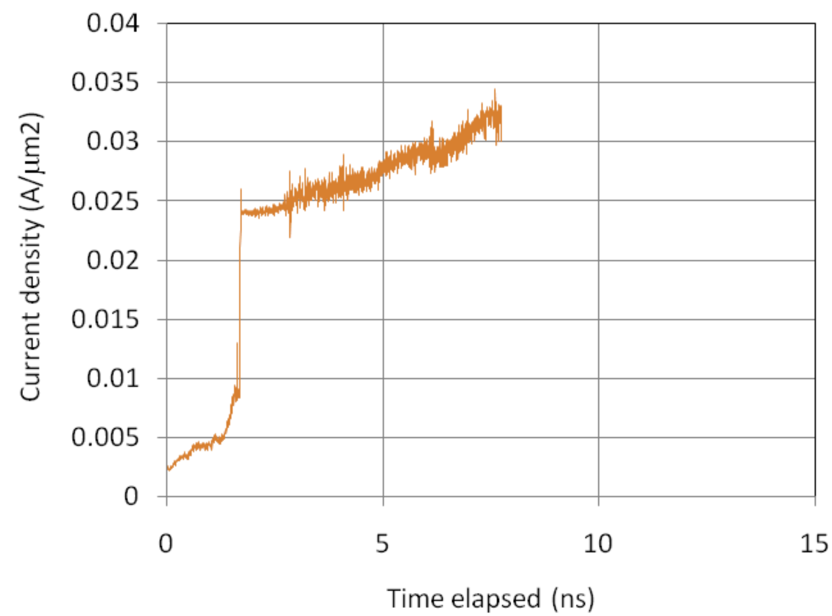
Old results comparison

From Helga



Our results (run 37)



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Possible sources of discrepancies

Simulation geometry:	Particle move dimensionality (1D, 2D)
	Field solve dimensionality (1D, 2D)
	Mesh elements (line segments, triangles)
	Mesh resolution (80 elements)
PIC technique details:	Field solver method (finite difference, finite element)
	Charge assignment method and order
	Field interpolation method and order
	Particle pusher (Boris method, velocity Verlet)
Input parameters:	(See parameters listed in Table 1.)
Particle boundary conditions:	Injection velocity distribution (truncated Maxwellian)
	At non-electrode boundaries (N/A, specular)
Collision methods:	Collision scheme (null-collision, no time counter)
	Cross section data (see [28])
	Cross section data interpolation method (linear, log)
	Cross section data extrapolation method (constant, zero)
	Post-collision energy partitioning
	Post-collision scatter procedure
Collision processes included:	Ionization collisions
(cf. Secs. 4.1 and 4.2)	Coulomb collisions
	Neutral-neutral elastic collisions
	Electron-neutral elastic collisions
	Neutral-ion charge exchange and momentum transfer

Discovered and fixed an error in Aleph's collision code

$$Z_{AB} = \frac{n_A n_B}{\sigma} d_{AB}^2 \left(\frac{8\pi kT}{m_{AB}^*} \right)^{1/2}$$

Where σ is a symmetry factor that is 1 for unlike molecules (B ≠ A) and 2 for like molecules (B = A).

Eq. 6.15b, Vincenti and Kruger, "Introduction to Physical Gas Dynamics"

(We had σ = 2 in all cases, so we were computing 2x too few A-B collisions)

What are the differences between the PIC algorithms?

PIC step	Aleph's method	Arc-PIC method
1. Interpolate charge to grid	Cloud-in-cell (CIC) (higher dimensional, unstructured version)	Cloud-in-cell (CIC)
2. Compute potential on grid	2D finite element	1D finite difference
3. Compute E	Constant field in element	Cloud-in-cell (CIC)
4. Compute F on particles	F = q E	F = q E

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Aleph field solver settings choices

Forward interpolation options (putting charge from particles on nodes or elements):

0) constant charge density in each element (this is the default, "0^{th} order" method)
1) Node-based interpolation of charge within each element (feels like a "1^{st} order" method)

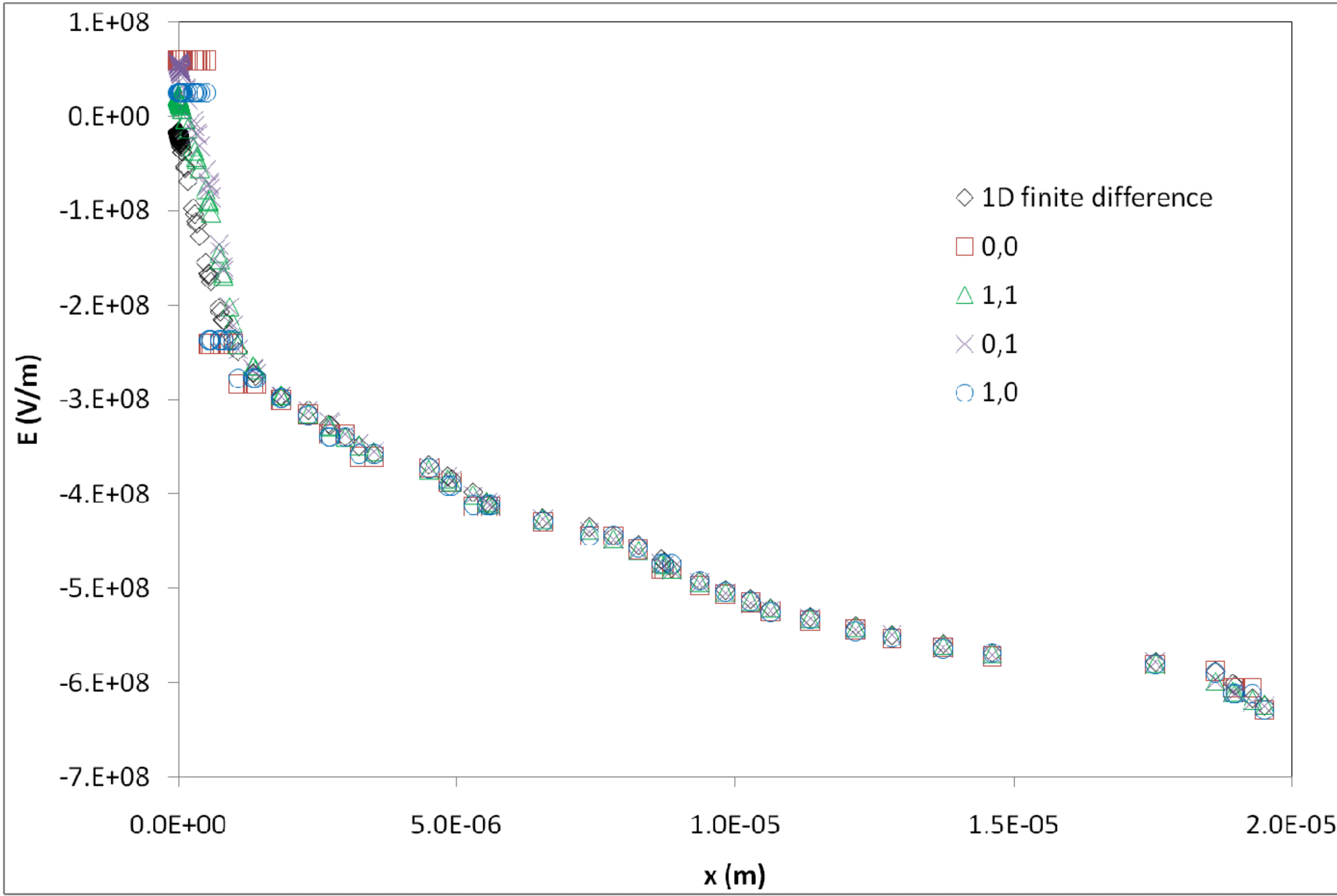
Here are the reverse interpolation options (putting E fields on particles):

0) constant electric fields within elements (this is the default, "0^{th} order" method)
1) volume-averaged electric field within elements (feels like a "1^{st} order" method)

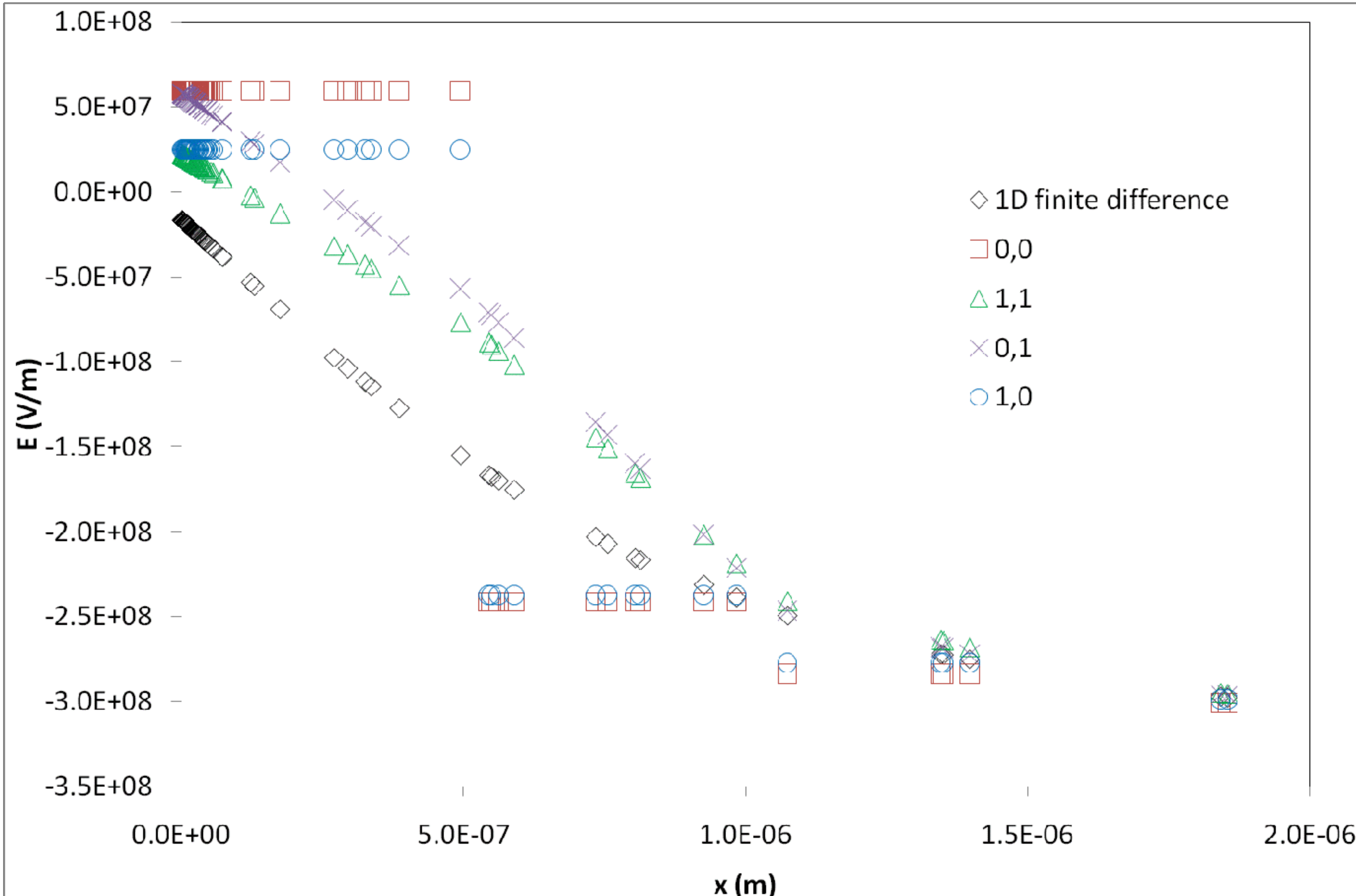
Tested all four combinations of (forward, reverse) interpolations:

(0,0)
(1,1)
(0,1)
(1,0)

How changes in field solver settings affect E



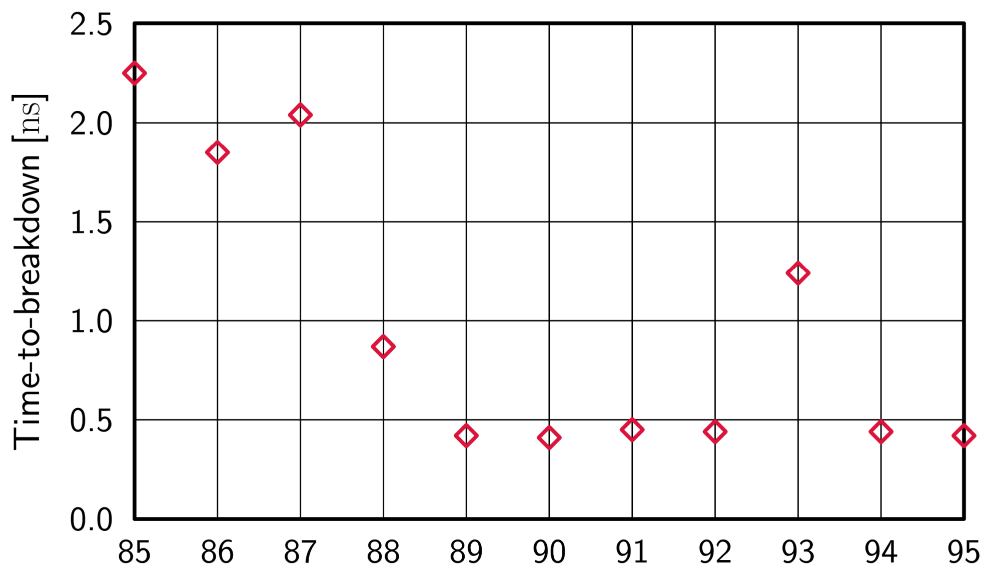
How changes in field solver settings affect E



PIC algorithm comparison observations

1. The computed potentials were usually similar, but not identical.
2. The computed times-to-breakdown were very different.
3. Method to compute E exhibited the biggest difference between the approaches.
4. <u>Constant-field-in-element approach produced insufficient accuracy for this problem at this mesh resolution.</u>

Changes in times-to-breakdown as computed by *Aleph*



Run number	85	86	87	88	89	90	91	92	93	94	95
Time-to-breakdown	2.25	1.85	2.04	0.87	0.42	0.41	0.45	0.44	1.24	0.44	0.42
Particle move dimensionality	1	1	1	2	1	1	2	2	2	2	2
Field solve dimensionality	2	2	2	2	1	1	2	2	2	2	2
Charge assignment order	0	0	0	0	1	1	1	0	1	1	1
Field interpolation order	0	0	0	0	1	1	1	1	0	1	1
Particle weighting / 276317917	1	1	1	1	1	0.1	1	1	1	0.1	10
Cross-section data interpolation	log	linear	linear	linear	linear	linear	linear	linear	linear	linear	linear
Threshold energy discrepancy	yes	yes	no	no	no	no	no	no	no	no	no

Lessons learned: causes of the big differences in computed times-to-breakdown

Differences in the:

1. Cross-section data, and its interpolation/extrapolation
2. Collision/chemistry methods
3. Post-collision scatter and energy disposal methods
4. PIC methodology

After remedying the major causes of the discrepancies, we observed much better agreement …

Code	Time-to-breakdown (ns)	Standard deviation in time-to-breakdown (ns)
Aleph	0.42	0.03
Arc-PIC	0.45	0.03

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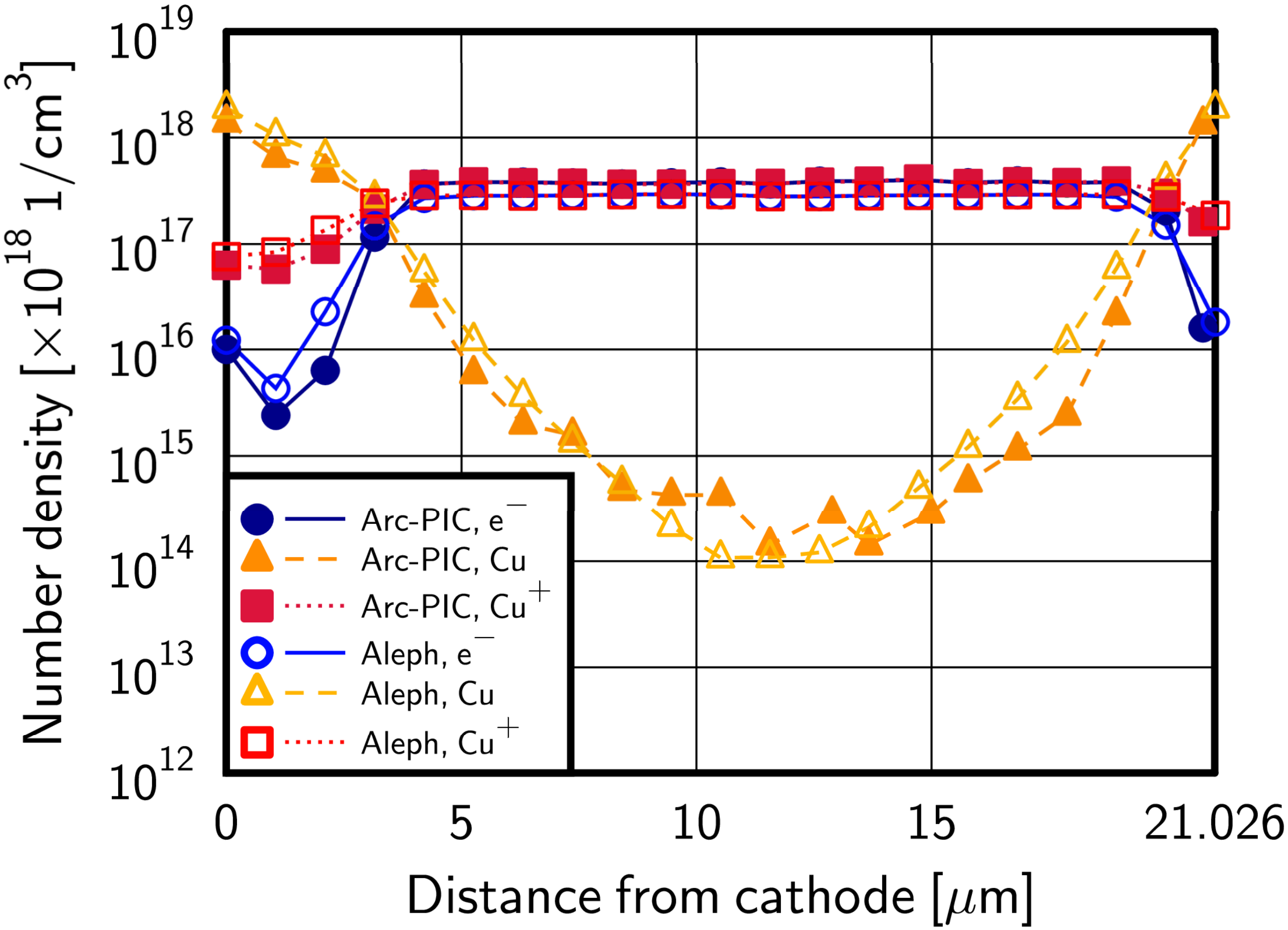
Spatial density distributions

Number densities across the discharge gap, averaged over the time interval between 3 and 3.5 ns.

Arc-PIC and Aleph show good qualitative agreement in all of the quantities, including the sheath region.



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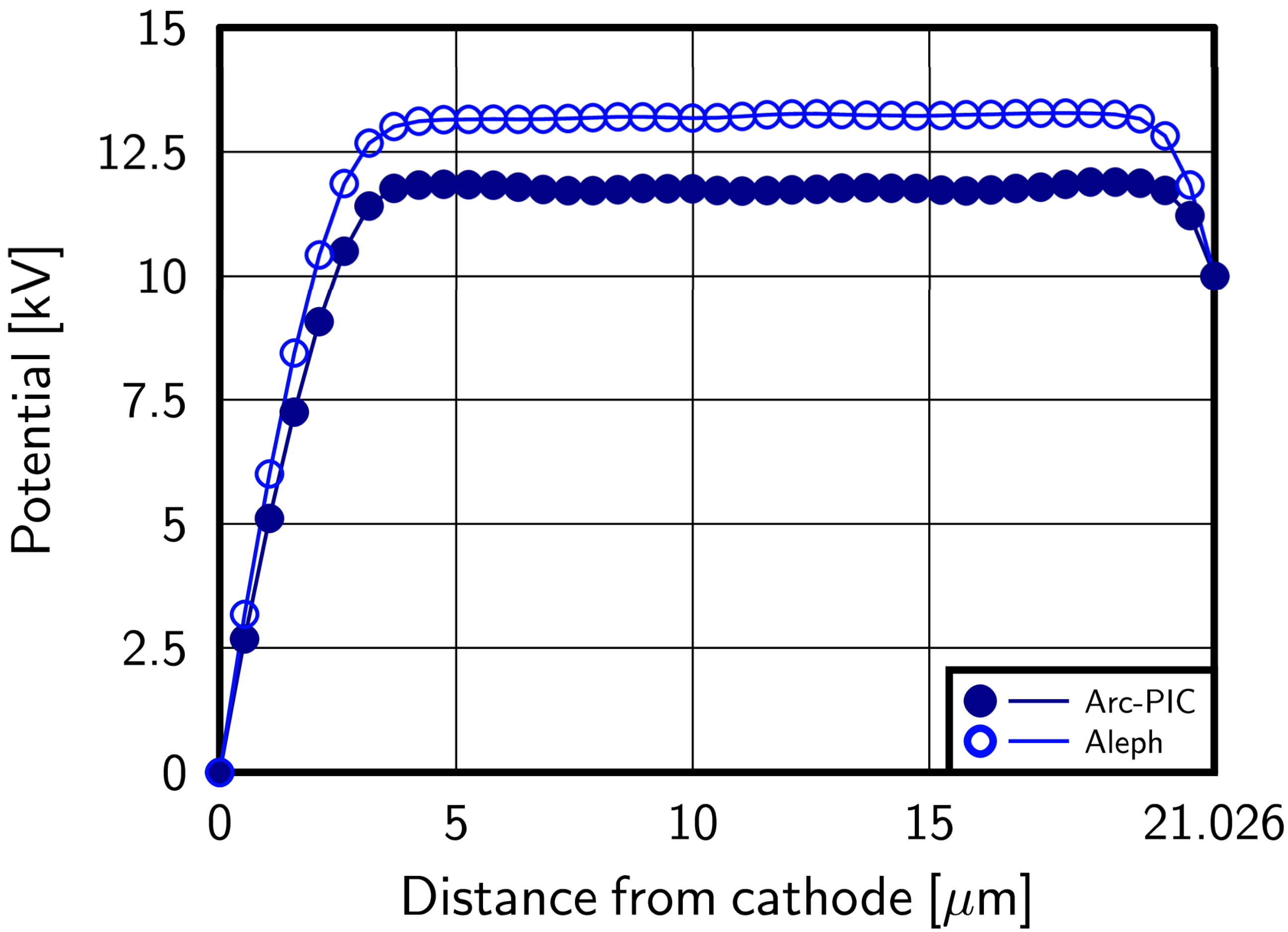
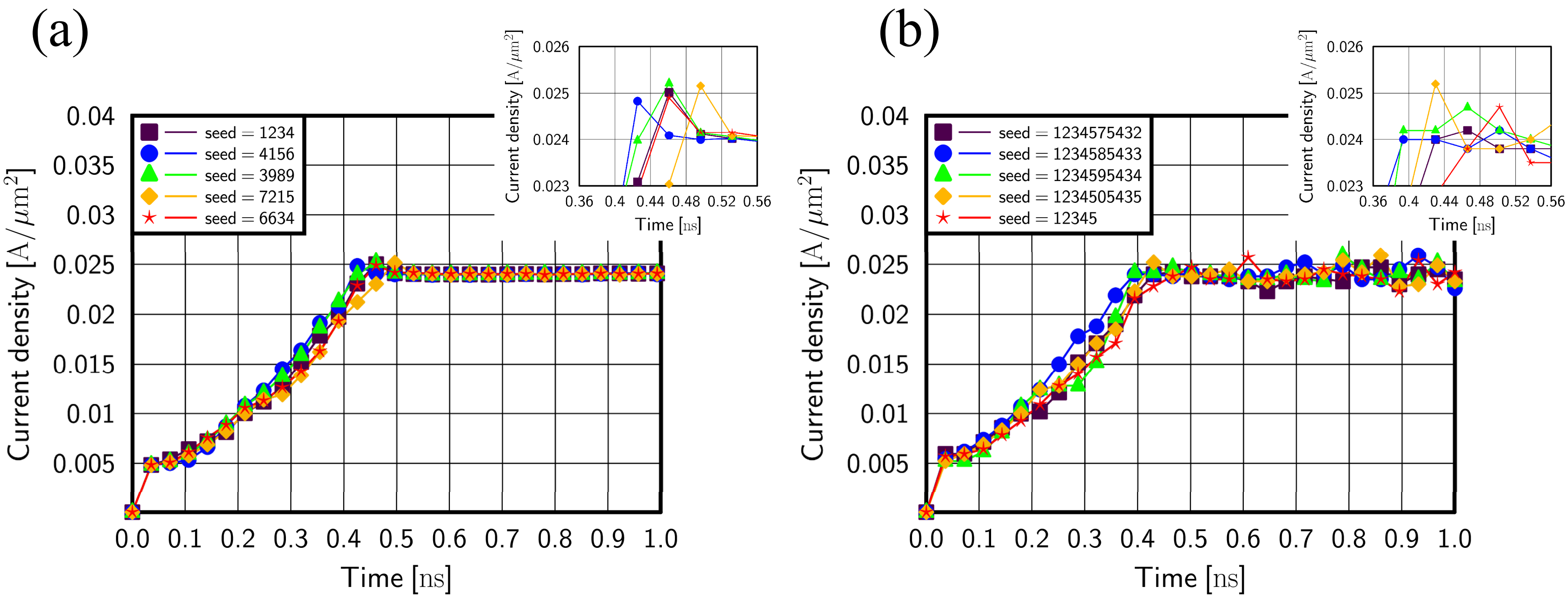
Potential profiles

Potential profiles across the discharge gap, averaged over the time interval between 3 and 3.5 ns.
Arc-PIC and Aleph show good qualitative agreement in all of the quantities, including the sheath region.
The plasma potentials differ slightly.



Time evolution of the current density across the gap



Figs.(a) and (b) show the statistical variation in current density with different seeds for Arc-PIC and Aleph, respectively.

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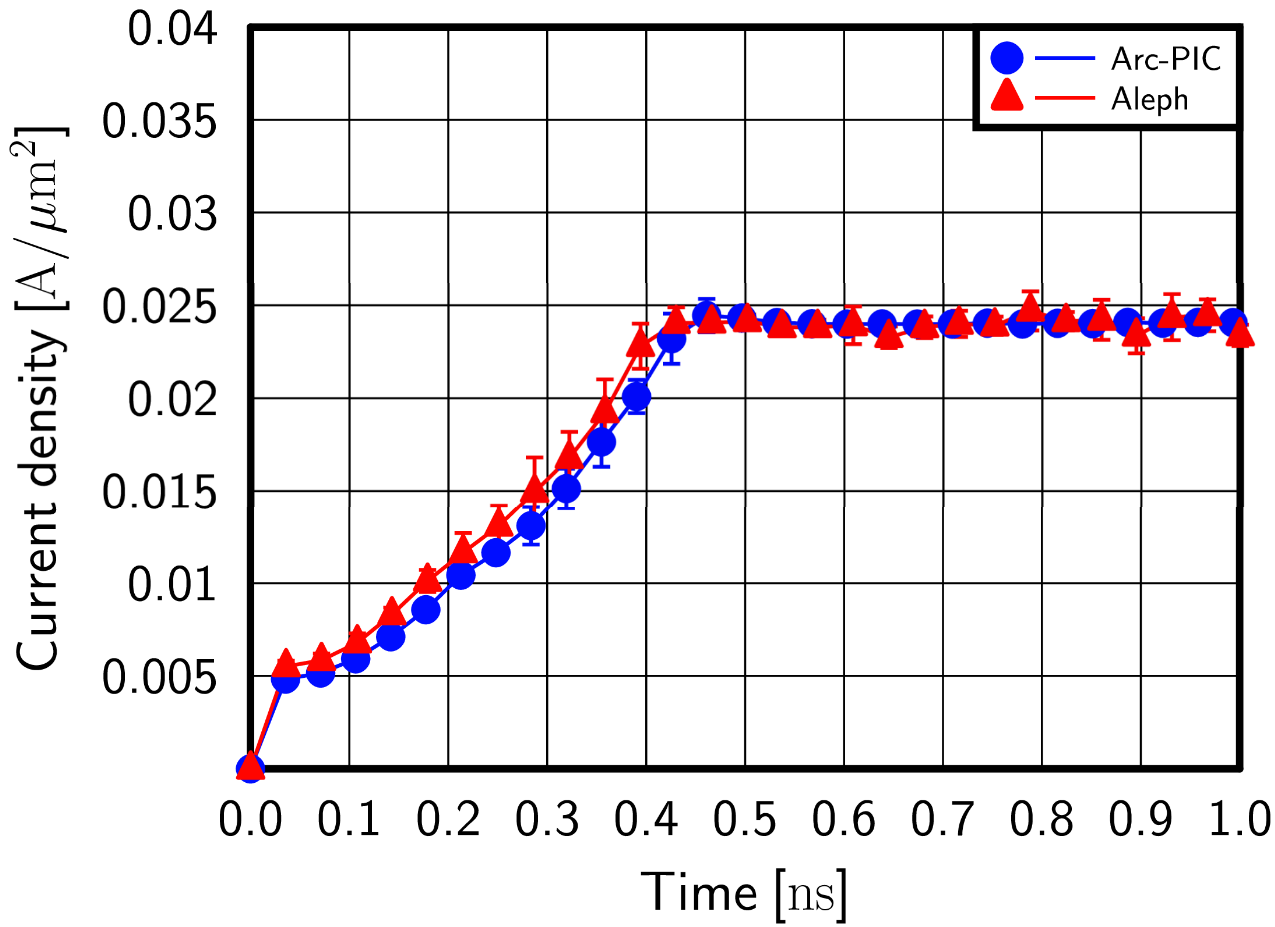
Time evolution of the current density across the gap

5-run average current densities for both codes.

The error bars represent the standard deviations produced by using different initial random number seeds.



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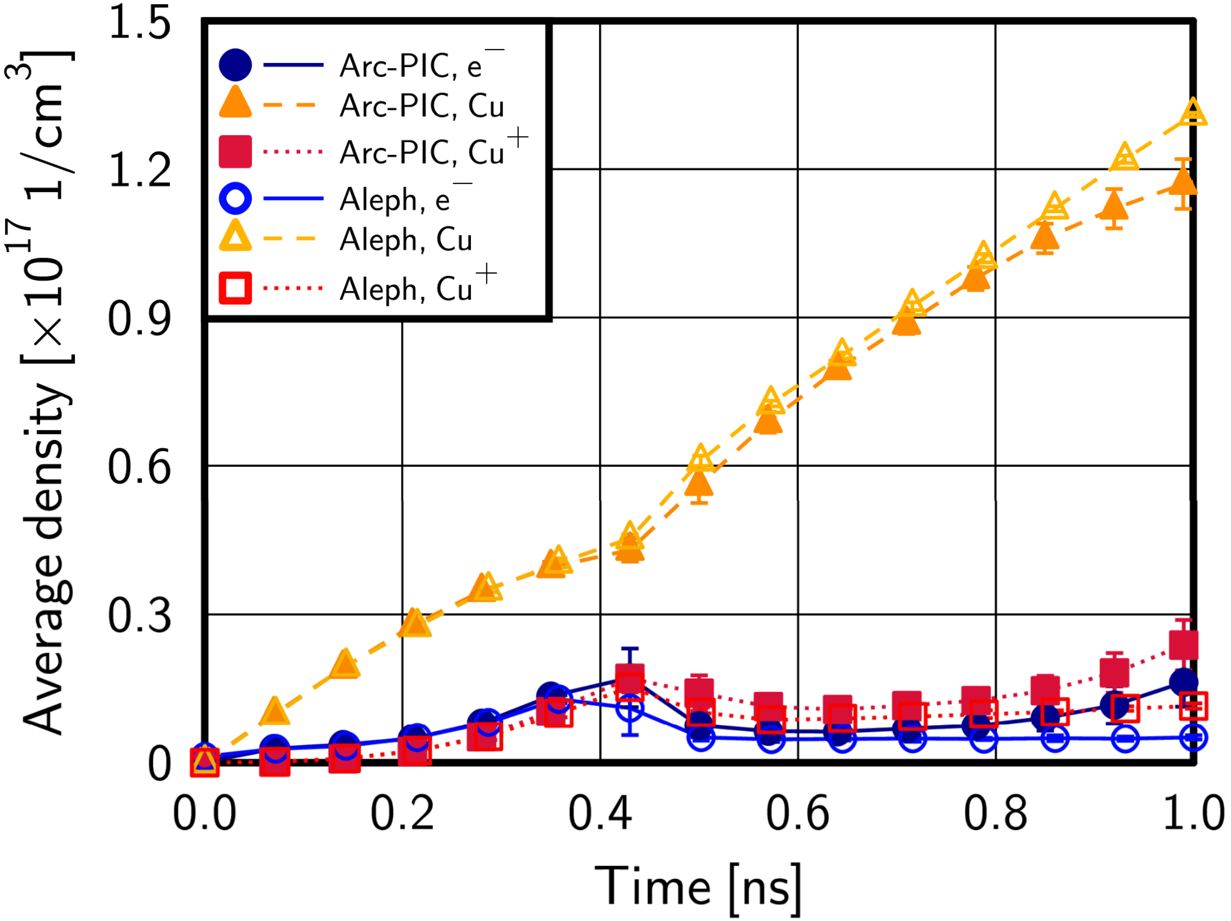
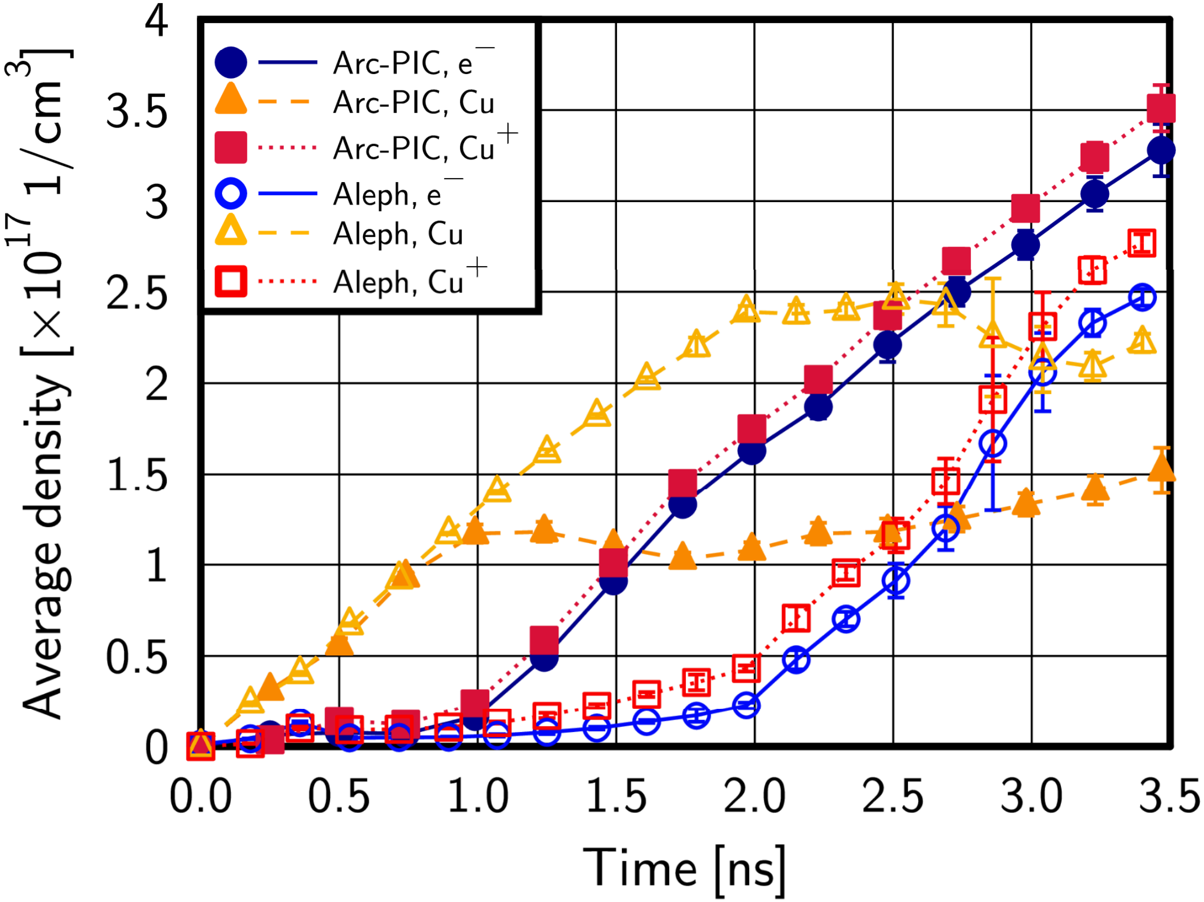
Early time particle densities

Time evolution of e⁻, Cu, and Cu⁺ average densities compared between Arc-PIC and Aleph. Each data point shows the 5-run average density calculated from the 5 simulations initialized with different random number seeds. The error bars represent the corresponding standard deviations.



Particle densities vs time

Time evolution of e$^-$, Cu, and Cu$^+$ average densities compared between Arc-PIC and Aleph. Each data point shows the 5-run average density calculated from the 5 simulations initialized with different random number seeds. The error bars represent the corresponding standard deviations.



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Conclusions

1. **Code-to-code comparison proved valuable.**
   - Increased confidence in codes and their ability to model non-linear phenomena.
   - Opened avenue for communication between research groups. Good way to collaborate.

2. **Essential to perform thorough V&V on PIC codes.**

3. **Simple 1D arc breakdown benchmark problem now well-defined for use by other research groups.**

4. **Vacuum arc discharge model very sensitive to small differences in input and methods.**

5. **Accurate PIC methodology and use of cross-section data especially crucial.**

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