Monte-Carlo vs. Bulk Conductivity Modeling of RF Breakdown of Helium*

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Motivation: Simulation of RF Breakdown of gases

• Goal is to simulate breakdown of gases at or near atmospheric pressure by GHz fields.

RF frequency	0-3 GHz
Gas pressure	0.5-1 atm
Electric field amplitude	10-50 kV/cm
Electric field/pressure (E/p)	10-100 kV/cm/atm
Pulse length	100 ns
Gases	He, Air, Ar, SF_6

•For strong enough fields seed electrons in the neutral gas are heated up to the ionization threshold. “Breakdown” occurs when the resulting weakly ionized plasma becomes large enough to affect the propagation of the RF field.

•At high enough densities the plasma becomes opaque. But the required density can be much higher than the “critical” density of a collisionless plasma.

Weakly ionized plasma regime

- In a weakly ionized plasma ($n_p << n_n$), collisionality of plasma species is dominated by collisions with neutrals.
- When energy dependent inelastic processes are significant the plasma particle distribution function can be quite non-Maxwellian

2 approaches to simulating weakly-ionized plasma

- Monte-Carlo collision (MCC) model in PIC code to simulate electron-neutral scattering and ionization in detail.
- Bulk conductivity (σ) model used to calculate Ohm's law current in EM solver.

Both approaches have been implemented in the code Lsp.

The two methods are compared in 0-D swarm calculations and 1-D RF breakdown simulations with He at STP.

Monte Carlo Scattering Algorithm*

- Implemented a Monte Carlo scattering algorithm for weakly ionized plasmas.
- Algorithm allows for an arbitrary number of elastic and inelastic processes, including ionization, excitation, and charge exchange. But must resolve collision frequency.
- Coulomb collisions assumed negligible. Recombination channels and multi-step processes not considered at present.
- Benchmarked against Boltzmann code for 0D swarm calculations. Good agreement in steady-state distribution function.
- Benchmarked against Berkeley plasma reactor code XPDP1 in 1D simulations of capacitively coupled plasma (CCP) reactor.

*Algorithm similar to that described in C. Birdsall, IEEE Trans. Plasma Sci. vol. 19, no. 2, p. 65, 1991.

Bulk Conductivity Model[1]

- In highly collisional regime ($\omega << \nu$) assume electron distribution function instantaneously reaches asymptotic state.
- Gas conductivity can be calculated from transport coefficients obtained from steady-state Boltzmann code EEDF[2].
- In this regime all transport coefficients are a function of only E/p. Lookup tables made for several gases (Air, He, Ar, SF_6)
- Electron density rate equation solved on grid using local E/p value. Conductivity used in Ohm's law current in EM field solve
- No macroparticles are necessary. Collision frequency need not be resolved.

[1]"N. Bruner et al. "Numerical Model of Microwave-Induced Gas Breakdown" (ICOPS 2004, paper 5P12; http://ewh.ieee.org/cmte/icops/ICOPSprogram.pdf)

[2]A. Napartovitch, "EEDF user's guide", unpublished

0-D swarm calculations with He at STP with Lsp

- 0-D velocity space simulation performed for He at STP
- Simulation performed in 1 cell. For MCC method particle velocities are updated but not positions.
- Prescribed electric field applied but No EM solve. The plasma current is not allowed to feed back on the fields.
- Algorithm allows for an arbitrary number of elastic and inelastic processes, including ionization, and excitation. But must resolve collision frequency.
- Compare the MCC and σ models with Boltzmann solver EEDF for DC field of 10 kV/cm
- Compare MCC and σ models for 10 kV/cm, 1 GHz field.

Cross-sections for e-He scattering

Collision frequency

$\nu = n_n \sigma v_{th}$

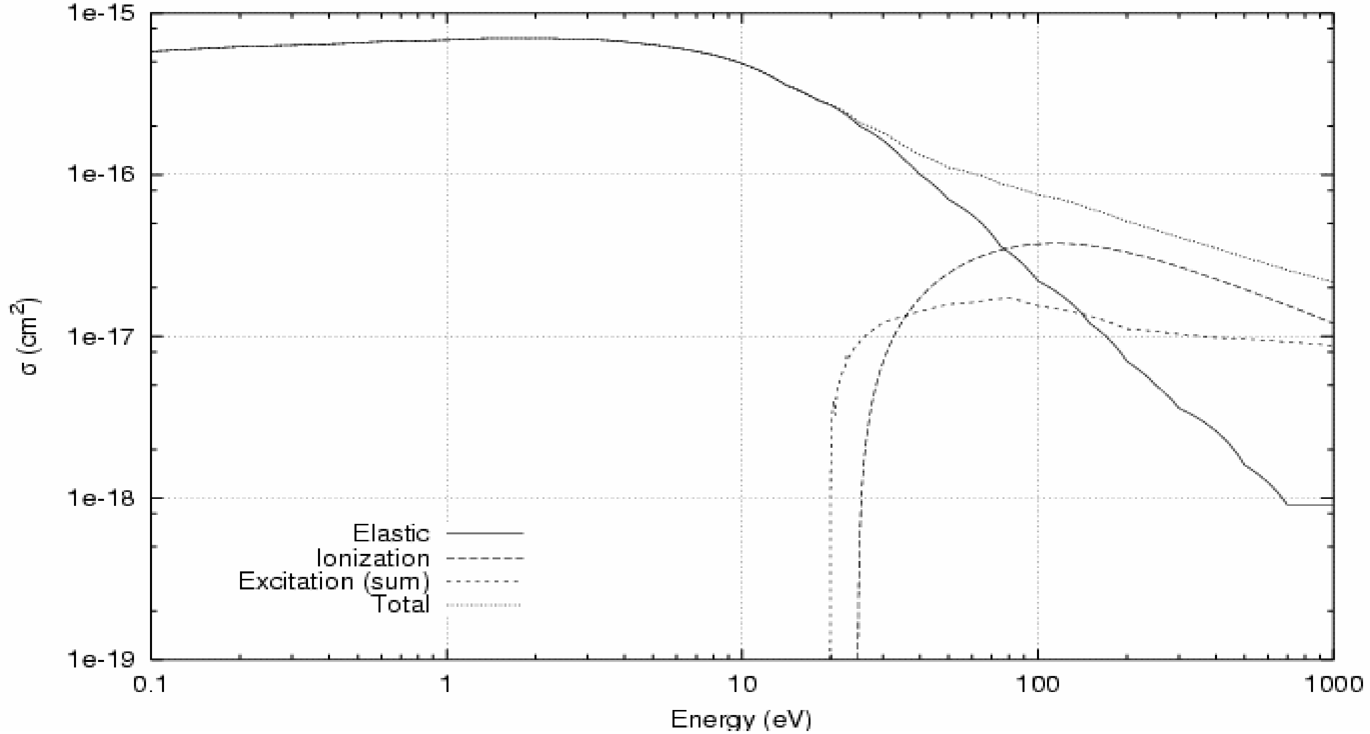
$\sigma \sim 10^{-15} cm^2$

For a few eV electrons

$v_{th} \sim 4 \times 10^7$ cm/s

and He at STP

$\nu \sim 10^{-12}$ s^{-1}

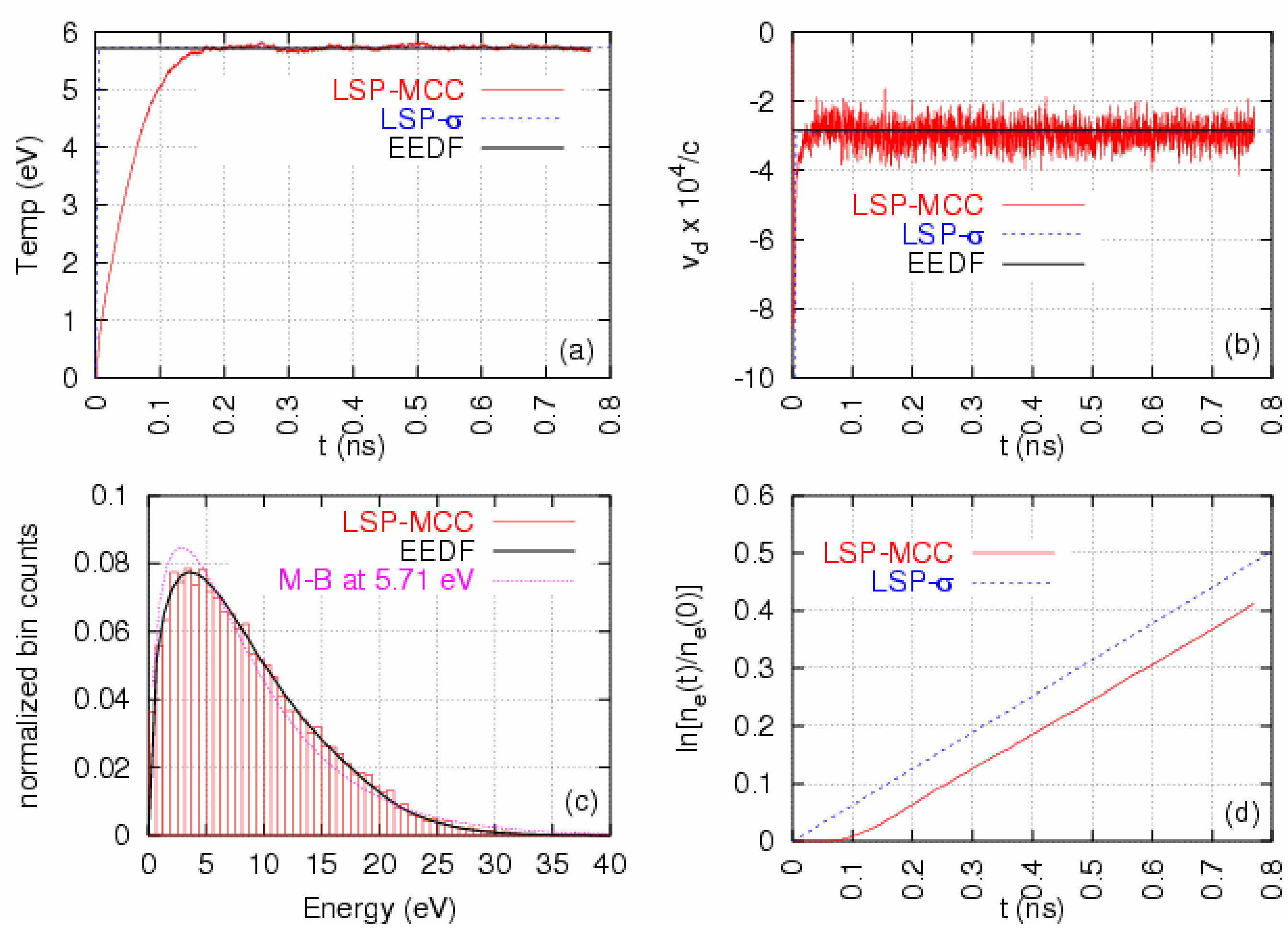


MCC model must resolve collision frequency

Ionization threshold 24.6 eV

Swarm calculation He at STP, E = 10 kV/cm DC

Seed electrons: $n_e = 10^{10}\ cm^{-3}$ at room temp.



0.1 ns transient time (a few hundred collision times) for electron heating up to ionization threshold.

Electron cooling due to equilibration with cold neutrals

If the field is shut off electrons will equilibrate with cold neutrals.

$$\frac{dT_e}{dt} = -Q_{en}$$

$$Q_{en} = \frac{m_e}{m_n}\nu(T_e - T_n)$$

For a few eV electrons and He at STP

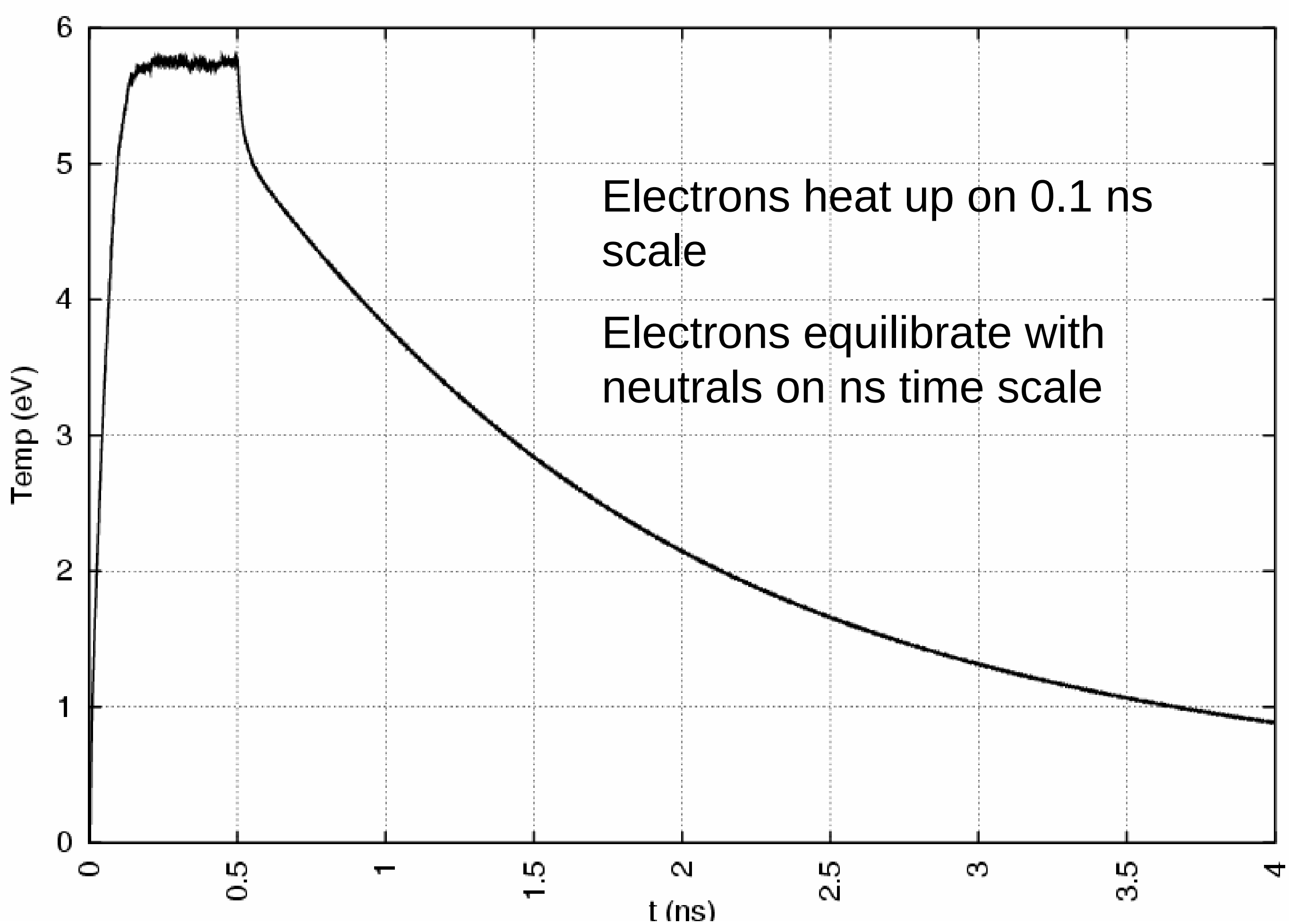
$$\nu \sim 10^{12}\,\mathrm{s}^{-1}$$

Equilibration time scale

$$\tau_E \sim \frac{m_n}{m_e}\frac{1}{\nu} \sim \text{ few ns}$$

Based on simple arguments there is an equilibration time on the order of 1 ns (thousands of collision times).

MCC swarm test: ns equilibration time



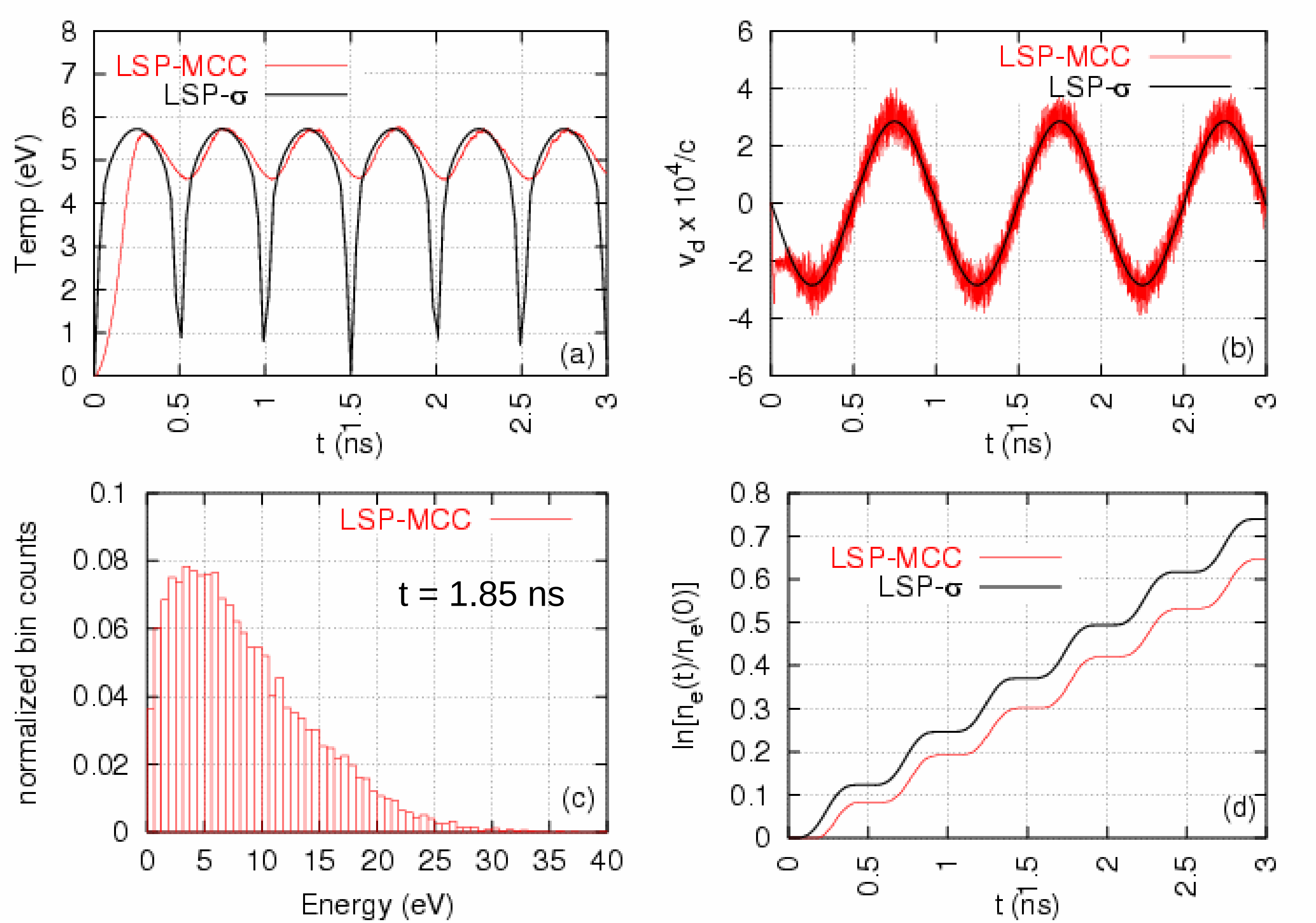
Electrons heat up on 0.1 ns scale

Electrons equilibrate with neutrals on ns time scale

Repeat swarm calculation with constant electric field 10 kV/cm. But abruptly shut off field at t = ½ ns.

Repeat with 1GHZ frequency on field

He at STP, E = 10 kV/cm sin(2 π 1 GHz t), ne(0) = 1e10 /cc



σ model lacks transient heating and cooling effects.

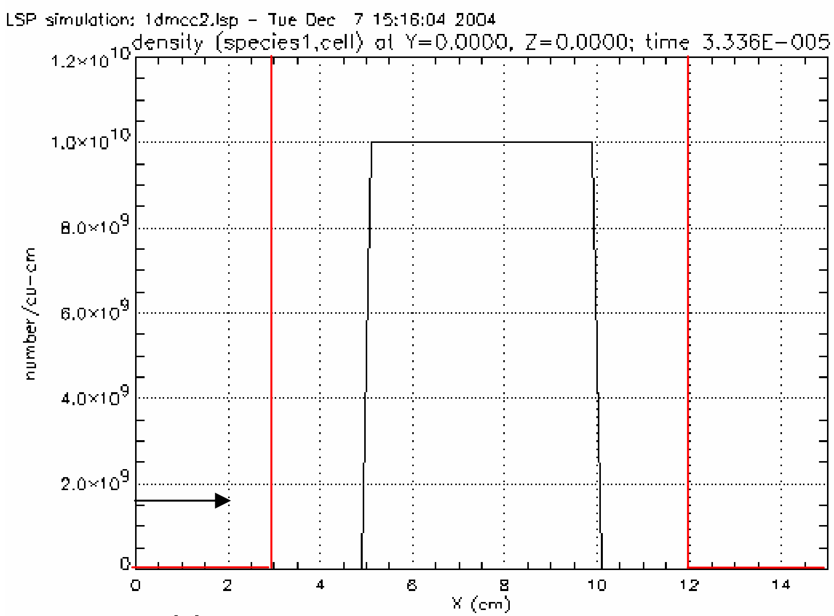
This results in slight overestimate of effective ionization rate.

He breakdown simulation

- 1D Lsp simulation of He breakdown
- He at STP
- Incident plane wave $|E|$=10 kV/cm, f = 1GHz
- Wave incident on 1-D slab of He gas with seed electron density.
- Again compare MCC and σ model.

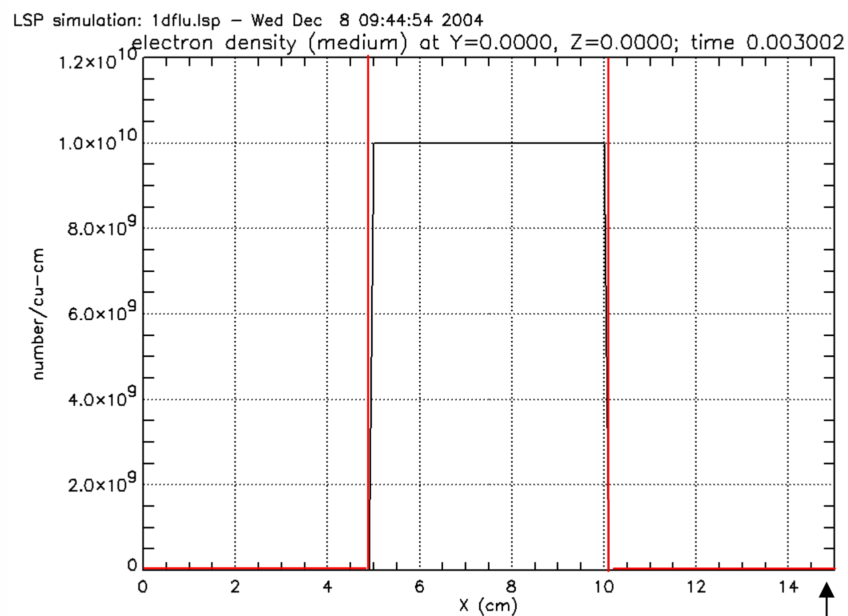
Initial density profiles

MCC simulation setup



Incident RF wave

Conductivity model simulation



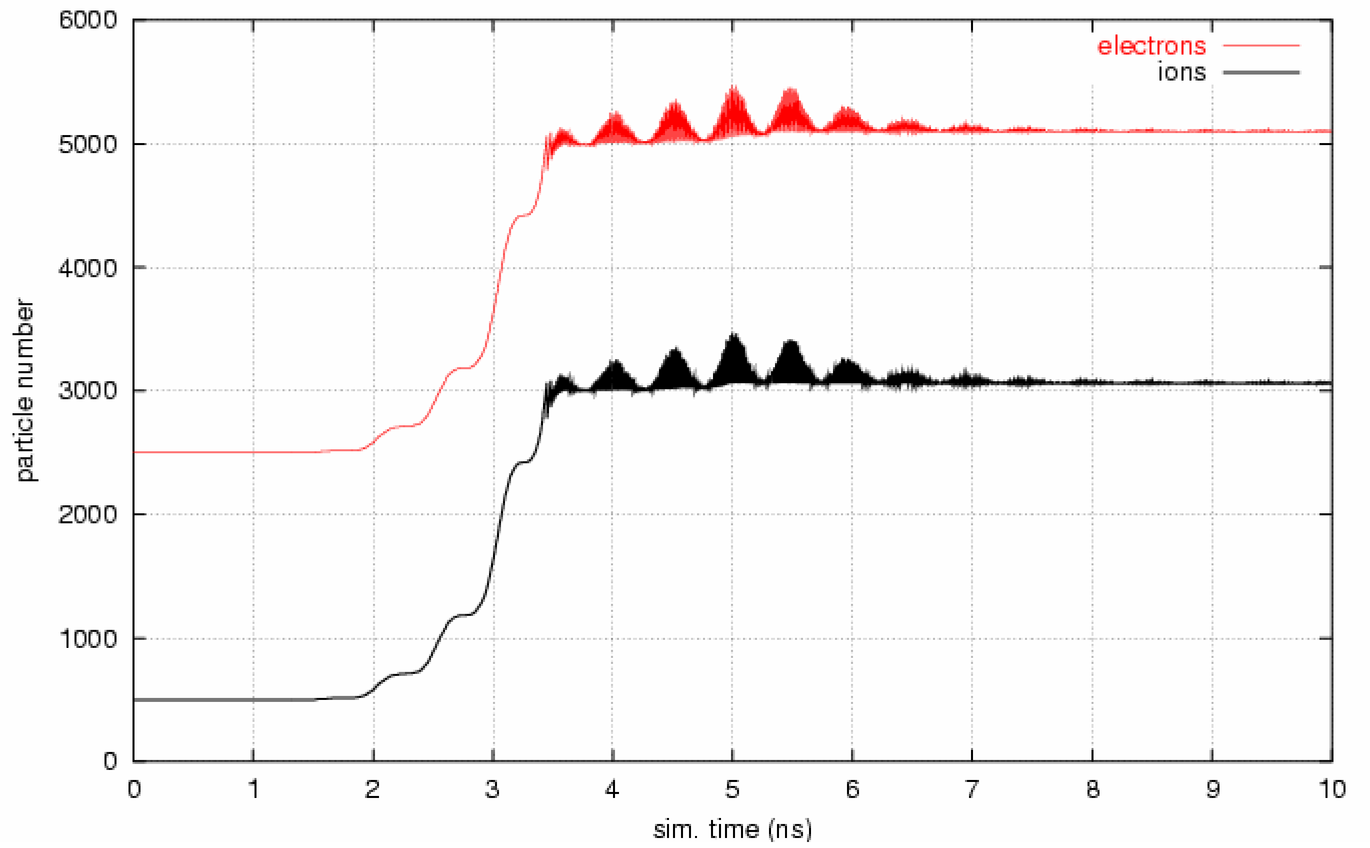
Neutral density profile

Seed electron profile

Wave transmitting boundary

Extra neutrals in MCC model here are just to keep the electrons from diffusing into the vacuum region where they are accelerated ballistically.

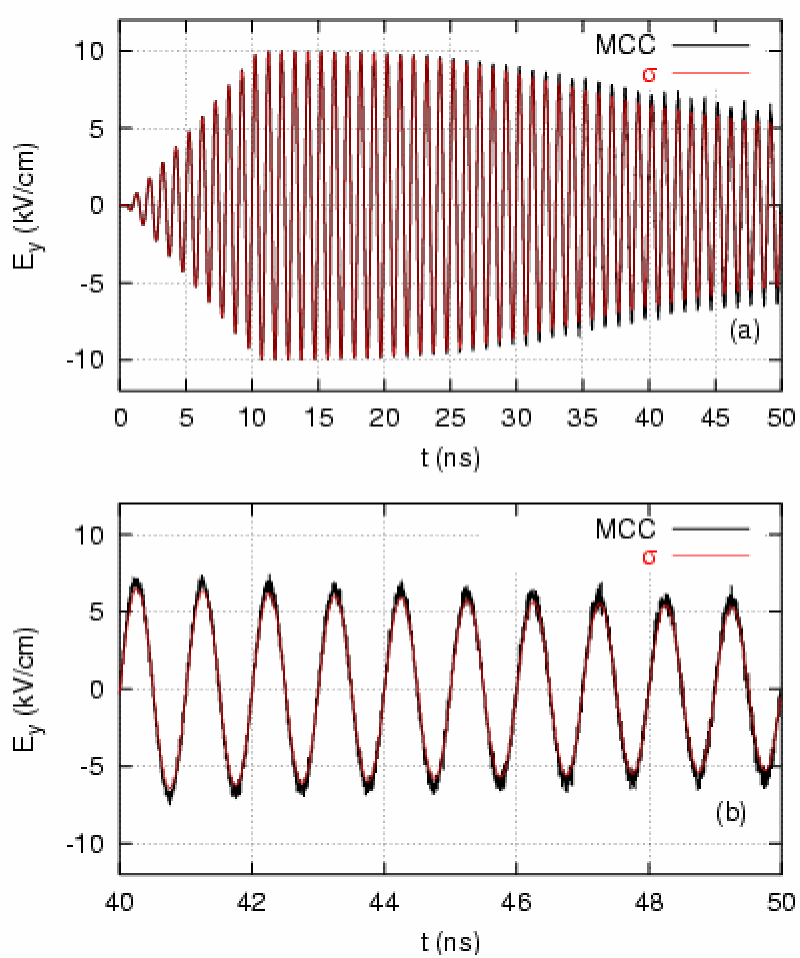
Particle number in MCC algorithm



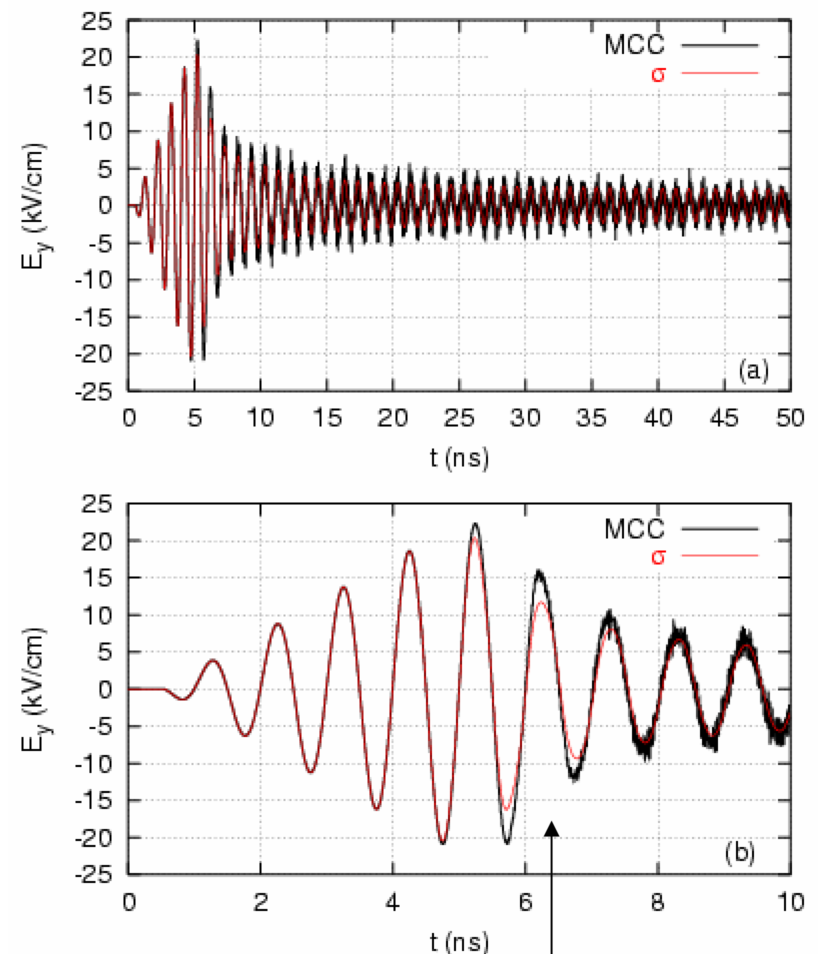
Lsp uses particle collapse algorithm to keep particle number from growing prohibitively large despite exponential growth in density.

Transmitted field amplitudes vs. t for 10 kV/cm, 50 kV/cm

10 kV/cm



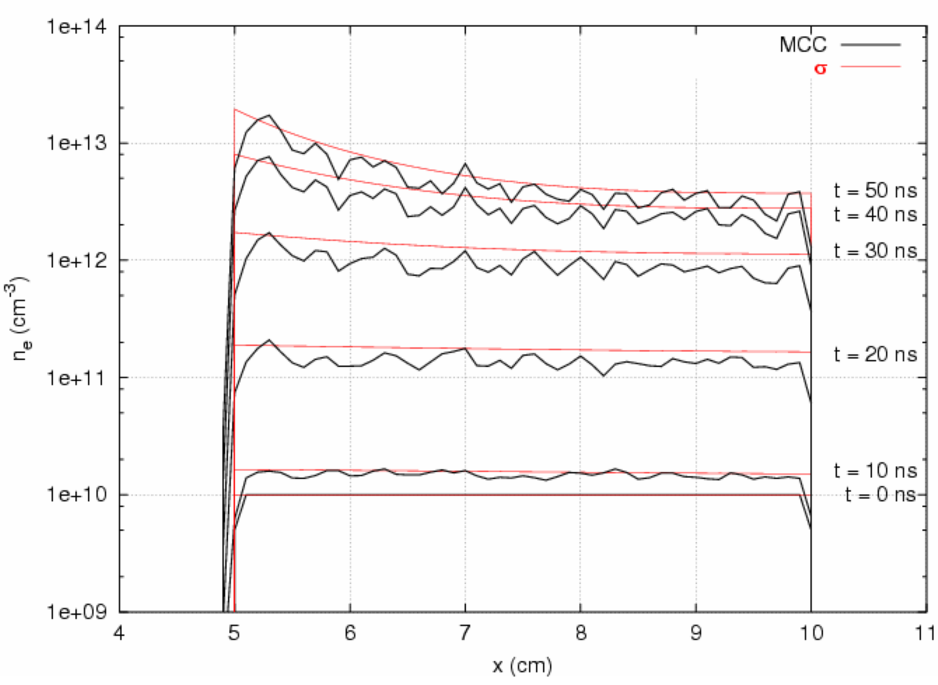
50 kV/cm



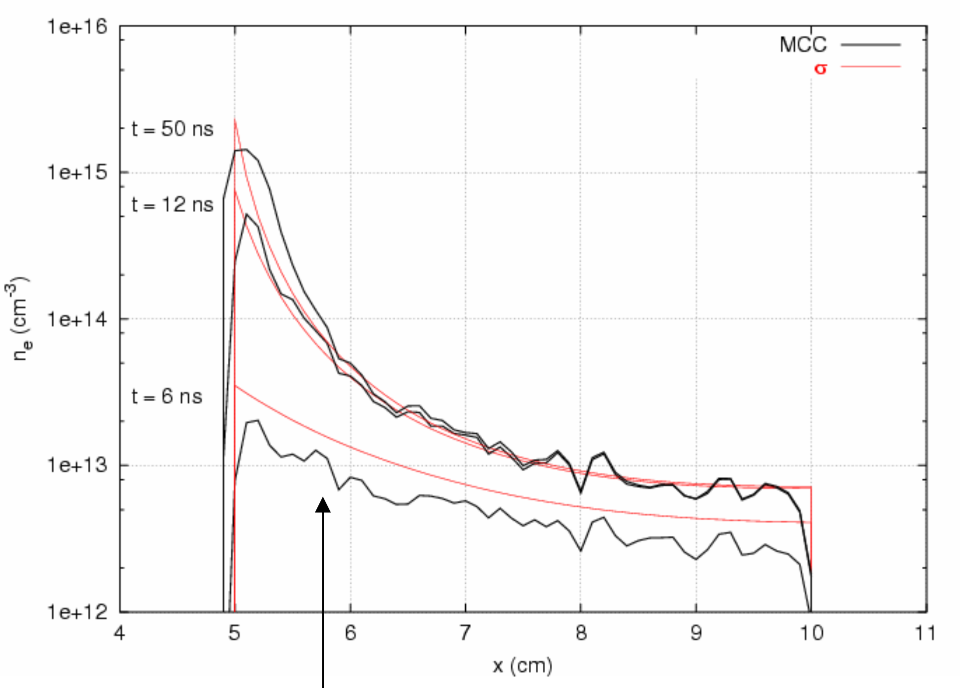
Small discrepancy due to elevated ionization rate for σ model.

Electron density vs. z for 10 kV/cm, 50 kV/cm

10 kV/cm



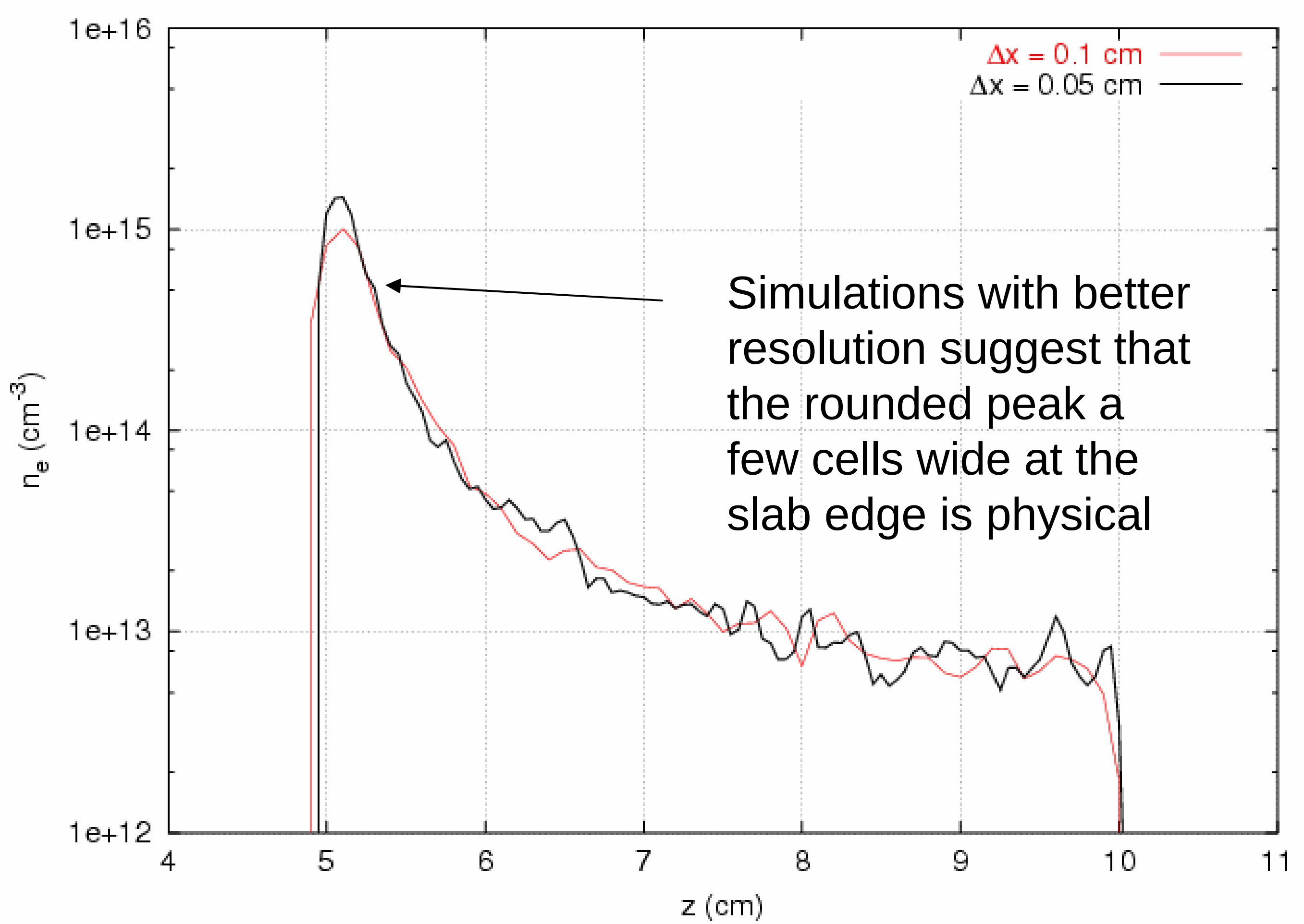
50 kV/cm



Discrepancy due to elevated ionization rate for σ model.

MCC model and edge effects

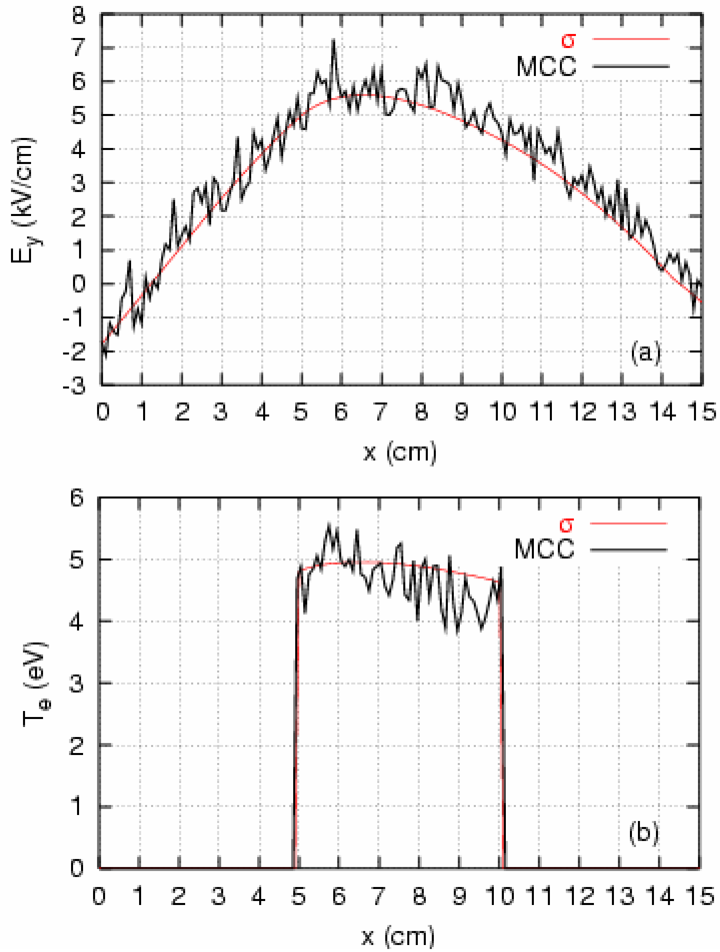
Neither Debye length nor collisional mean free path are resolved on grid for MCC model



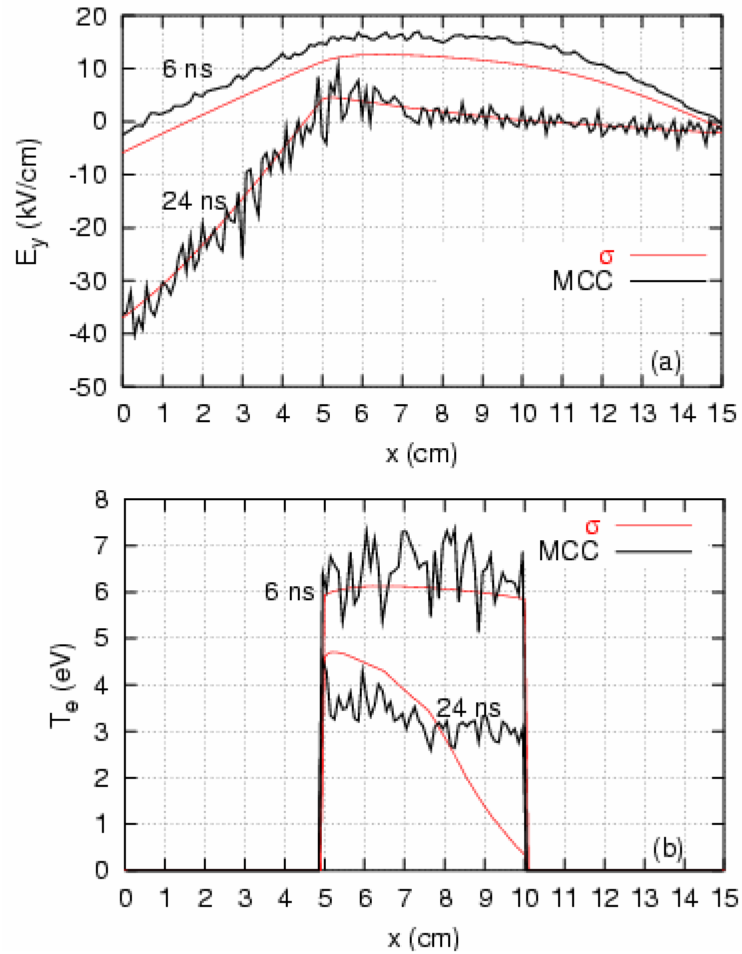
Simulations with better resolution suggest that the rounded peak a few cells wide at the slab edge is physical

Electric field and electron temperature vs. z

10 kV/cm



50 kV/cm



As field value is reduced in slab, electron temperature drops.
Transient cooling time neglected in σ model

Thermal Conductivity: too slow

Is thermal conductivity significant in the slab?

$$\frac{dT_e}{dt} \sim -K\nabla^2 T_e$$

$$K \sim \frac{T_e}{m_e \nu} \sim \frac{v_{th}^2}{\nu}$$

For He at STP and electron energy of a few eV

$$\nu \sim 10^{-12}\text{s}^{-1}$$

$$K \sim 1600 \text{ cm}^2\text{/s}$$

Slab width $L = 5$ cm

Thermal conduction time scale

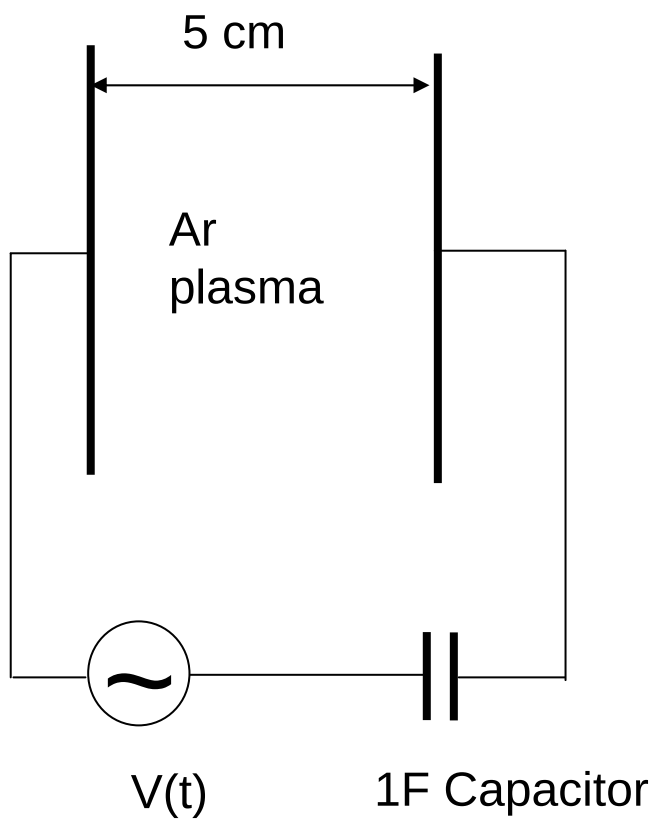
$$\tau_K \sim \frac{L^2}{K} \sim 10^{-2} s$$

Thermal conduction takes too long to be significant.

Same argument holds for spatial diffusion (ambipolar or not)

Compare LSP with MCC model and Berkeley code XPDP1* for 1D capacitively coupled plasma reactor

1-D simulation of weakly ionized Ar plasma between capacitor plates driven by RF voltage source



*J. Verboncoeur, M. Alves, V. Vahedi, and C. Birdsall, J Comp. Phys. Vol 104, p. 321, 1993

Download available at http:/ptsg.eecs.berkeley.edu

Cross sections for electron-neutral collisions for Ar gas

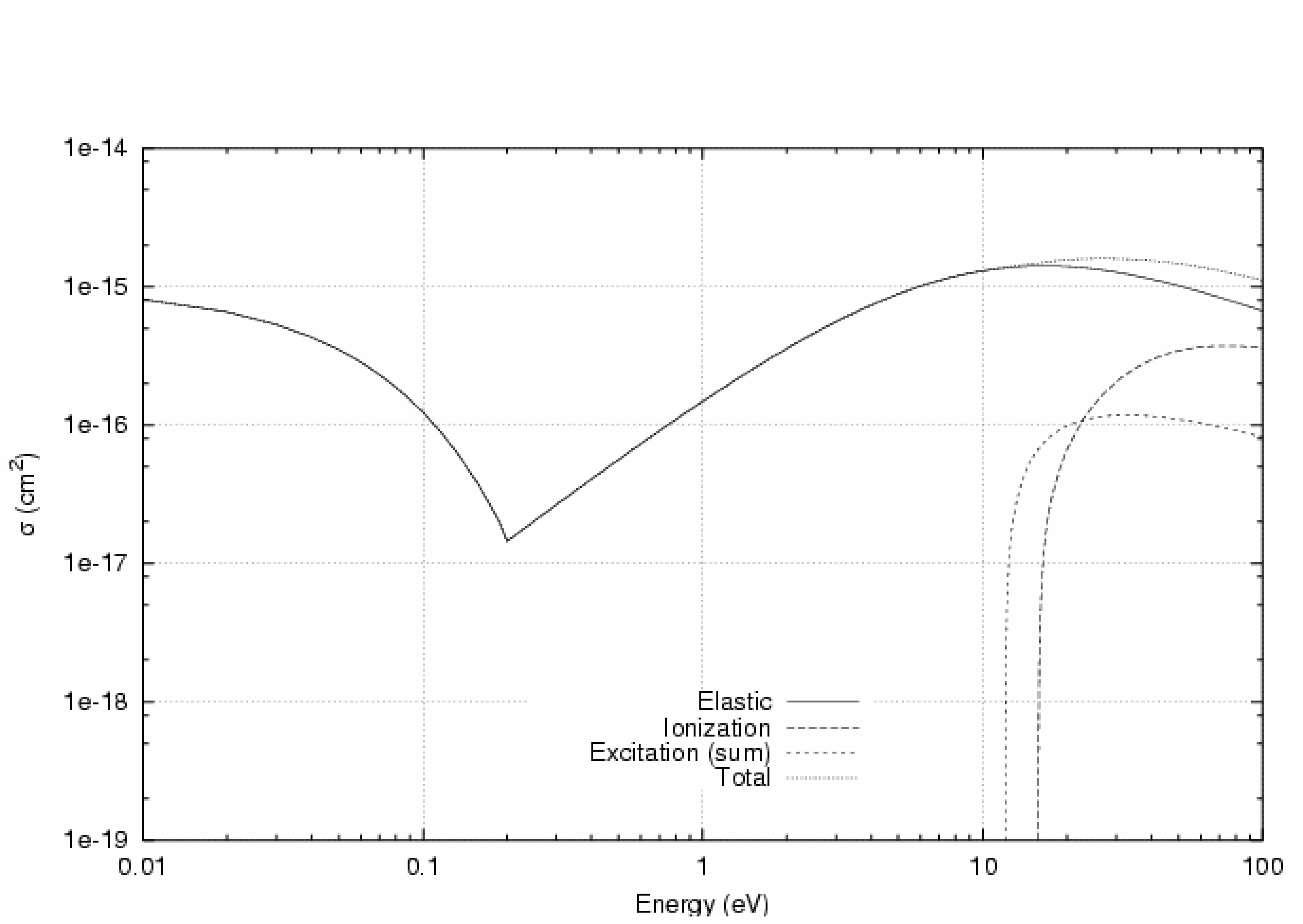
Important processes are

1) Elastic scattering of electrons and neutrals
2) Ionization
3) Sum of Excitation

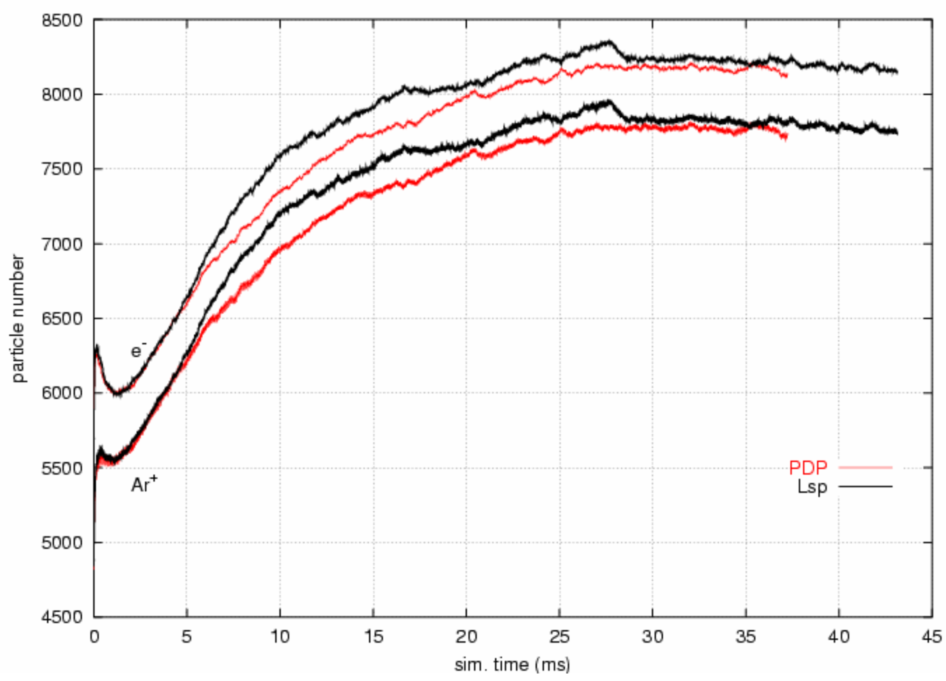
processes

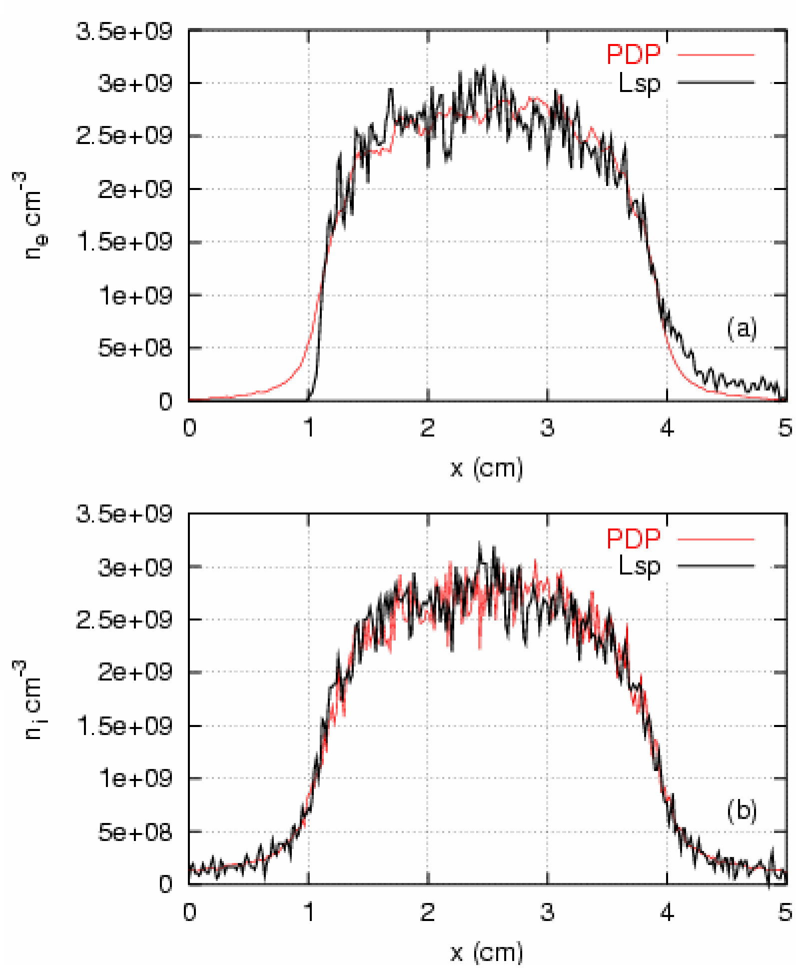
Ionization threshold
~ 15.7 eV

Excitation threshold
~ 11.6 eV



Comparison of Lsp with MCC and XPDP1





Conclusions

- Described Monte-Carlo collision model and Bulk conductivity model for simulation weakly-ionized plasmas.
- Compared the two approaches for RF breakdown simulations. Overall agreement is good. Conductivity model is faster (no macroparticles, needn’t resolve collision frequencies) but lacks proper treatment of transient plasma heating and cooling.
- MCC benchmarked in CCP simulations

Lsp info: http://www.lspsuite.net