

# **Numerical Solution of the Boltzmann Equation:**

## **Kinetic Simulation of Plasmas**

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# Outline

- **Propagator Method**
- **Kinetic Model (Convective Scheme – CS) using propagator method**
  - **Energy Conservation**
  - **Long Lived Moving Cell Technique – reduce ND**
  - **Collisions**
- **Fluid Model using Propagator Method**
  - **Ballistic movement and energy conservation**
  - **Propagator method VS Finite Difference**
  - **Can be used over wide range of  $\Delta x$  and  $\Delta t$**
- **N-Capacitor Model to observe ‘local’ and ‘non-local’ behaviors of discharge**
  - **Analytic calculation**
  - **Fluid/Capacitor Model**
- **Comparison among models**

# Propagator Method

- Kinetic behavior of gas discharge described by Boltzmann Equation (BE) :

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{a} \cdot \frac{\partial f}{\partial \mathbf{v}} = C(f)$$

- Solution for each particle species (for short time step)

$$f(\mathbf{x}, \mathbf{v}, t) = \iint P(\mathbf{x}, \mathbf{v}, t; \mathbf{x}', \mathbf{v}', t') f(\mathbf{x}', \mathbf{v}', t') d\mathbf{x}' d\mathbf{v}'$$

Where  $t > t'$

# Convective Scheme vs Particle Methods

- **Particle Methods (Monte Carlo, P-I-C models)**
  - Use super particles – unbreakable entities which collide statistically using random number generators
  - Statistical noise in number of particles in a small region (of phase space) can be significant issue
- **Convective Scheme (CS)**
  - Uses cells
  - Free of statistical noise, but finite size and discreteness of phase space mesh can cause numerical diffusion (ND)
  - Long-Lived Moving Cells (LLMC) can reduce ND by reducing the number of times redistribution occurs

# Convective Scheme (CS)

- **Ballistic Transport**

- **BE numerically integrated along ‘characteristic curves’**

$$\begin{aligned}\frac{dz}{dt} &= \mathbf{v} \\ \frac{d\mathbf{v}}{dt} &= \frac{q}{m} (\mathbf{E} + \mathbf{v} \times \mathbf{B})\end{aligned}$$

- **Total energy is conserved**

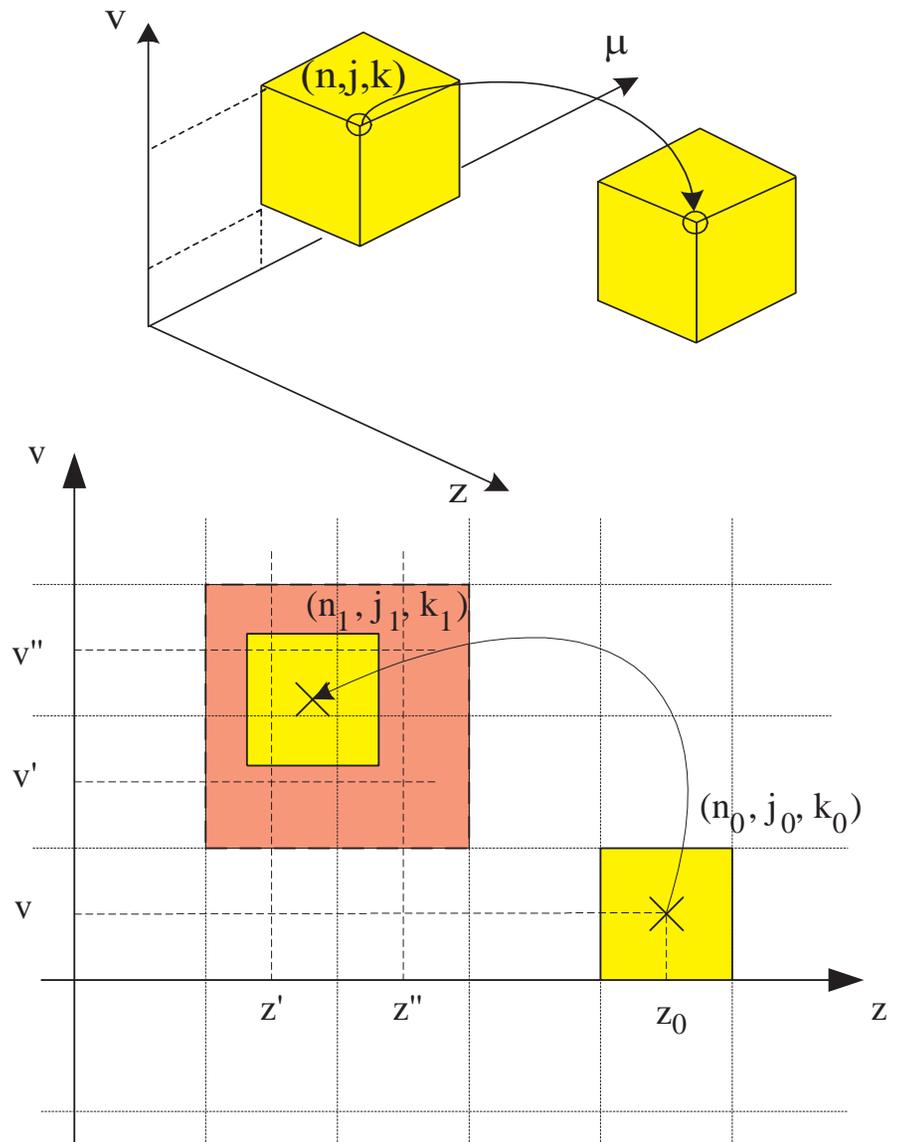
$$\frac{1}{2} m v_z'^2 = \frac{1}{2} m v_z''^2 + q\Phi(z'') - q\Phi(z')$$

- **Use staircase potential profile**

**Potential set to be uniform in each spatial cell**

# Construct Mesh and Cells

- **e.g. Mesh** constructed from
  - $z$  : position on spatial  $z$  axis
  - $v$  : speed of electron
  - $\mu$  :  $\cos \theta$  ( $= v_z/v$ ),  
 $(n,j,k)$  associated with  $(z|_j, v|_l, \mu|_k)$
- **Mesh Cell** : cell fixed on mesh
- **Initial Cell** : cell before ballistic motion carries it away from its original mesh cell
- **Moving cell** : cell during or after ballistic motion
- **Final Cell** : mesh cell overlapped by moving cell at end of ballistic motion

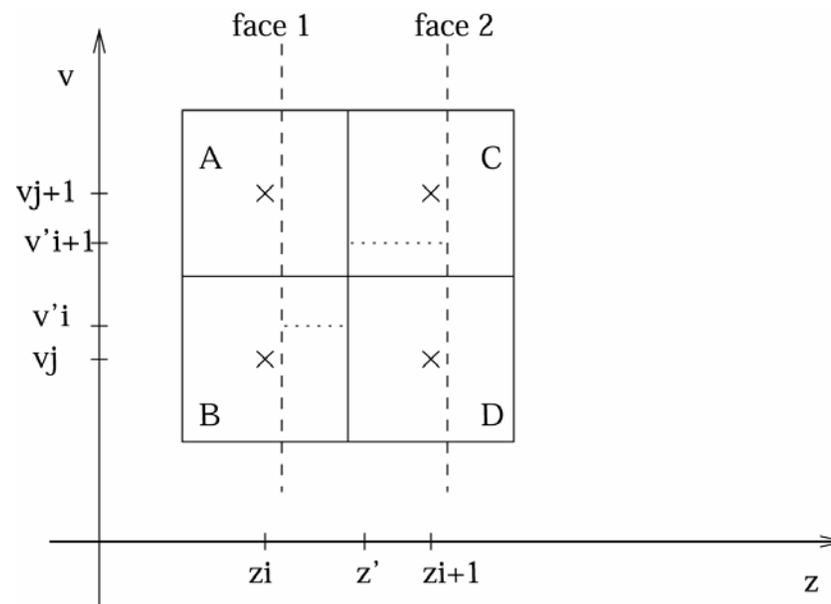


# Particle Redistribution

- **Electrons in moving cell at  $(z', v', k')$  shared between neighboring cells on  $(z, v)$  mesh, cells A, B, C, and D.**
- **Particle number and kinetic energy conserved - contents of initial cell carefully put back, one initial cell at a time**
- **In each spatial cell, particles are additionally mapped over  $v$  and  $\mu$  cells such that ‘parallel’ and ‘perpendicular’ components of average kinetic energy unchanged**

# Energy Conservation During Particle Redistribution

- **Overlap in energy is determined from energy conservation in each spatial cell separately – allowing for different potential energy in each spatial cell**



- **$v'_i$  is the speed which conserves energy in the left hand spatial cell;  $v'_{i+1}$  conserves energy in the right hand spatial cell**

- **The overlap in space and energy determine fraction ‘ $F_A$ ,  $F_B$ ,  $F_C$ , and  $F_D$ ’**

$$F_A = \left( \frac{z|_{i+1} - z'}{z|_{i+1} - z|_i} \right) \left( \frac{(v'_i)^2 - v|_j^2}{v|_{j+1}^2 - v|_j^2} \right), \quad F_B = \left( \frac{z|_{i+1} - z'}{z|_{i+1} - z|_i} \right) \left( \frac{v|_{j+1}^2 - (v'_i)^2}{v|_{j+1}^2 - v|_j^2} \right)$$

$$F_C = \left( \frac{z' - z|_i}{z|_{i+1} - z|_i} \right) \left( \frac{(v'_{i+1})^2 - v|_j^2}{v|_{j+1}^2 - v|_j^2} \right), \quad F_D = \left( \frac{z' - z|_i}{z|_{i+1} - z|_i} \right) \left( \frac{v|_{j+1}^2 - (v'_{i+1})^2}{v|_{j+1}^2 - v|_j^2} \right)$$

where  $(v'_i)^2 = (v')^2 + (2q/m)\Phi(z') - (2q/m)\Phi(z|_i)$ , and

$(v'_{i+1})^2 = (v')^2 + (2q/m)\Phi(z') - (2q/m)\Phi(z|_{i+1})$

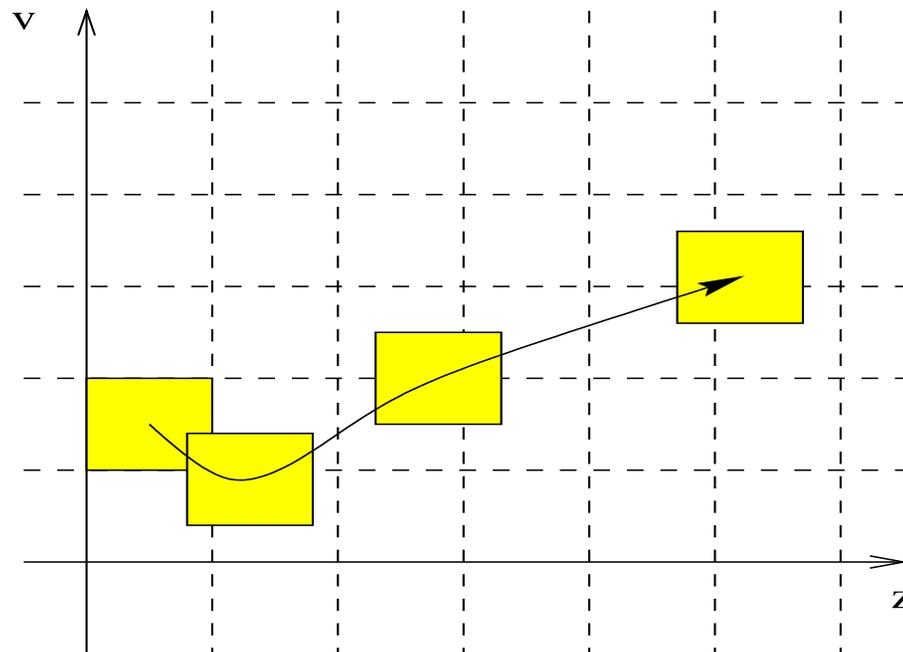
- **If one spatial cell is energetically forbidden,  $\frac{1}{2}m(\mu'v')^2 + q\Phi(z') < q\Phi(z|_i)$  or  $q\Phi(z|_{i+1})$ , particles remapped to other spatial cells with newly calculated  $v$  and  $v_z$**

# Cell Faces or Cell Centers

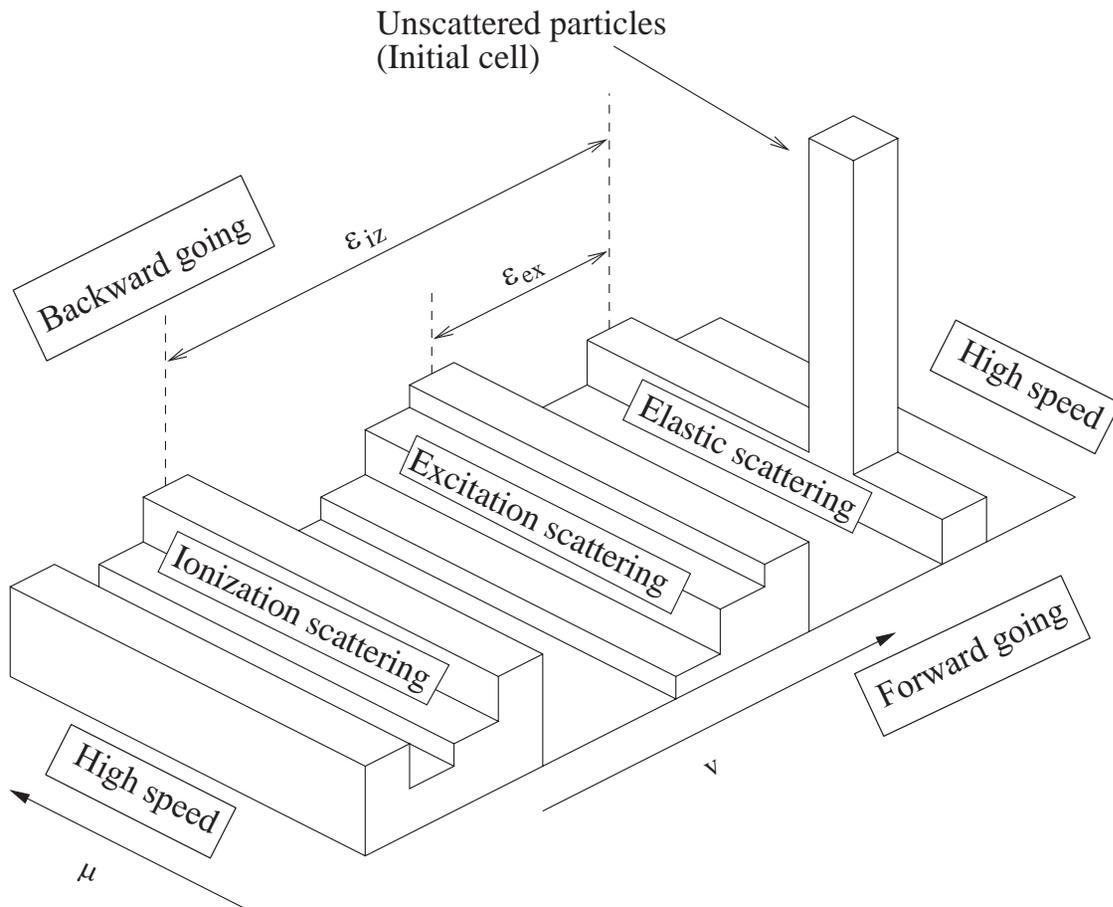
- **Spatial cell boundaries/faces at  $z|_j - \Delta z|_j / 2$  and  $z|_j + \Delta z|_j / 2$  can be moved either**
  - I. Together according to initial velocity and local electric field at cell center**
  - II. Independently according to initial velocity and local electric field at each face position**
- **If we move cell center and keep length of moving cell fixed, then gaps can open up between moving cells**
- **If we move cell faces independently , we may be able to avoid gaps but e.g., if one face bounces but not the other the moving cell acquires complex shape – has to be mapped back as two parts moving in opposite directions**

# CS Using Long-Lived Moving Cells (LLMC)

- **Train of LLMC launched, one cell at most launched each time step for each mesh cell (LLMC can be launched less often)**
- **Number of unscattered particles in moving cell decays exponentially**
- **Particles in leading moving cell remapped back to the mesh when new moving cell is added to the train**
- **Remapping happens less often compare to regular CS**
- **Numerical diffusion highly reduced**



# Electron Collision Operator



- In one time step  $\Delta t$ , fraction of particles  $v\Delta t$  ( $\ll 1$ ) is scattered out of each cell and put back into other cells
- Electrons leaving a scattering event is distributed isotropically; isotropic elastic scattering described through elastic-momentum-transfer x-section
- Electrons involved in inelastic processes are distributed according to differential energy scattering x-sections

●  $\epsilon_{iz}$  and  $\epsilon_{ex}$  are ionization and excitation threshold energies

# CS Implementation Guideline

- I. **Find Constants of Motion** : conserved quantities should remain constant during ballistic motion and remapping
- II. **Choose Mesh Coordinates** : if mesh coordinate is constant of motion, remapping procedures should not distribute particles across different regions of that coordinate
- III. **Choose Mesh Size** : to resolve velocity mesh at low energy, we set  $\Delta v/v = C$ , then  $v|_l = v_{\min} \exp(C'l)$ ,  $l = 0, \dots, N$   
 $C'$  is chosen so that  $C \sim 0.1$

**Note:** lowest velocity mesh where  $v = 0$  is necessary for energy conservation; it's needed to be handled carefully

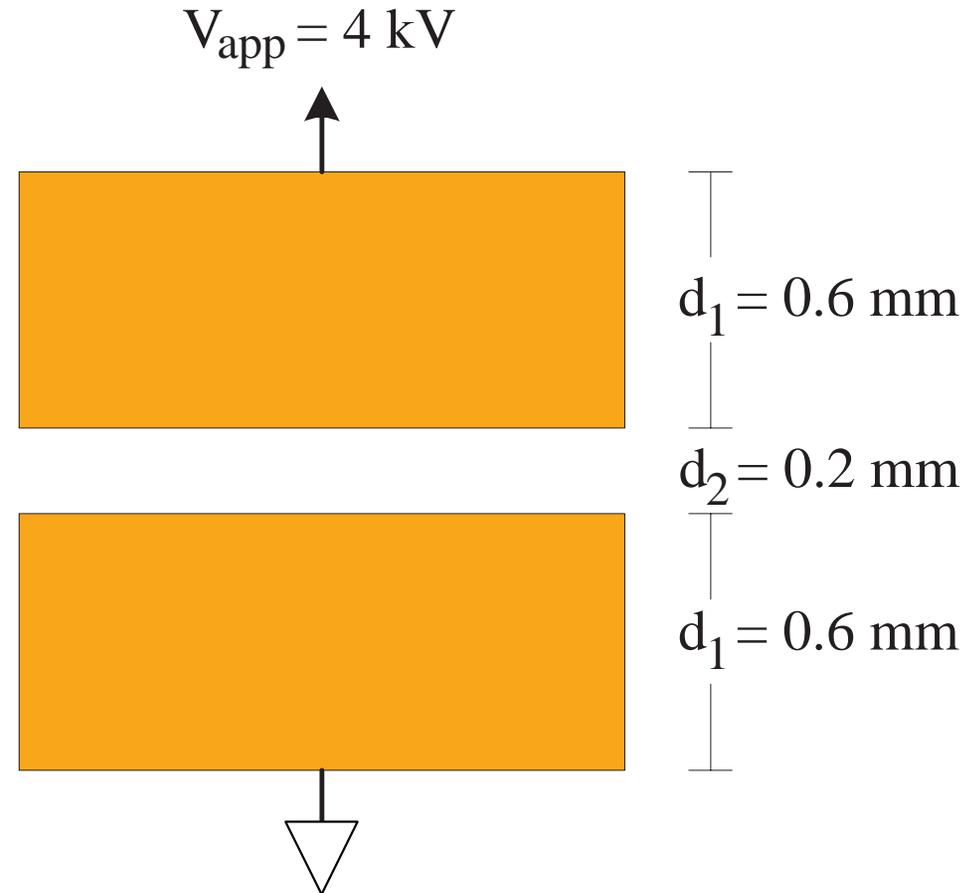
- IV. Remapping Rules** : energy mesh can be used instead of velocity mesh so it does not change other constants of motion
- V. Ballistic Transport** : value of velocity of electrons is not determined by integrating equation of motion, but by conservation of energy (conservation of momentum law is usually employed for ions)
- VI. Collisions** : use  $N_2$  collision cross-section data (elastic, inelastic (e.g., rotational, vibrational etc.), and ionization). At each time step, fraction ' $v\Delta t$ ' of particles collide and is put back into other cell at same spatial position with new  $v$

## VII. Time Step : depends on basic characteristic frequencies

- Collision frequency :  $\Delta t \ll \nu_s^{-1} = [N \nu \sigma(\nu)]^{-1}$
- Total collision frequency :  $\Delta t \sim 0.2\tau < e^{-1}\tau < \tau$ , where  
total collision time  $\tau = \nu^{-1}$
- Plasma frequency :  $\Delta t < \frac{2\pi}{\omega_e} = 2\pi \left( \frac{n e^2}{\epsilon_0 m} \right)^{-\frac{1}{2}}$
- Dielectric relaxation time :  $\Delta t < \tau_d = \frac{\epsilon_0}{n e \mu_e}$

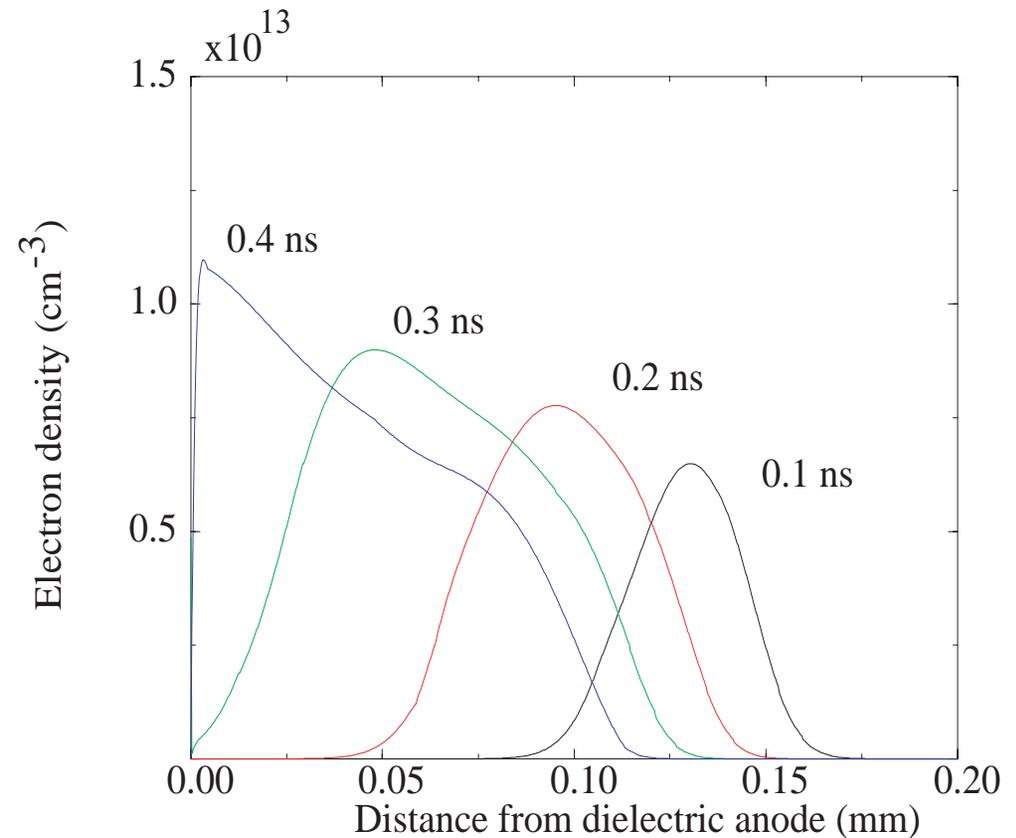
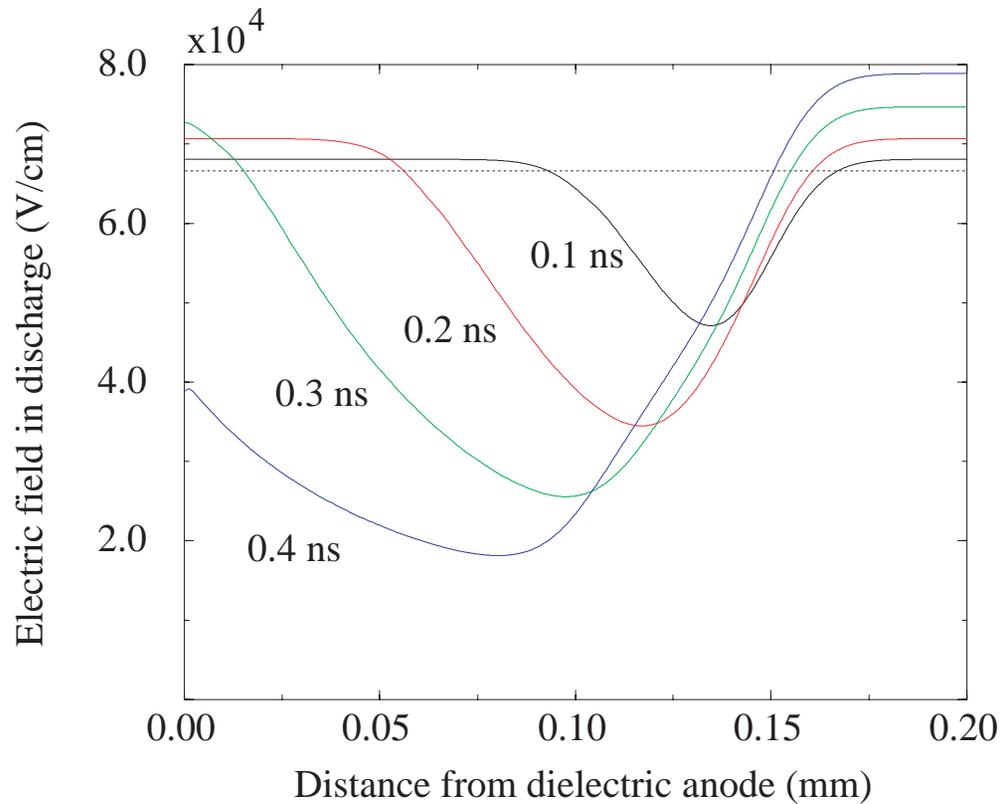
# Dielectric Barrier Discharge Geometry

- $\text{N}_2$  gas
- At atmospheric pressure
- (DC) Applied Voltage = 4 kV
- Dielectric layer width = 0.6 mm ( $\epsilon_r \sim 3$ )
- Capillary diameter = 0.2 mm
- No initial charge on dielectric surface
- Initial density  $\sim 1 \times 10^{10} \text{ cm}^{-3}$

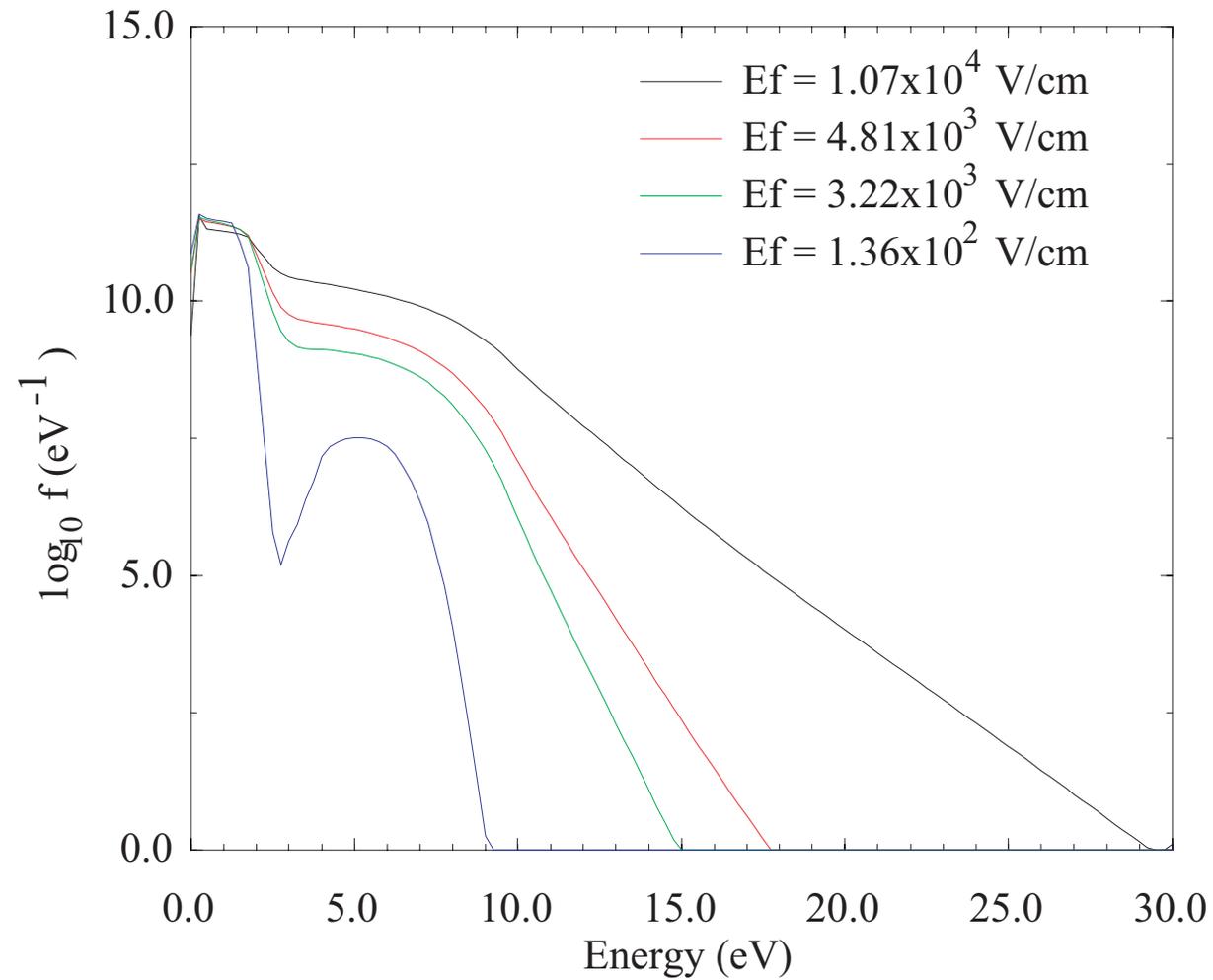


**Note:**  $d_1$  and  $d_2$  may be varied e.g.  $(d_1, d_2) = (0.9, 0.3) \text{ mm}$  or  $(1.5, 0.5) \text{ cm}$ .  $V_{\text{app}}$  is set to keep the electric field the same for each discharge length

# Time Evolution of Electric field and Electron Density in Discharge



# Electron Energy Distribution Function



# Fluid Simulation Using Propagator Method

- **Ballistic motion of propagator approximated by**

- **Drift Distance :**

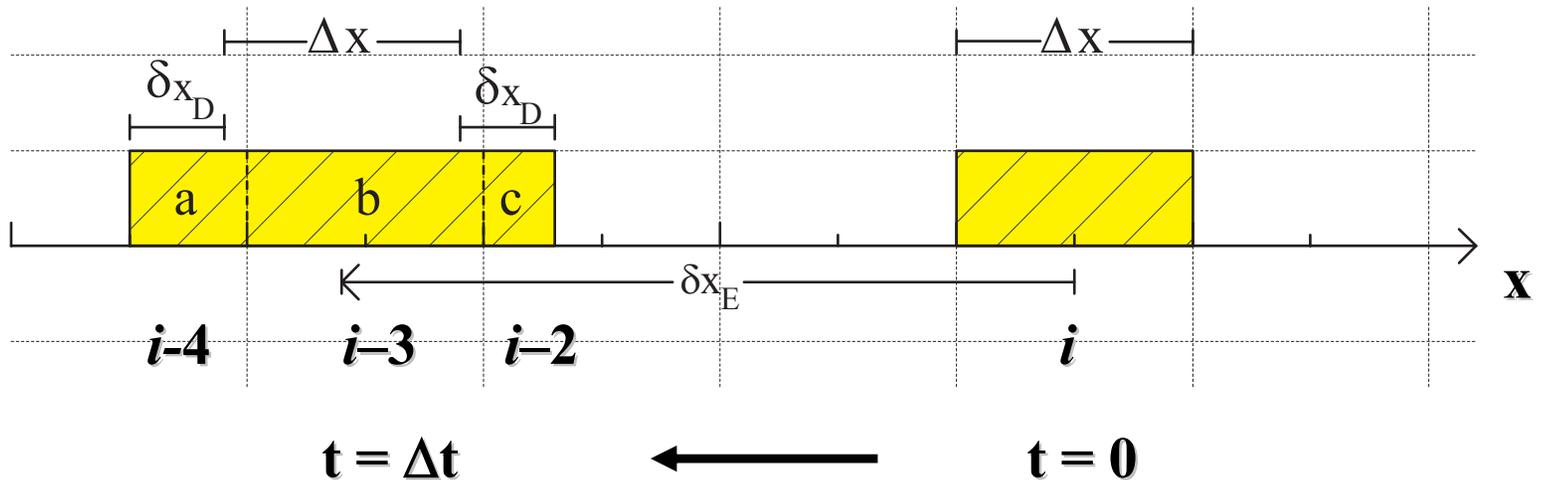
$$\delta x_E = \mu_{\text{eff}} E \Delta t$$

- **Diffusion (both ends of propagator expand outward by) :**

$$\delta x_D = \begin{cases} D_{\text{eff}} \frac{\Delta t}{\Delta x}, & \text{if } \Delta t \text{ is small} \\ \sqrt{2 D_{\text{eff}} \Delta t}, & \text{if } \Delta t \text{ is large} \end{cases}$$

- $\mu_{\text{eff}}$  and  $D_{\text{eff}}$  denote effective mobility and effective diffusion coefficient calculated from electron density pulse from kinetic simulations (as functions of electric field,  $E$ , and mean kinetic energy,  $\kappa$ )

# Ballistic Movement



- By simple overlap rule, fractions of particles,  $F_j$ , going to neighboring cells  $j$  in one time step is

$$F_j = \frac{\delta x_j}{C_l}$$

- $\delta x_j$  is length of moving cell which overlaps final cell  $j$
- $C_l = \Delta x + 2\delta x_D$

# Mean Displacement Determination

- For this example, mean displacement is

$$\delta \bar{x} = F_{i-4} (-4 \Delta x) + F_{i-3} (-3 \Delta x) + F_{i-2} (-2 \Delta x)$$

where

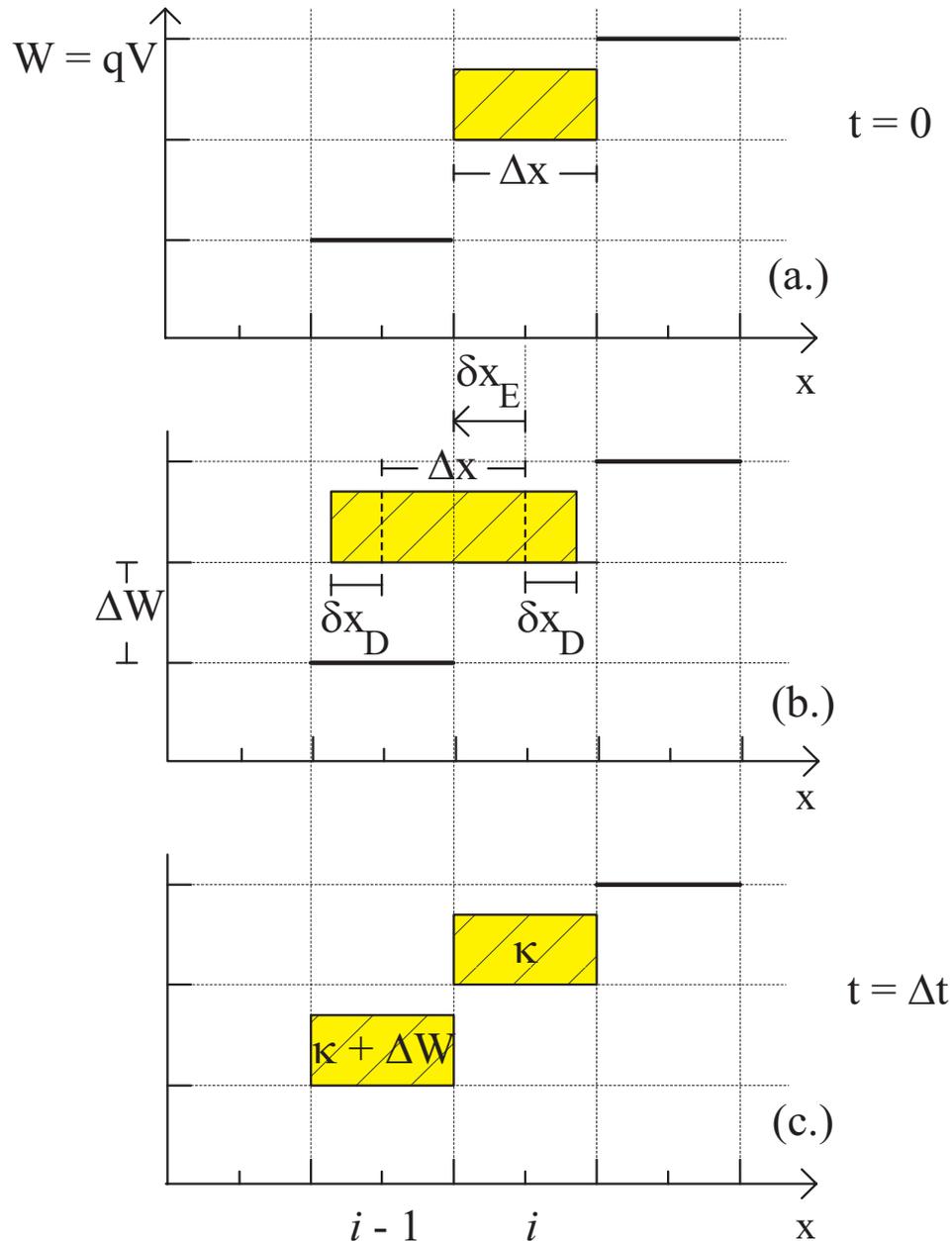
$$F_{i-4} = \frac{|\delta x_E| + \delta x_D - 3 \Delta x}{\Delta x + 2 \delta x_D}$$

$$F_{i-3} = \frac{\Delta x}{\Delta x + 2 \delta x_D}$$

$$F_{i-2} = \frac{\delta x_D - |\delta x_E| + 3 \Delta x}{\Delta x + 2 \delta x_D}$$

- When  $\delta x_E$  and  $\delta x_D \leq \Delta x$  (both  $\delta x_E > \delta x_D$  and  $\delta x_E < \delta x_D$ ), only simple overlap rule yields  $\delta x \neq \delta x_E$ 
  - Corrections must be applied!!

# Conservation of Energy



- Use stair-case potential profile
- Particles initially at cell  $i$  have mean kinetic energy  $\kappa$
- Particles fall from cell  $i$  to  $i - 1$  and pick up potential energy difference between cells  $\Delta W$ , and have final mean energy of  $\Delta W + \kappa$
- The rest of the group stays at cell  $i$  with same mean energy  $\kappa$

# Propagator & Finite Difference Schemes

- When  $\delta x_E$  and  $\delta x_D$  are both less than  $0.5\Delta x$ , propagator gives reasonable FD expressions

(Consider  $\delta x_E = 0$  and  $\Delta t$  very small,  $\delta x_E = D \frac{\Delta x}{\Delta t}$  )

- Particle sharing aspect

- Propagator approach:** fraction  $f$  of contents in cell  $i$  put into  $i+1$ ,

where  $f = \frac{\delta x_D}{\Delta x + 2\delta x_D}$ . Then for  $\delta x_D \ll \Delta x$ ,

$$f = \frac{D \Delta t}{(\Delta x)^2}$$

- FD approach:** initial  $n_i$  in cell  $i$ , then Flux  $\Gamma_D = \frac{D n_i}{\Delta x}$

thus, change in density in neighbor cell is

$$\Delta n = \frac{D \Delta t}{(\Delta x)^2} n_i$$

• Energy conserving aspect

Propagator scheme can be reduced to FD scheme,

when  $\delta x_E, \delta x_D \ll \Delta x$ , and  $\delta x_D < \delta x_E$

• **Propagator approach:** change in energy of cell i due to cell i+1 is

$$\Delta(\bar{n}\bar{\varepsilon})_i = \frac{\bar{n}_{i+1} \bar{\varepsilon}_{i+1} \delta x_{i+1}}{\Delta x} = \frac{\bar{n}_{i+1} \bar{\varepsilon}_{i+1} v_{dr}}{\Delta x} \Delta t$$

( $\delta x_{i+1} = v_{dr} \Delta t$ ;  $v_{dr} \rightarrow$  drift velocity which denotes net effect of mobility and diffusion)

Then change in energy in cell i due to particle losses and heating in one time step is

$$\Delta(\bar{n}\bar{\varepsilon})_i = Q_i \Delta t - \frac{\bar{n}_i \bar{\varepsilon}_i \delta x_i}{\Delta x}$$

• **FD approach:** Upwind equation of conservation of energy

$$\frac{\partial(\bar{n}\bar{\varepsilon})}{\partial t} + \frac{\partial(\bar{n}\bar{\varepsilon} v_{dr})}{\partial x} = Q_i$$

$Q_i$  is heating rate

# Fitting Fluid Parameters from Kinetic Model

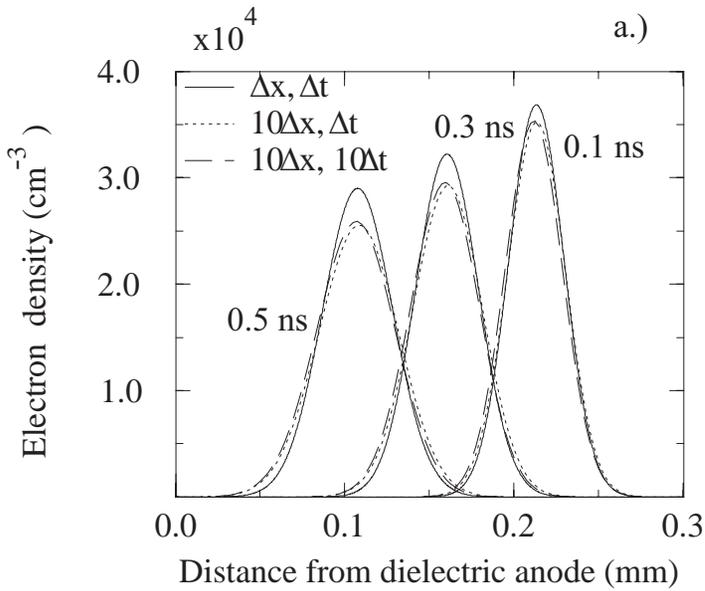
## ● Procedures :

- I. Steady state of EEDF,  $f_e$  generated in homogeneous  $N_2$  gas for given electric field  $E$
- II. Load  $f_e$  into single spatial cell  $i$  and calculate fraction of particles moving into neighboring cells in  $N$  time steps
- III.  $\mu_{\text{eff}}$  and  $D_{\text{eff}}$  calculated from mean position and width of density pulse
- IV.  $\mu_{\text{eff}}$ ,  $D_{\text{eff}}$ , Ionization rate ( $I$ ), fraction of energy going to ionization ( $\alpha$ ) obtained as functions of  $E$  and mean energy  $\kappa$

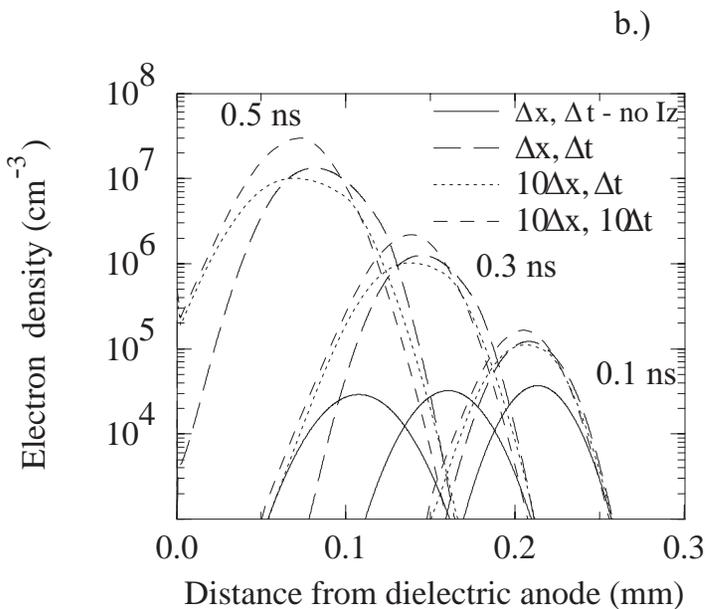
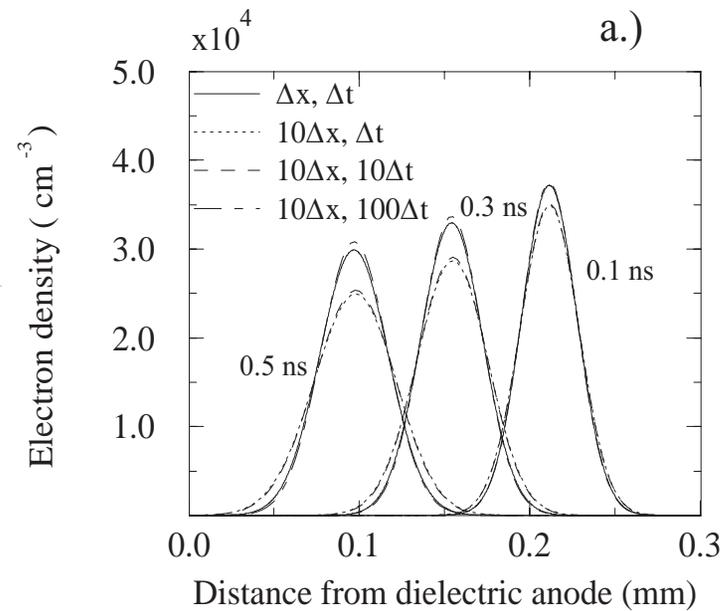
## ● 2 Options for running fluid code

- Fluid -  $R(E) \rightarrow$  use  $(\mu_{\text{eff}}, D_{\text{eff}}, I, \alpha)$  as functions of  $E$
- Fluid -  $R(\kappa) \rightarrow$  use  $(\mu_{\text{eff}}, D_{\text{eff}}, I, \alpha)$  as functions of  $\kappa$

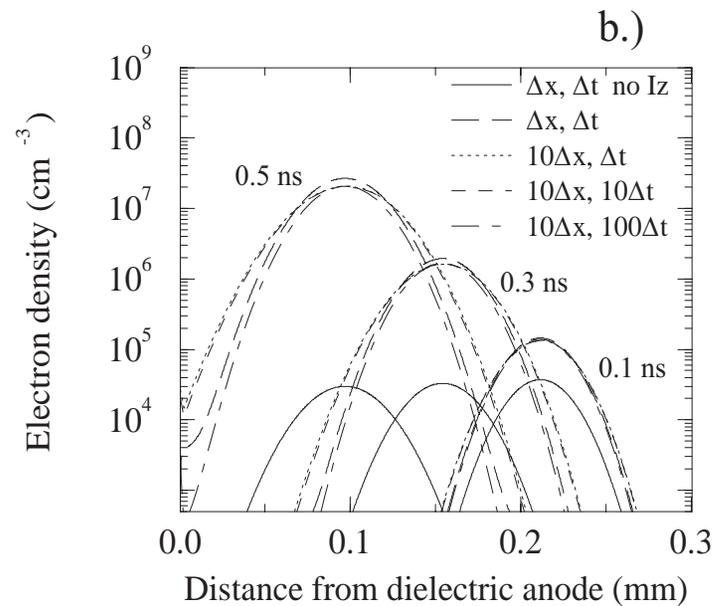
# Using Fluid Scheme Over Wide Range of $\Delta x$ and $\Delta t$



**w/o Ionization**



**w/ Ionization**

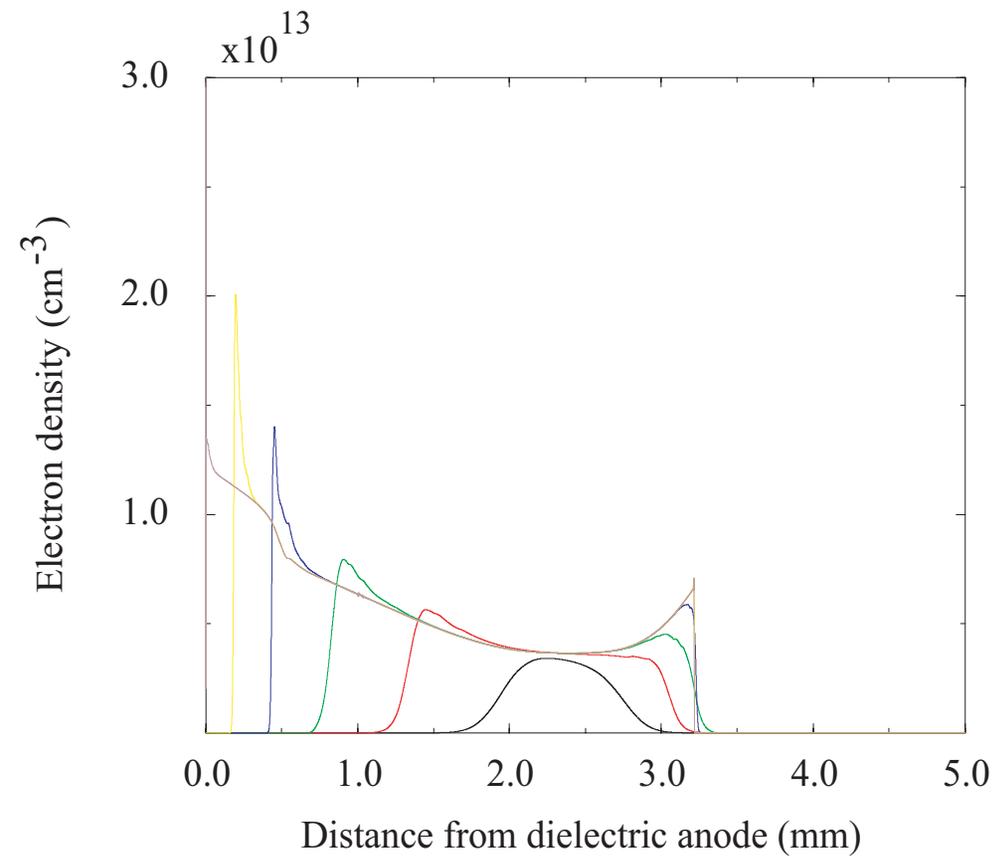
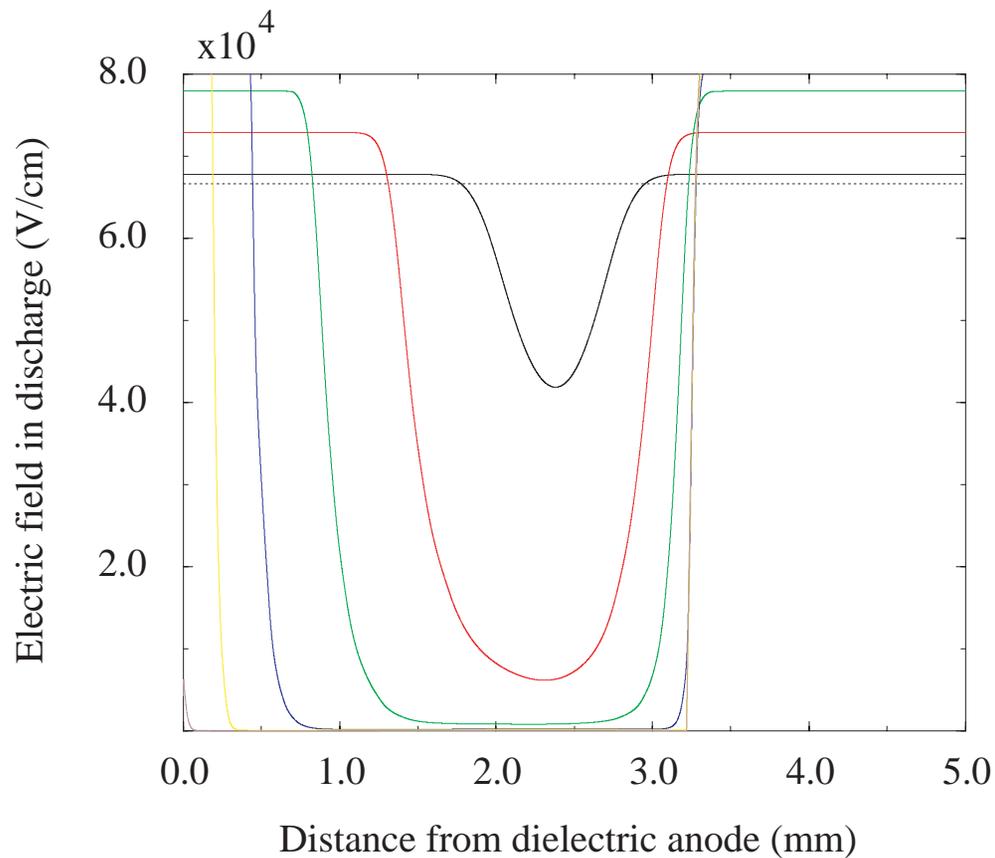


**Fluid –  $R(\kappa)$**

**Fluid –  $R(E)$**

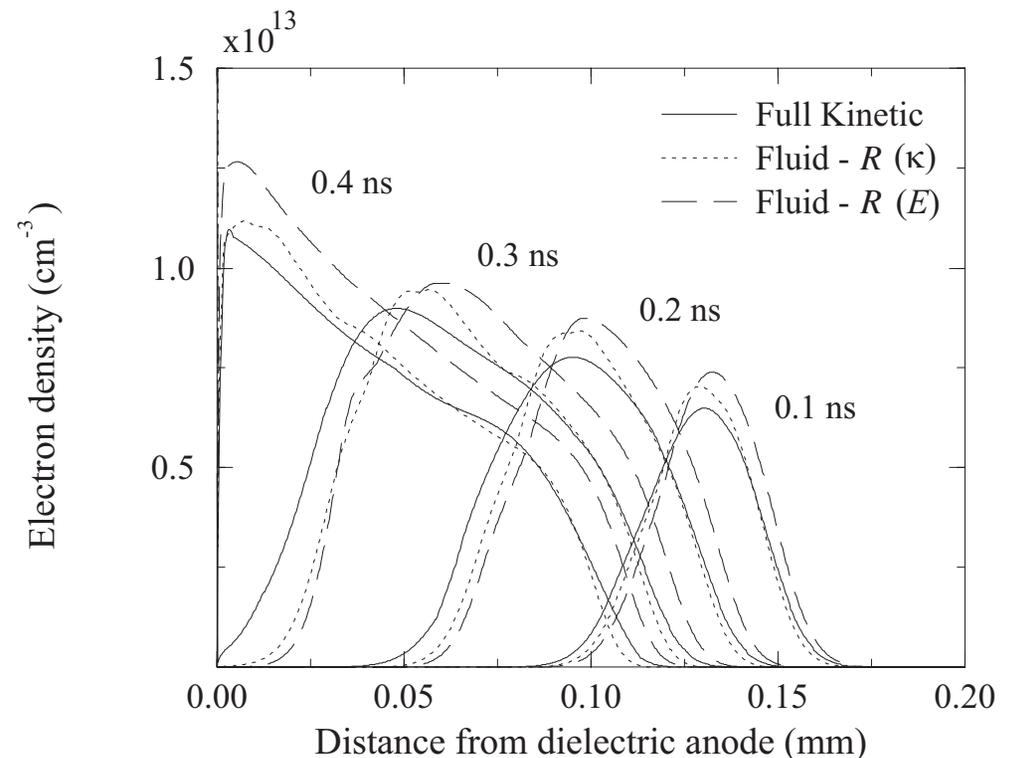
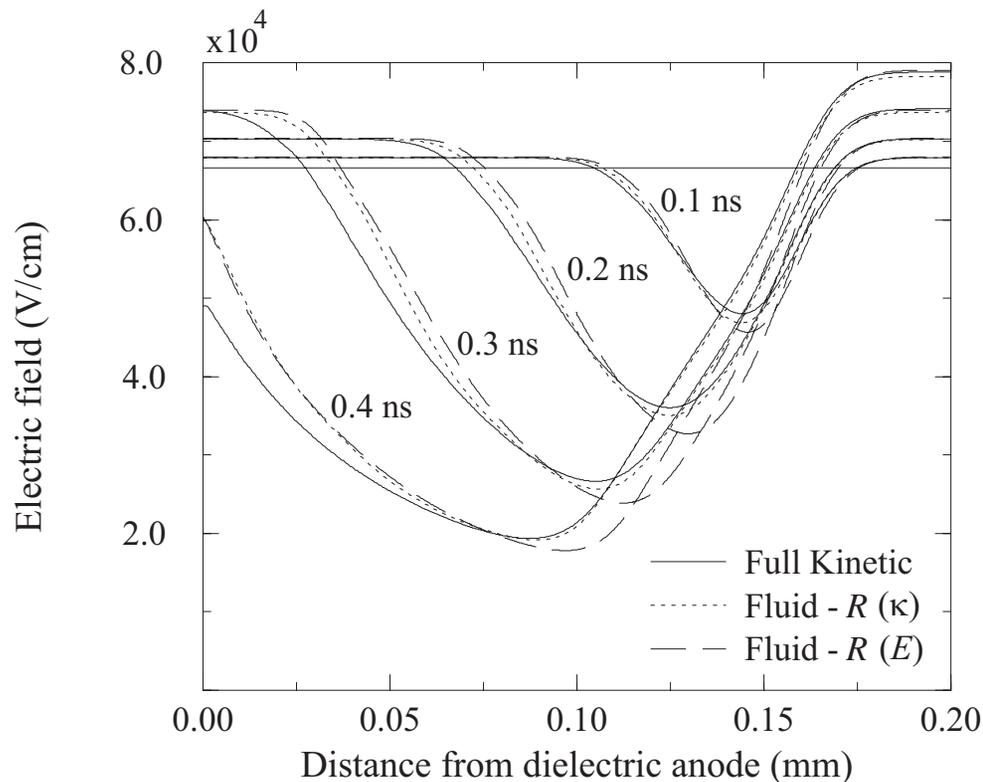
# Time Evolution of Breakdown from Fluid Simulation

## Electric field and electron density in 5mm N<sub>2</sub> discharge

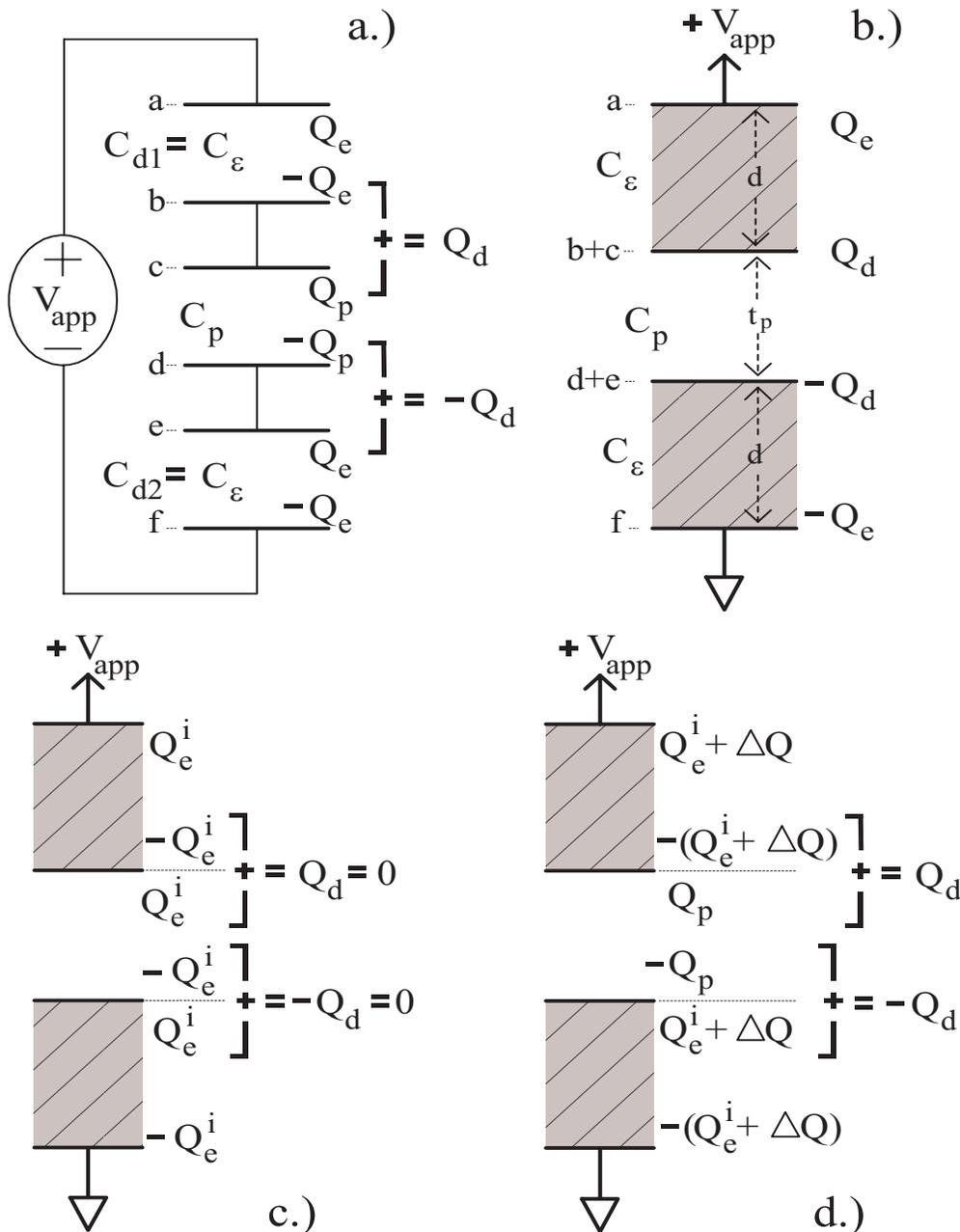


# Comparison of Kinetic and Fluid Simulations

Electric field and electron density in 0.2 mm N<sub>2</sub> discharge is illustrated



# Analytic Capacitor Model



- Discharge is considered as a series of 3 capacitors; plasma capacitor ( $C_p$ ) and 2 dielectric capacitors ( $C_d$ )

- $\Delta Q = C_d(V_p^i - V_p)$ , where

$$C_d = \left( \frac{1}{C_{d1}} + \frac{1}{C_{d2}} \right)^{-1}$$

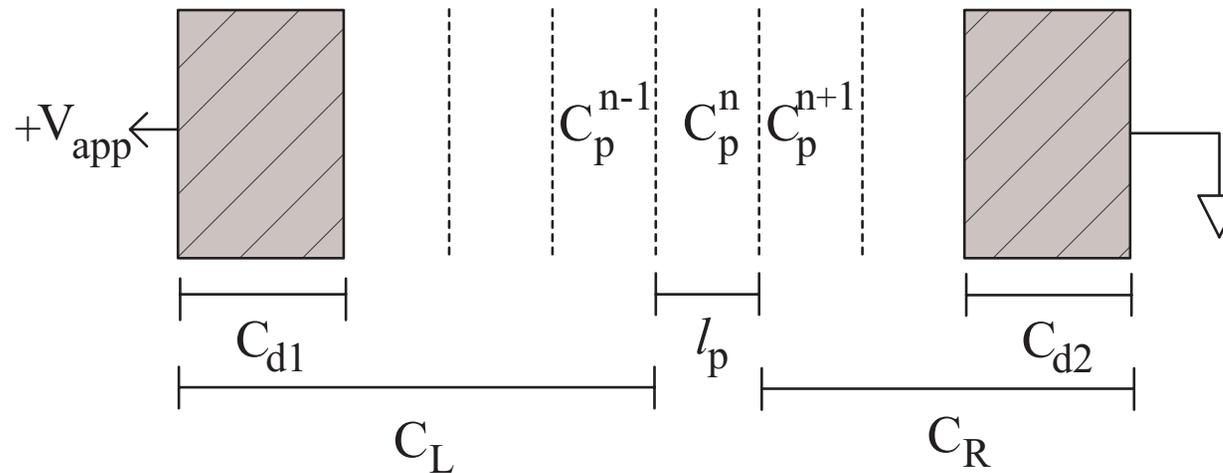
- Energy put into plasma,

$$W_p = W_s^i - W_s + V_{app} \Delta Q$$

$$= \frac{1}{2} \left( 1 + \frac{C_d}{C_p} \right) (W_1^i - W_1)$$

$$= \frac{1}{2} \left( 1 + \frac{C_d}{C_p} \right) \left( \frac{Q_p^i{}^2 - Q_p^2}{C_p} \right)$$

# N – Capacitor Model



- $C_p$  is separated into  $N$  small capacitors
- Order of breakdown depends on the highest density in each capacitor,  $C_p^n$

● Energy put into plasma is

$$W_p = \frac{1}{2} \left( 1 + \frac{C_d^n}{C_p^n} \right) \left( \frac{(Q_p^{i^n})^2 - Q_p^{n^2}}{C_p^n} \right)$$

where

$$Q_p^{i^n} = Q_e^{i^n} = Q_e^i \prod_{n'} \left( \frac{C_d^{n'}}{C_p^{n'}} + 1 \right) \quad \text{and} \quad C_d^n = \left( \frac{1}{C_L^n} + \frac{1}{C_R^n} \right)^{-1}$$

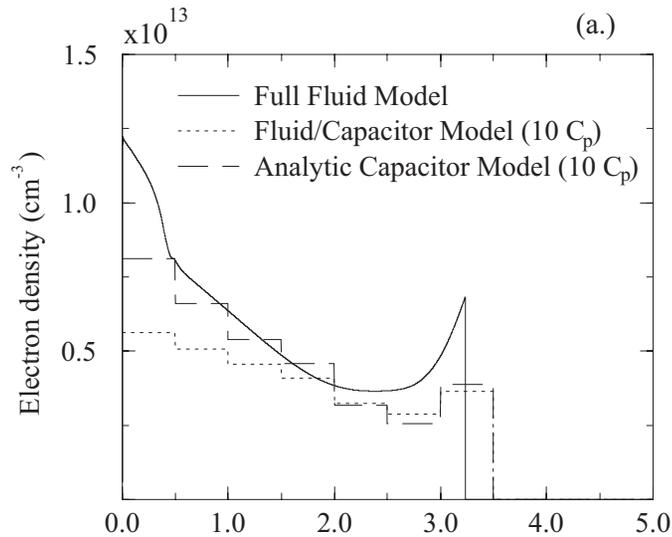
● Total number of ionizations before the field reaches value  $D_p'$

$$N_{iz}(D_p') = \frac{1}{\epsilon_{iz}} \int_{D_p^i}^{D_p'} \alpha_{iz}(D_p) \frac{\partial W_p}{\partial D_p} dD_p$$

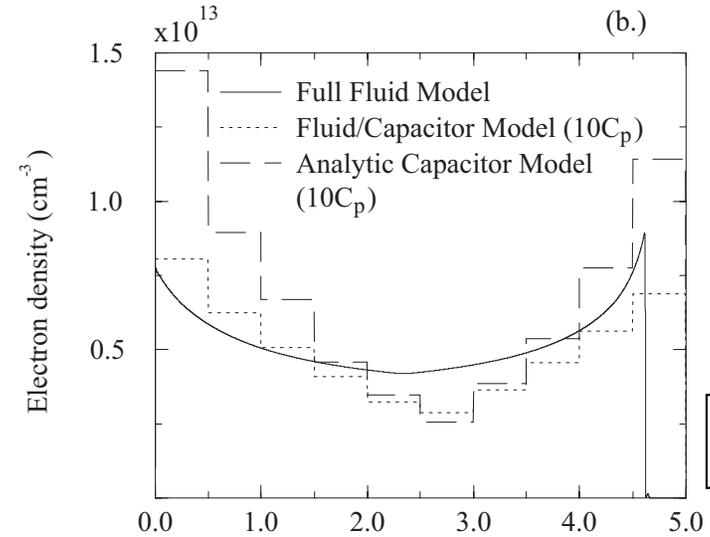
# Comparison of Analytic calculation and Fluid simulation

- Electron density calculated from full fluid – R(k), fluid – R(k)/Capacitor, and fully analytic N – Capacitor models for the first breakdown phase in 5mm discharge for different initial densities

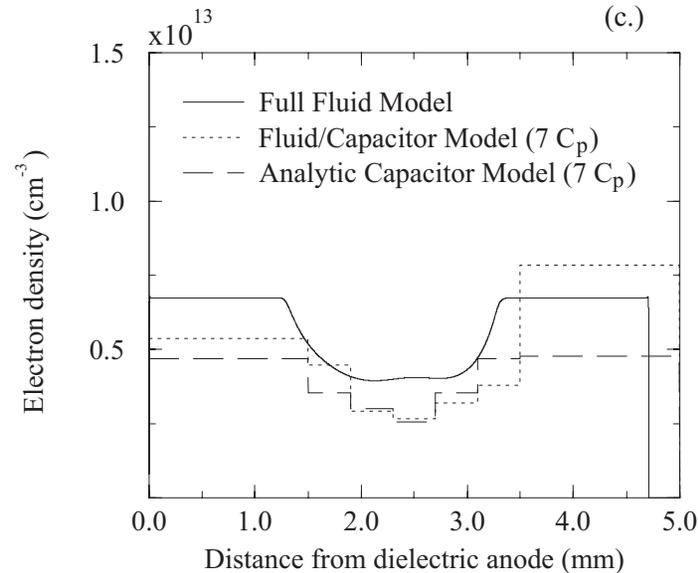
Gaussian



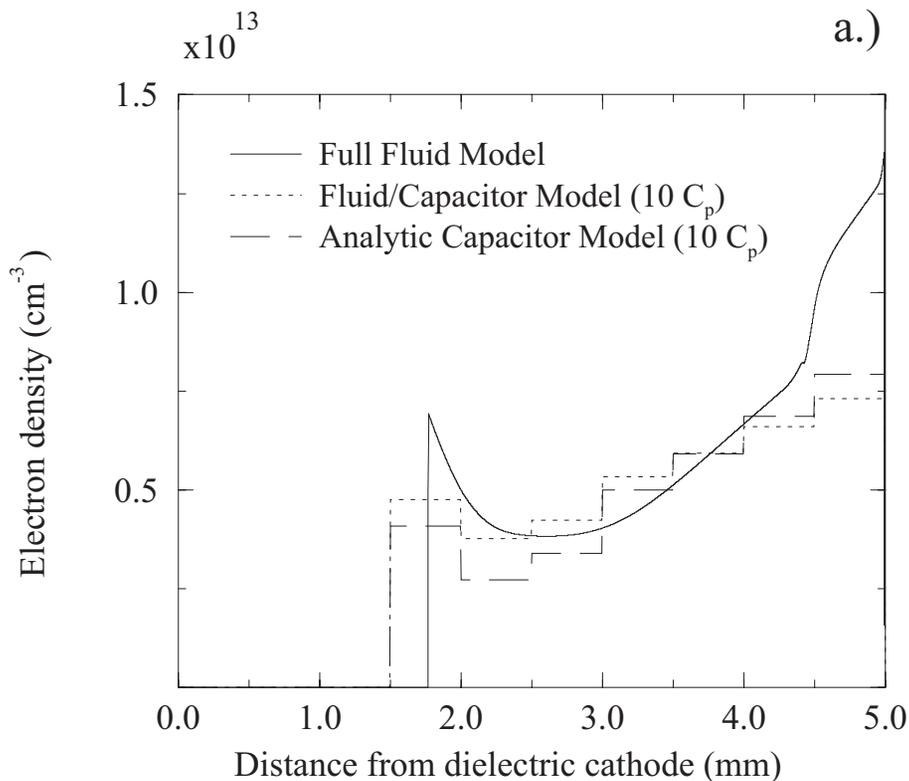
Pyramidal



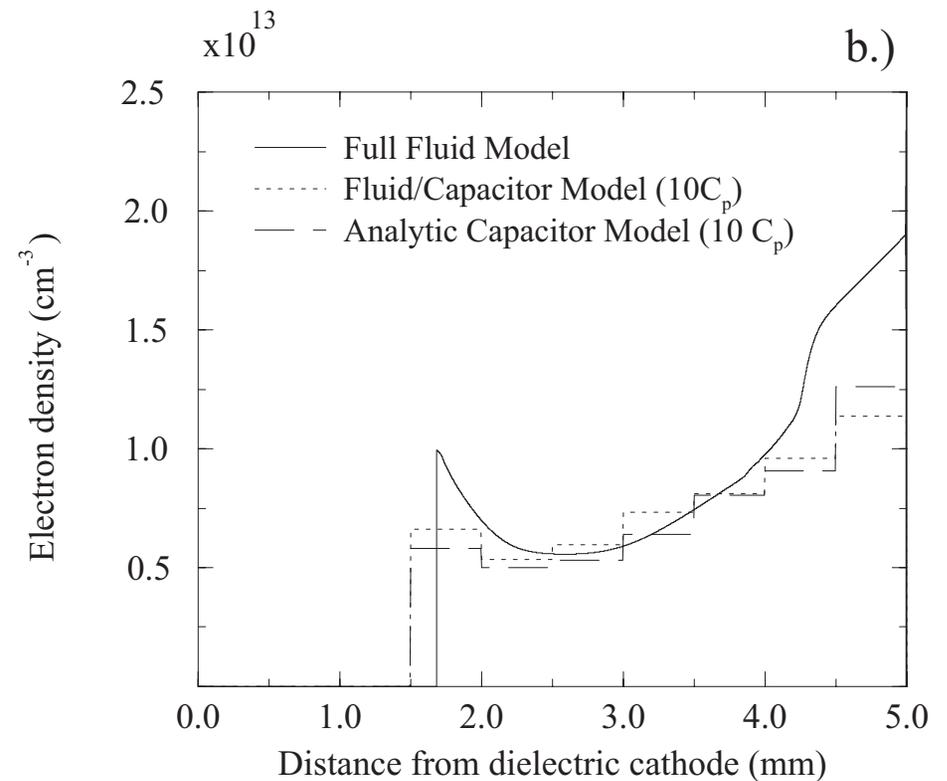
Semi-homogeneous



- Electron density calculated from full fluid – R(k), fluid – R(k)/Capacitor, and fully analytic N – Capacitor models with initial charge 8.84 C/m<sup>2</sup> on dielectric surface (left from first breakdown cycle) – for Gaussian density initialization**



**a.)  $V_{app} = -100 \text{ V}$**



**b.)  $V_{app} = -1 \text{ kV}$**

# Summary

- Propagator method has been employed to set up kinetic and fluid simulations
- Kinetic model is the most accurate, but takes considerable time and computer resources
- LLMC can reduce numerical diffusion in CS
- Fluid model using propagator can be used over wide range of  $\Delta x$  and  $\Delta t$  (without ionization); during breakdown only very small  $\Delta x$ ,  $\Delta t$  work well
- Fluid simulation gives a good agreement with CS when its transport and collision parameters are functions of  $\kappa$
- ‘Local’ model (N – capacitor model) agrees well with ‘non-local’ model (fluid – R( $\kappa$ )) in middle of the discharge, and agrees within 40% in last capacitor (close to dielectric surface)