MONTE CARLO METHODS
FOR ELECTRON TRANSPORT

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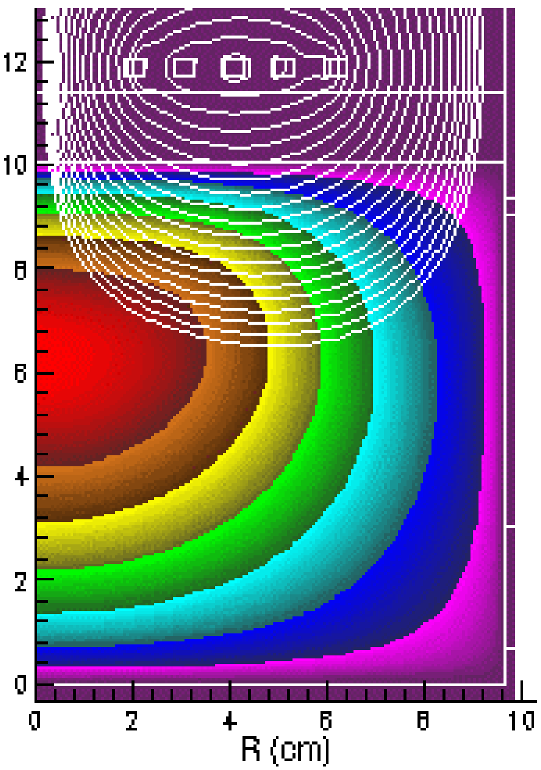
MONTE CARLO METHODS FOR ELECTRON TRANSPORT

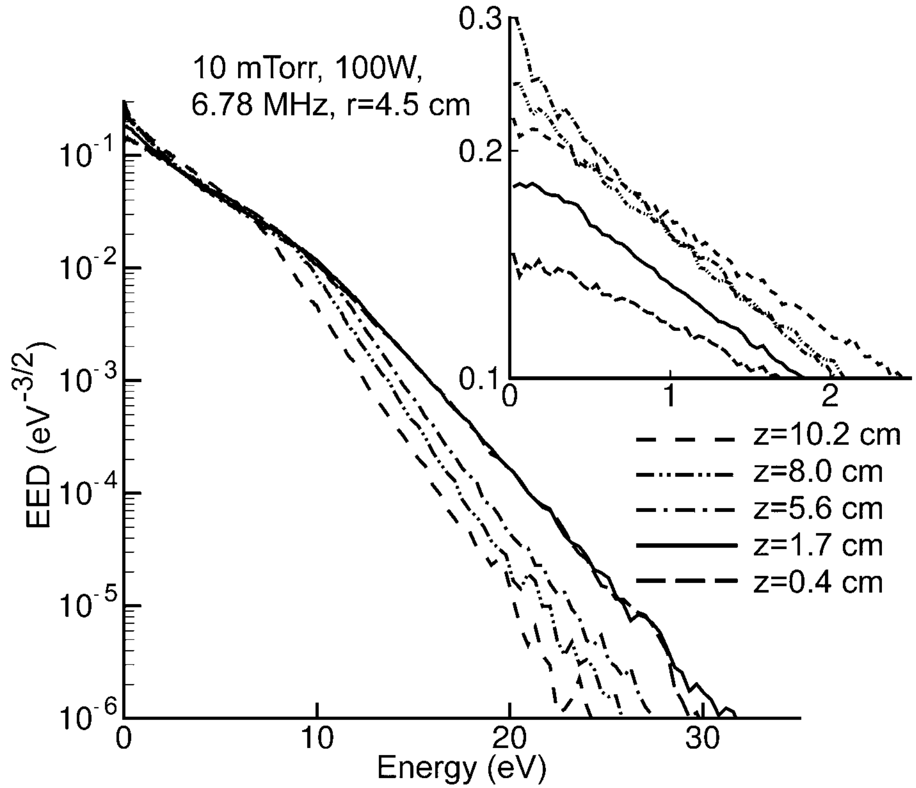
- **The Monte Carlo (MC) method was developed during WWII for analysis of neutron moderation and transport.**
- **MC methods enable direct simulation of complex physical phenomena which may not be amenable to conventional PDE analysis.**
- **The method relies upon knowledge of probability functions for the phenomena of interest to statistically (randomly) select occurrences of events whose ensemble average is “the answer”.**
- **These methods are extensively used in simulating electron transport do obtain, for example, electron energy distributions.**

EXAMPLE: ELECTRON ENERGY DISTRIBUTION IN ICP

- **Inductively Coupled Plasma: Ar, 10 mTorr, 6.78 MHz**



- **Electric field (overlay) and ion density (max = 1.7 x 10^{11} cm^{-3})**



- **EED at r= 4.5 cm vs Distance from Window**

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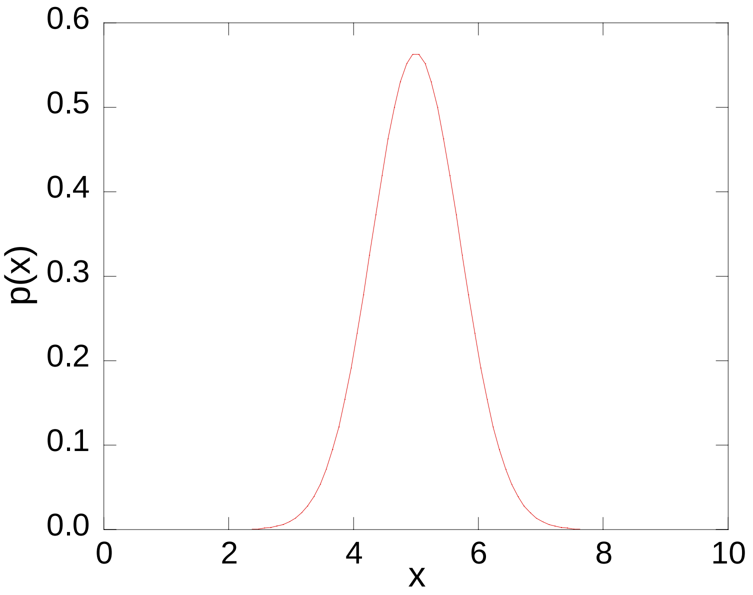
MONTE CARLO METHOD REFERENCES

- **J. P. Boeuf and E. Marode, J. Phys. D 15, 2169 (1982)**
- **G. L. Braglia, Physica 92C, 91 (1977)**
- **S. R. Hunter, Aust. J. Phys. 30, 83 (1977)**
- **S. Lin and J. Bardsley, J. Chem. Phys 66, 435 (1977)**
- **S. Longo, Plasma Source Science Technol. 9, 468 (2000)**
- **J. Lucas, Int. J. Electronics 32, 393 (1972)**
- **J. Lucas and H. T. Saelee, J. Phys. D 8, 640 (1975)**
- **K. Nanbu, Phys. Rev E 55, 4642 (1997)**
- **M. Yousfi, A. Hennad and A. Alkaa, Phys Rev E 49, 3264 (1994)**

- **Computational Science and Engineering Project**
  http://csep1.phy.ornl.gov, http://csep1.phy.ornl.gov/CSEP/MC/MC.html

BASICS OF THE MONTE CARLO METHOD: p(x)

- **A physical phenomenon has a known probability distribution function p(x) which, for example, gives the probability of an event occurring at position x.**



$$\int_{0}^{\infty} p(x)dx = 1$$

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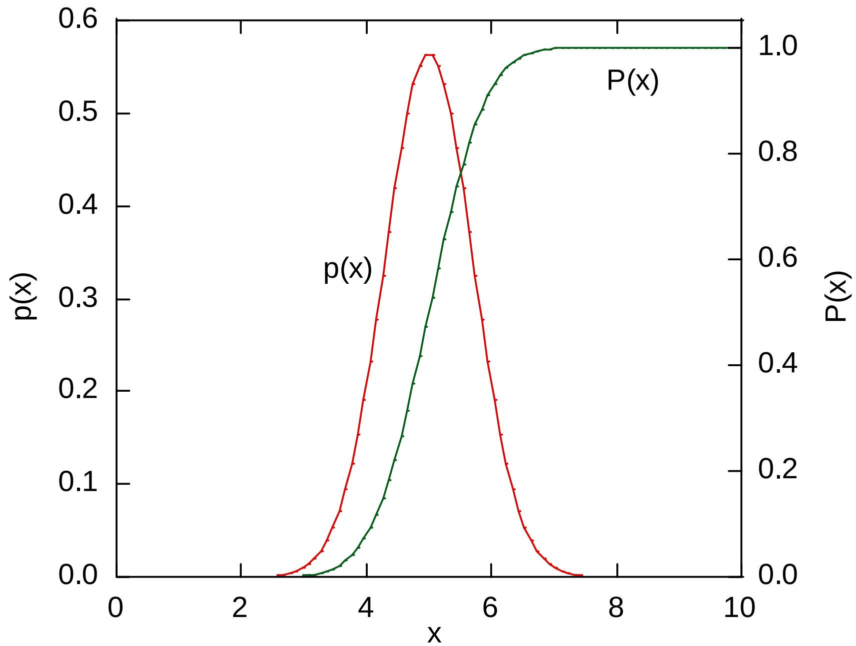
BASICS OF THE MONTE CARLO METHOD: P(x)

- **The cumulative probability distribution function P(x) is the likelihood that an event has occurred prior to x.**



$$P(x) = \int_{o}^{x} p(x')dx'$$

$$P(0) = 0, \;\; P(\infty) = 1$$

- **Since p(x) is always positive, there is a 1-to-1 mapping of r=[0,1] onto P(x = 0 $\rightarrow$x = ∞).**

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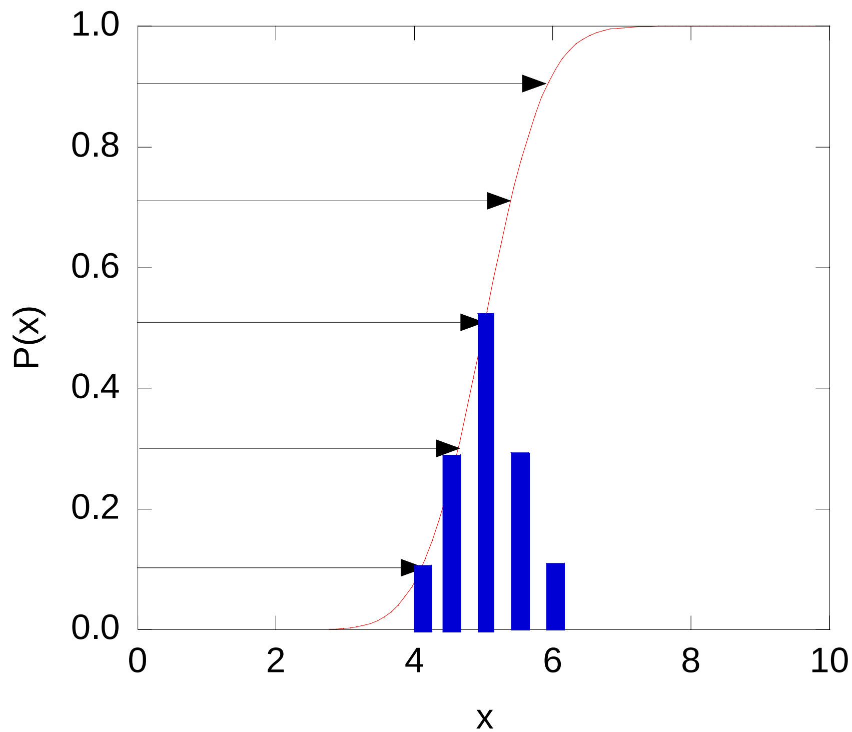
RANDOM USE OF P(x) TO REGENERATE p(x)

- By randomly choosing "product values" of P(x) (distributed [0,1]) and binning the occurrences of the argument x, we reproduce p(x).



- The function which, given a random number r=[0,1], provides a randomly selected value of x is:

$$x = P^{-1}(r)$$

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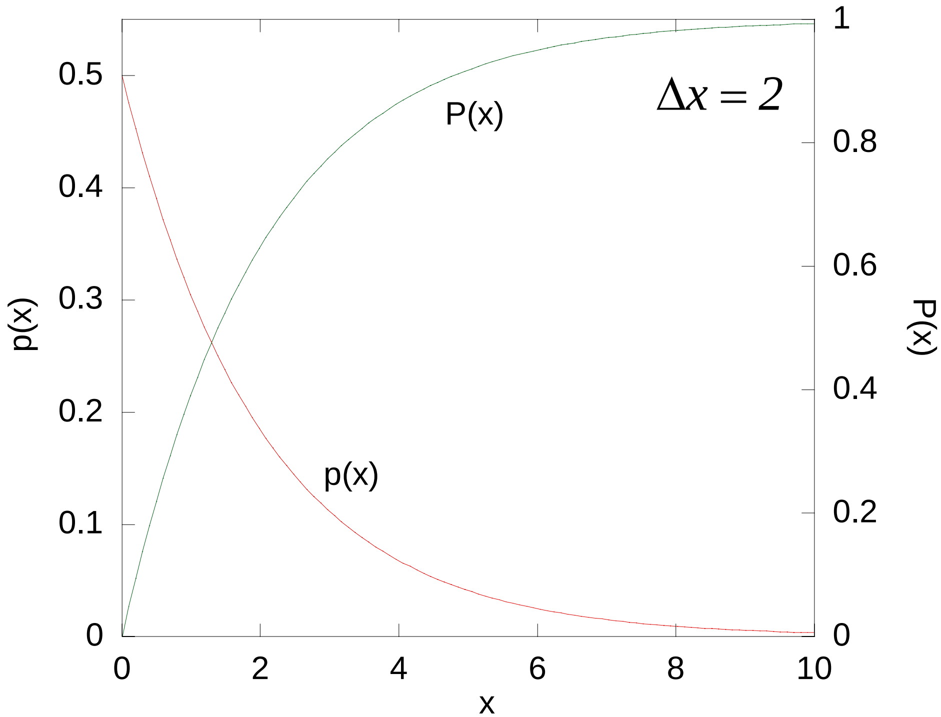
EXAMPLE: RANDOM P(x) TO REGENERATE p(x)



$$p(x) = \frac{1}{\Delta x}\exp(-\frac{x}{\Delta x})$$

$$P(x) = 1 - \exp(-\frac{x}{\Delta x})$$

$$x = P^{-1}(r) = -\Delta x \cdot \ln(1-r)$$

$$r = [0,1]$$

- **WARNING!!! In practical problems, p(x) cannot be analytically integrated for P(x) and/or P(x) cannot be analytically inverted for $P^{-1}(x)$. These operations must be done numerically.**

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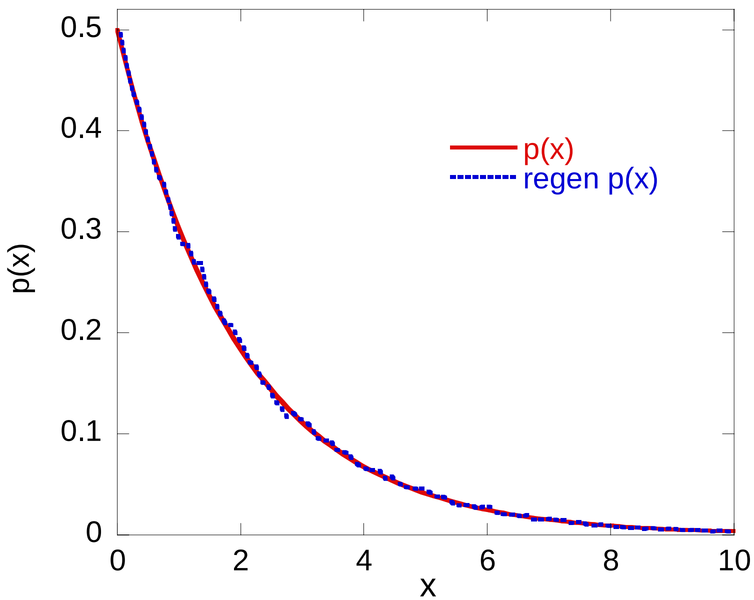
EXAMPLE: RANDOM P(x) TO REGENERATE p(x)

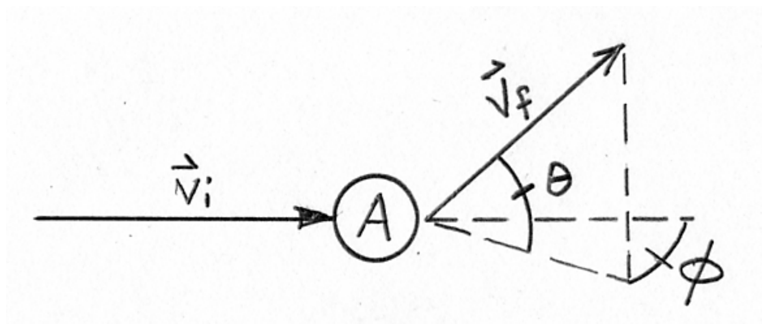


- **p(x) is reproduced within random statistical error ($n^{-1/2}$=0.01).**

```
ibins=100
itrials=10000
deltax=2
xmax=10.
dx=xmax/ibins
ynorm=0.
do i=1,itrials
  r = random(iseed)
  x=-deltax*alog(1.-r)
  ibin=x/dx
  ynorm=ynorm+dx
  y(ibin)=y(ibin)+1.
end do
do i=1,ibins
  y(i)=y(i)/ynorm
end do
```

ELECTRON SCATTERING

- **An electron with energy ε collides with an atom with differential cross section $\sigma(\varepsilon, \theta, \phi)$**



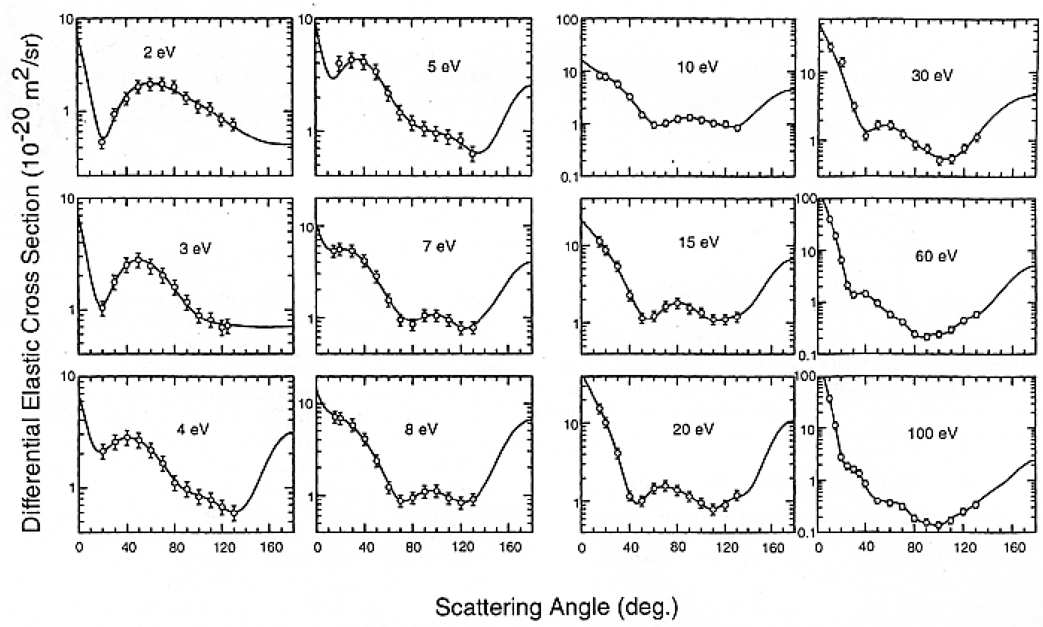
providing the likelihood of scattering into the solid angle centered on (θ, ϕ) .

Note: Typically only the explicit dependence on polar angle θ is considered. Scattering with azimuthal angle φ is usually assumed to be uniform.

DIFFERENTIAL SCATTERING

- $\sigma(\varepsilon,\theta)$ **for real atoms and molecules can be quite complex (C_2F_6)**

Christophorou, J. Chem. Phys. Ref. Data 27, 1, (1998)



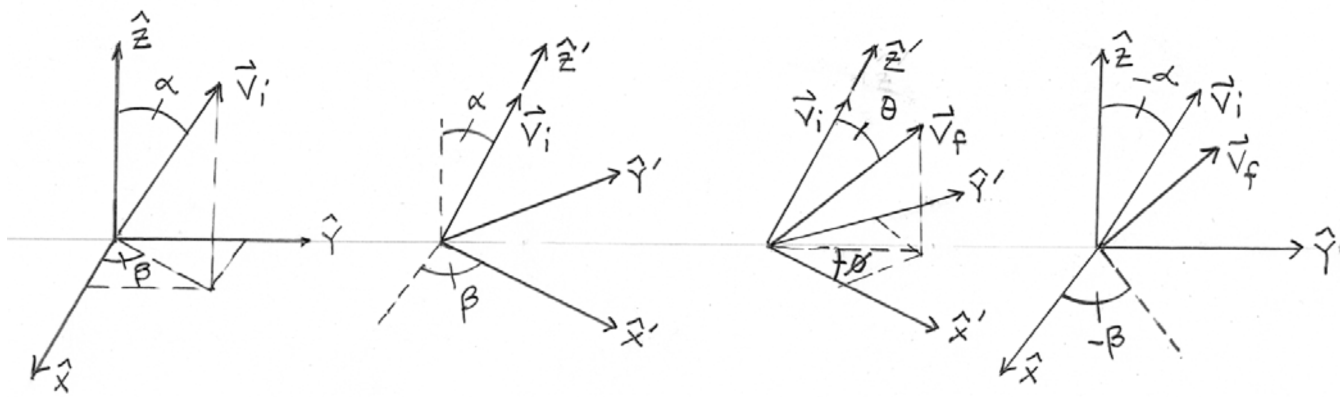
- **Accounting for forward scattering at higher energies (> 10s eV) is very important in simulating electron transport.**

- **Assuming Isotropic scattering in the polar direction yields:**

$$\sigma(\theta)=\sigma_o,\ \ P(\theta)=\frac{1}{2\sigma_o}\int_0^{\theta}\sigma_o\sin(\theta')d\theta',\quad \theta=\mathrm{acos}(2r-1)$$

COLLISION DYNAMICS

- **To account for the change in velocity of an electron following a collision:**



1. **Determine Eularian angles** (β, α) **of** $\vec{v}_{initial}$
2. **Rotate frame by** (β, α) **so z-, x-axes align with** $\vec{v}_{initial}$
3. **Rotate** $\vec{v}_{initial}$ **by** (θ, ϕ) **to yield direction of** $\vec{v}_{final}$
4. **Account for change in speed** $\left|\vec{v}_{final}\right|^2 = \left|\vec{v}_{initial}\right|^2 - 2\Delta\varepsilon / m_e$
5. **Rotate frame by** $(-\alpha, -\beta)$ **to original orientation**

COLLISION DYNAMICS

- **End result is the "scattering matrix" which transforms initial velocity to final velocity:**

$$\vec{v}_{final} = \left|\vec{v}_{final}\right| \cdot \begin{bmatrix} \cos(\beta)\cos(\alpha)\sin(\theta)\cos(\phi) + \cos(\beta)\sin(\alpha)\cos(\theta) - \sin(\beta)\sin(\theta)\sin(\phi) \\ \sin(\beta)\cos(\alpha)\sin(\theta)\cos(\phi) + \sin(\beta)\sin(\alpha)\cos(\theta) - \cos(\beta)\sin(\theta)\sin(\phi) \\ -\sin(\alpha)\sin(\theta)\cos(\phi) + \cos(\alpha)\cos(\theta) \end{bmatrix}$$

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EXAMPLE: ELECTRON SWARM

- A swarm of electrons drifts in a uniform electric field in a gas having a constant elastic collision frequency and isotropic collisions. What is the average drift velocity?

- For constant collision frequency ν, the randomly selected time between collisions is:

$$\Delta t = -\frac{1}{\nu} \cdot alog(1 - r)$$

- The change in energy in an elastic collision is

$$\Delta \varepsilon = \left(1 - \frac{2m_e}{M} \left(1 - \cos(\theta) \right) \right)$$

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EXAMPLE: PROGRAM DRIFT

```
      PROGRAM DRIFT
C
C     Initialize randmom number generators. IMPORTANT: Use a different
C     sequence of random numbers for different processes
C
      DO I=1,3
        CALL INIT_RAN(I)
      END DO
C
      XMASSE=0.911E-27                ! Electron mass (g)
      XMASSN=20.*1.67E-24             ! Atomic mass (g)
C
C     Select electric field and collision frequency.
C
      EFIELD=5.                       ! V/cm. Assume in the x-direction
      COLF=1.E9                       ! 1/s
      ACX=EFIELD*1.6E-12/XMASSE       ! Acceleration
      IELECTRONS=1000                 ! Number of electron particles
      XEND=20.                        ! Drift distance (cm)
      TTOTAL=0.                       ! Drift time (s)
      VDRIFT=0.                       ! Drift velocity
      XNORM=0.                        ! Normalization constant
C
```


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EXAMPLE: PROGRAM DRIFT

```
      DO I=1,IELECTRONS
        X=0.
        TTOTAL=0.
        VX=0.
        VY=0.
        VZ=0.
C
C     Randomly choose time to next collision
C
   50   DT=-(1./COLF)*LOG(1.-RAN(1))
C
C     Update position, speed of particle
C
        X=X+VX*DT+0.5*ACX*DT*DT
        VX=VX+ACX*DT
        TTOTAL=TTOTAL+DT
C
C     Electron has not reached XEND. Perform Scatter
C
        IF (X.LT.XEND) THEN
          V=SQRT(VX**2+VY**2+VZ**2)
C
C     Eularian Angles
C
          BETA=ATAN2(VY,VX)
          ALPHA=ACOS(VZ/V)
C
C     Randomly choose scattering angles
C
          THETA=ACOS(2.*RAN(2)-1.)
          PHI=2*PI*RAN(3)
```


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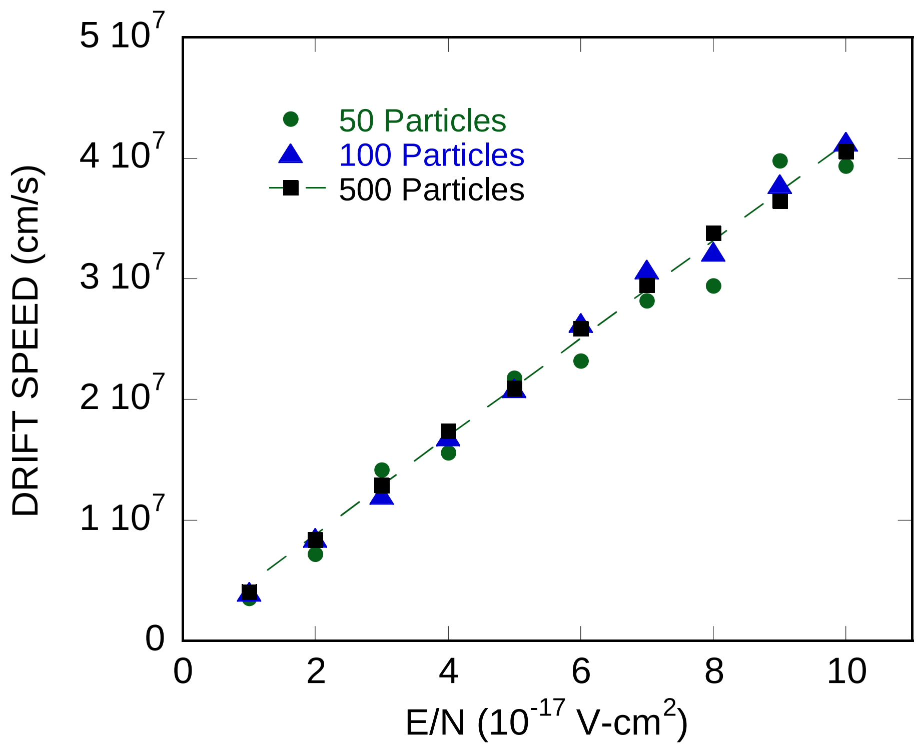
EXAMPLE: PROGRAM DRIFT

```
C
C       Account for energy loss during elastic collision
C
            V=V*SQRT(1.-(2.*XMASSE/XMASSN)*(1.-COS(THETA)))
C
C       Perform scatter
C
            VX=V*(COS(BETA)*COS(ALPHA)*SIN(THETA)*COS(PHI)+
     +          COS(BETA)*SIN(ALPHA)*COS(THETA)-SIN(BETA)*SIN(THETA)*SIN(PHI))
            VY=V*(SIN(BETA)*COS(ALPHA)*SIN(THETA)*COS(PHI)+
     +          SIN(BETA)*SIN(ALPHA)*COS(THETA)+COS(BETA)*SIN(THETA)*SIN(PHI))
            VZ=V*(-SIN(ALPHA)*SIN(THETA)*COS(PHI)+COS(ALPHA)*COS(THETA))
C
C       Advance trajectories until the next collision
C
            GO TO 50
C
          END IF
C
C       Electron has drifted at least XEND
C
          VDRIFT=VDRIFT+X/TTOTAL
          XNORM=XNORM+1.
        END DO
C
        VDRIFT=VDRIFT/XNORM
        PRINT *, 'VDRIFT=',VDRIFT,' cm/s'
C
        END
```

EXAMPLE: ELECTRON SWARM

- Collision frequency = 1.048 x 10^9 s^{-1}
- Drift distance = 20 cm
- E/N (Electric field/gas number density) = 1-10 x 10^{-17} V-cm3
- Electron particles=50-500 per E/N



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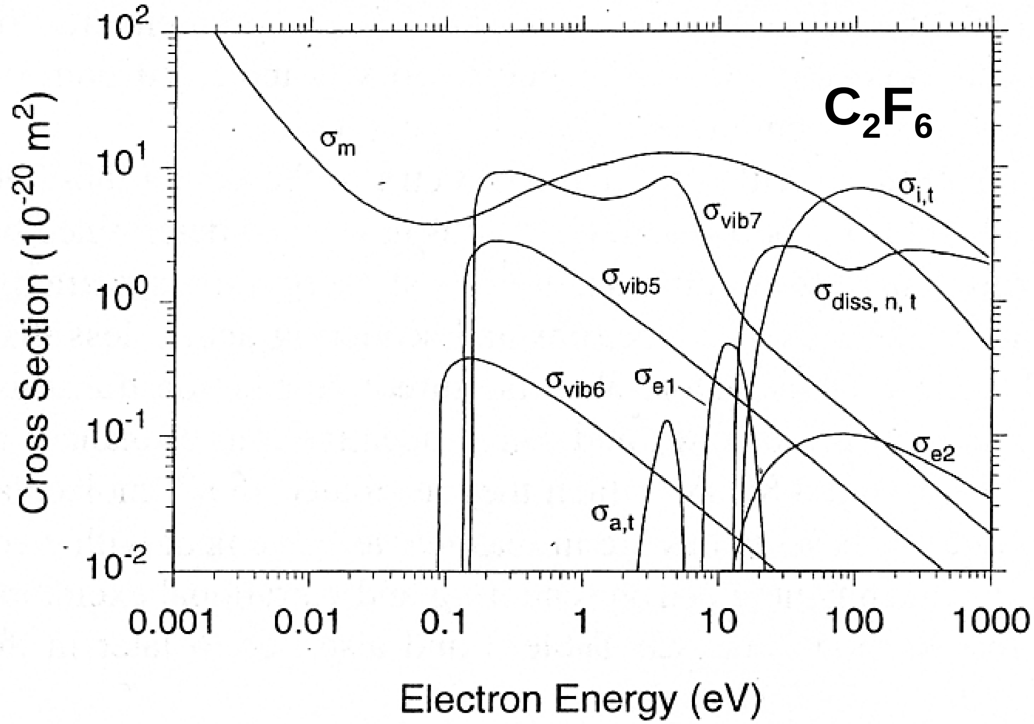
MUTIPLE COLLISIONS

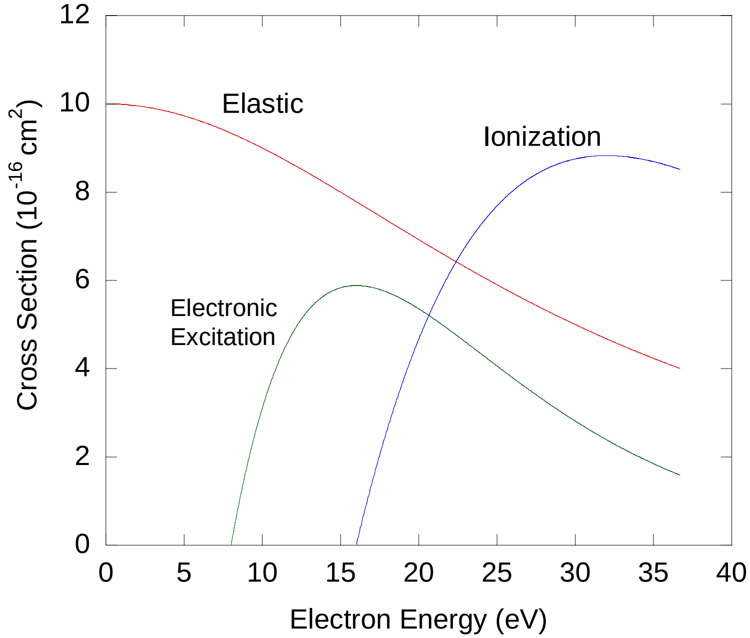
- **Real atoms/molecules have many electron collision processes (elastic, vibrational excitation, electronic excitation, ionization) with separate differential cross sections.**

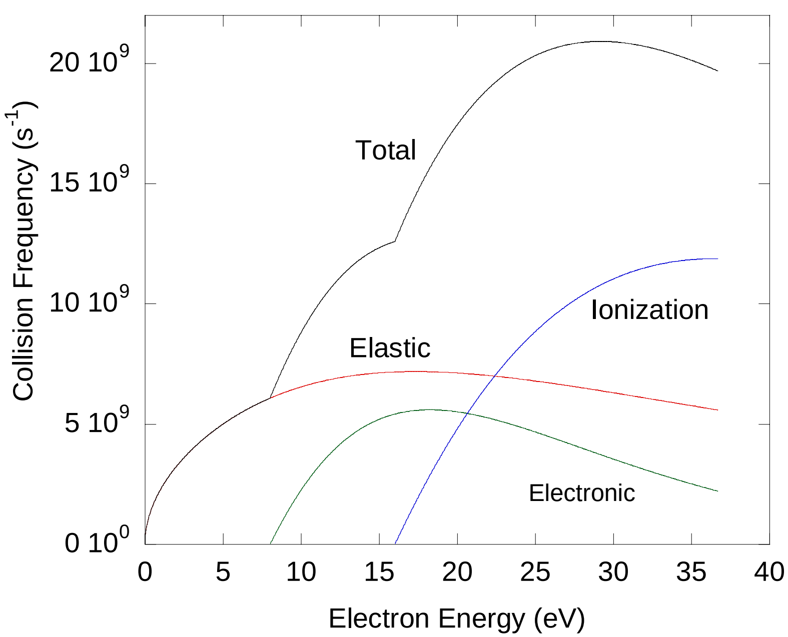


Christophorou, J. Chem. Phys. Ref. Data 27, 1, (1998)

- **These processes can be statistically accounted for using MC techniques**

MODEL CROSS SECTIONS

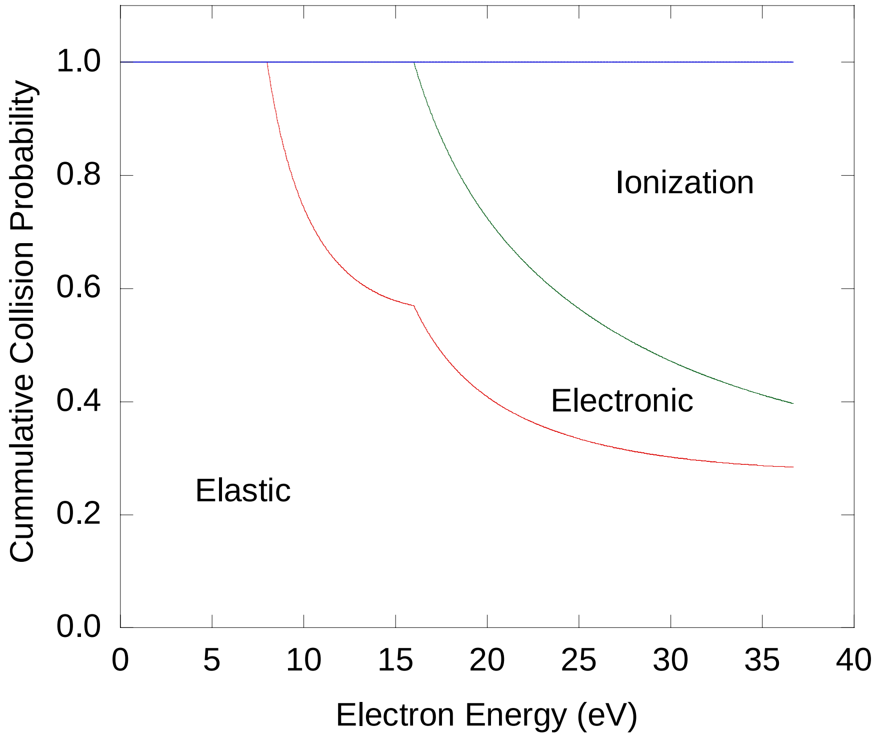




- **Compute collision frequencies for each process j having collision partner density N_j,**

$$\nu_j(\varepsilon) = \left(\frac{2\varepsilon}{m_e}\right)^{1/2} \sigma_j(\varepsilon) N_j, \quad \nu_{total}(\varepsilon) = \sum_j \nu_j(\varepsilon)$$

CUMULATIVE COLLISION PROBABILITY



$$p_j(\varepsilon) = \frac{\sum_{i=j-1}^{j} \nu_j(\varepsilon)}{\nu_{total}(\varepsilon)}$$

- **Cumulative collision probability is sum of probability of experiencing “yours” and all “previous” collisions. (Note: Order of summation is not important.)**

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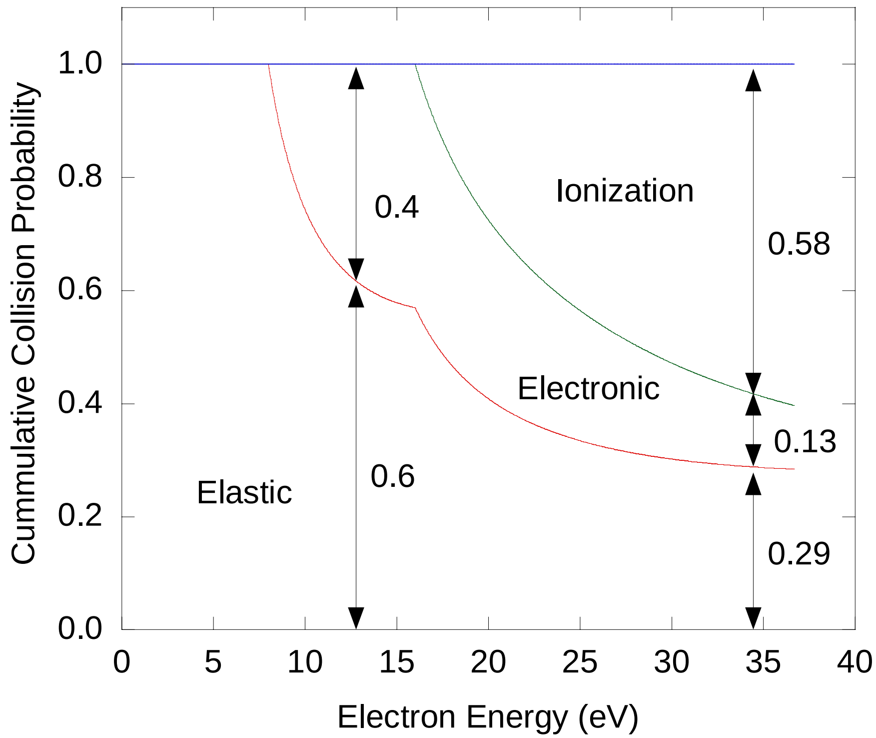
COLLISION SELECTION PROCESS



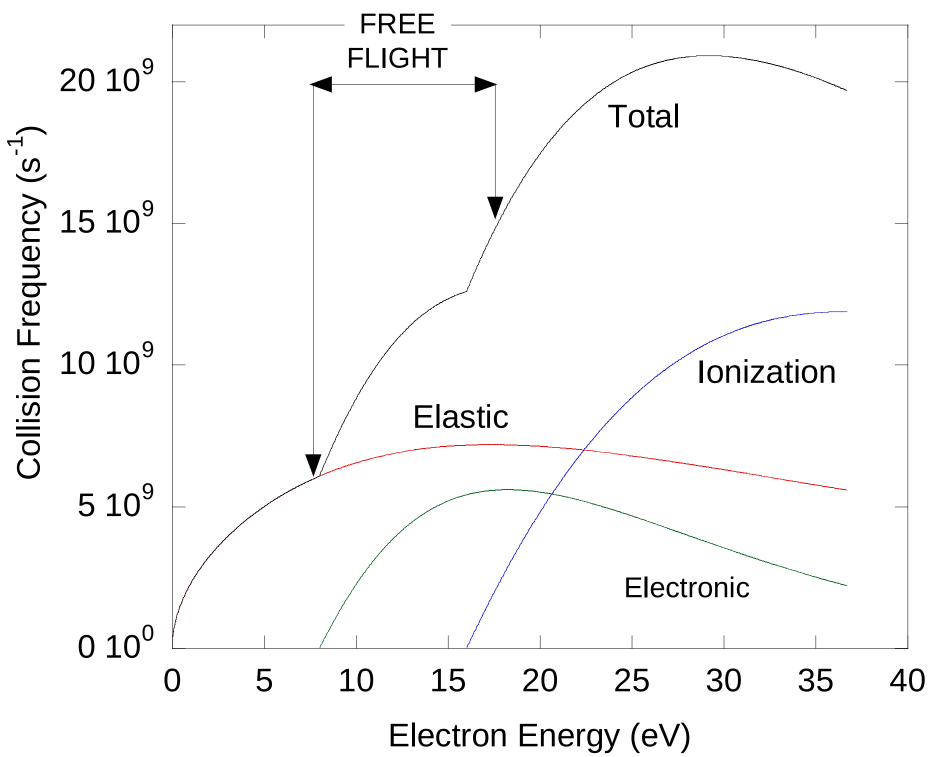
- **Choose time between collisions based on total collision frequency.**

$$\Delta t = \frac{-1}{\nu_{total}(\varepsilon)} \log(1 - r_1)$$

- **The collision which occurs is that which satisfies**

$$p_{j-1}(\varepsilon) < r_2 \le p_j(\varepsilon)$$

NULL COLLISION FREQUENCY



- **The electron energy and collision frequency can change during the free flight between collisions.**
- **There is an ambiguity in choosing the time between collisions.**
- **The ambiguity is eliminated by the "null collision frequency" (NCF).**

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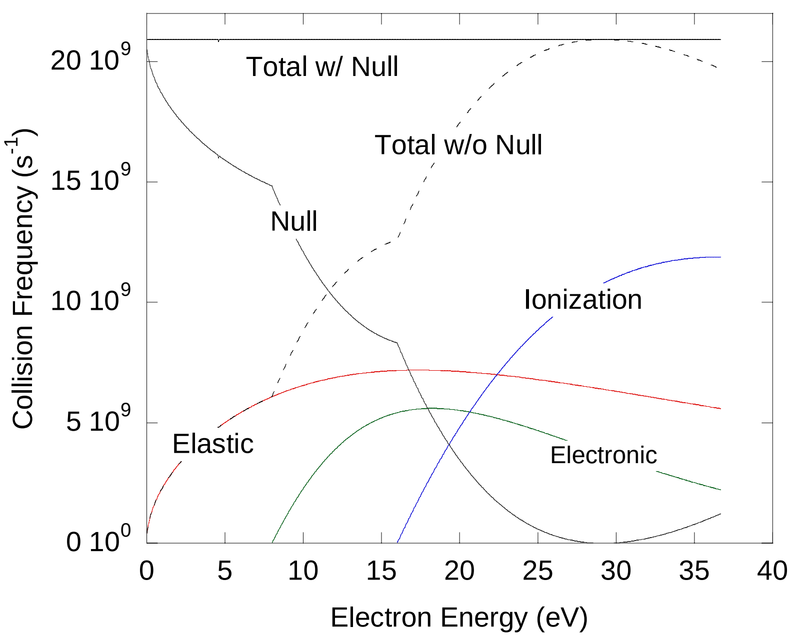
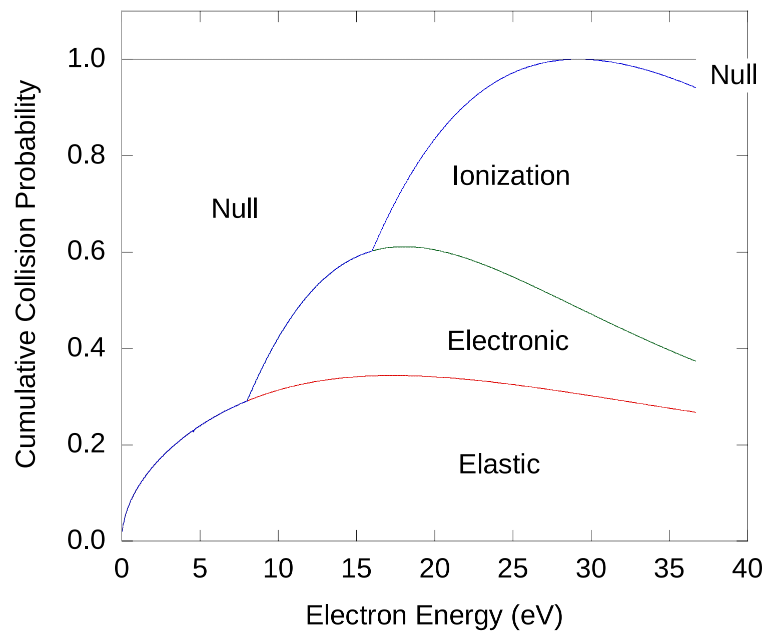
NULL COLLISION FREQUENCY

- **The NCF is a fictitious process used to make it appear that all energies have the same collision frequency.**

$$\nu_{null}(\varepsilon) = Max[\nu_{total}(\varepsilon)] - \nu_{total}(\varepsilon)$$



- **Collision frequencies with Null.**



- **Cumulative Probabilities with Null.**

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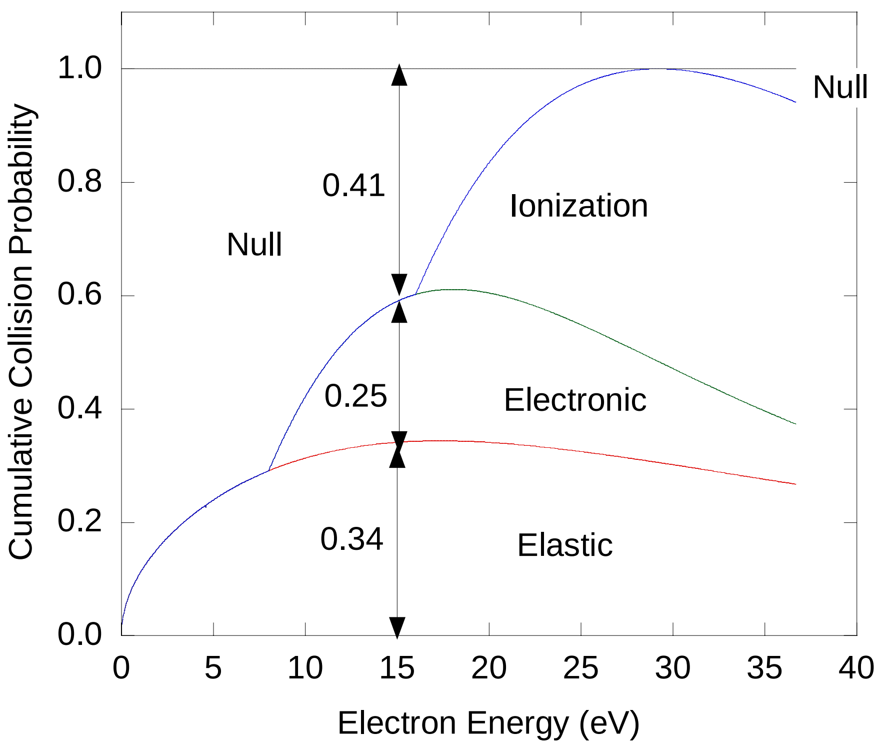
COLLISION SELECTION PROCESS WITH NULL



- **Choose time between collisions based on maximum total collision frequency.**

$$\Delta t = \frac{-1}{Max\left[\nu_{total}(\varepsilon)\right]}\log(1-r_1)$$

- **The collision which occurs is that which satisfies.**

$$p_{j-1}(\varepsilon) < r_2 \le p_j(\varepsilon)$$

- **If the null is chosen, disregard the collision. Allow the electron to proceed to the next free flight without changing its velocity.**

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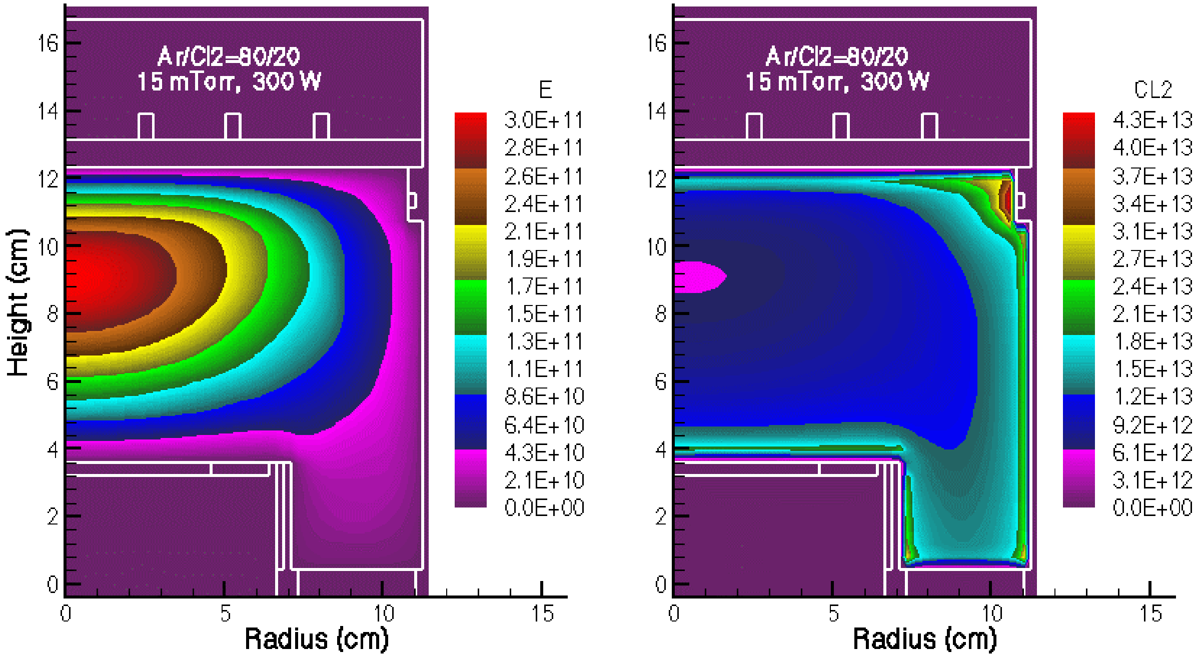
SPATIALLY VARYING COLLISION FREQUENCY



- **[e] and Cl_2 densities in an ICP for etching (Ar/Cl_2=80/20, 15 mTorr)**

- **In many of the systems of interest, the density of the collision partner depends on position and time.**

$$\nu_j(\varepsilon, x, t) = \left(\frac{2\varepsilon}{m_e}\right)^{1/2} \sigma_j(\varepsilon) N_j(x,t)$$

- **The choice of $\nu_{total}(\varepsilon)$ can be ambiguous.**

EXTENSION OF NULL METHOD TO ACCOUNT FOR N(x,t)

- **Sample time/space domain to determine** $Max[N_j(x,t)]$**.**
- **Compute** $\nu_j(\varepsilon), \quad \nu_{total}(\varepsilon), \quad Max[\nu_{total}(\varepsilon)], \quad \nu_{null}(\varepsilon)$ **using** $Max[N_j(x,t)]$**.**
- $Timestep: \quad \Delta t = \dfrac{-1}{Max[\nu_{total}(\varepsilon, x)]} \log(1 - r_1)$
- $x = x + v \cdot \Delta t, \quad v = v + a \cdot \Delta t$
- $Collision: \quad p_{j-1}(\varepsilon) < r_2 \le p_j(\varepsilon)$
- $j = Null \rightarrow next\ trajectory$
- $r_3 > \dfrac{N_j(x,t)}{Max[N_j(x,t)]} \rightarrow Null \rightarrow next\ trajectory$
- $scattering(\theta, \phi) = F^{-1}(r_4, r_5)$
- $Scattering\ Matrix$

SAMPLING AND INTEGRATION METHODS

- **Electron distributions are obtained by sampling the particle trajectories; binning particles by energy, velocity, position to obtain** $f\left(\varepsilon,\vec{r},t\right)\ or\ \ f\left(\vec{v},\vec{r},t\right)$**.**
- **How you sample affects the distribution function you derive.**
- **Integration Δt should be less than: Δt_{col}, fraction of $1/\nu_{rf}$, fraction of** $\left[\frac{v}{E}\frac{dE}{dx}\right]^{-1}$ **or other constraining frequencies.**
- **Δt can be different for each particle. Particles can "diverge in time" until they reach a time when they must be coincident.**
- **Recommended sampling and integration strategy:**
  - **Choose t(next collision) = t(last collision) + Δt_{col}**
  - **Integrate using $\Delta t \leq$ t- t(next collision)**
  - **Sample particles for every Δt weighting the contribution by Δt .**
  - **When reach t(next collision), collide and choose new Δt_{col}**

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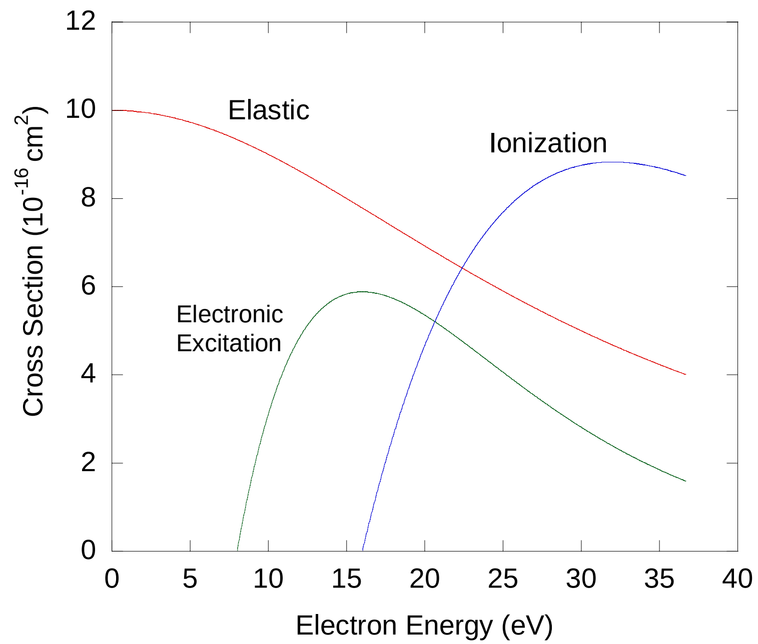
EXAMPLE: ELECTRON ENERGY DISTRIBUTION

- **Compute electron energy distribution and rate coefficients for idealized cross sections.**

- **Conditions:**

- **E/N: 100 x 10^{-17} V-cm^2 (100 Td)**
- **Drift distance: 3 cm (sample after 0.5 cm)**
- **Number of Particles: 2000**



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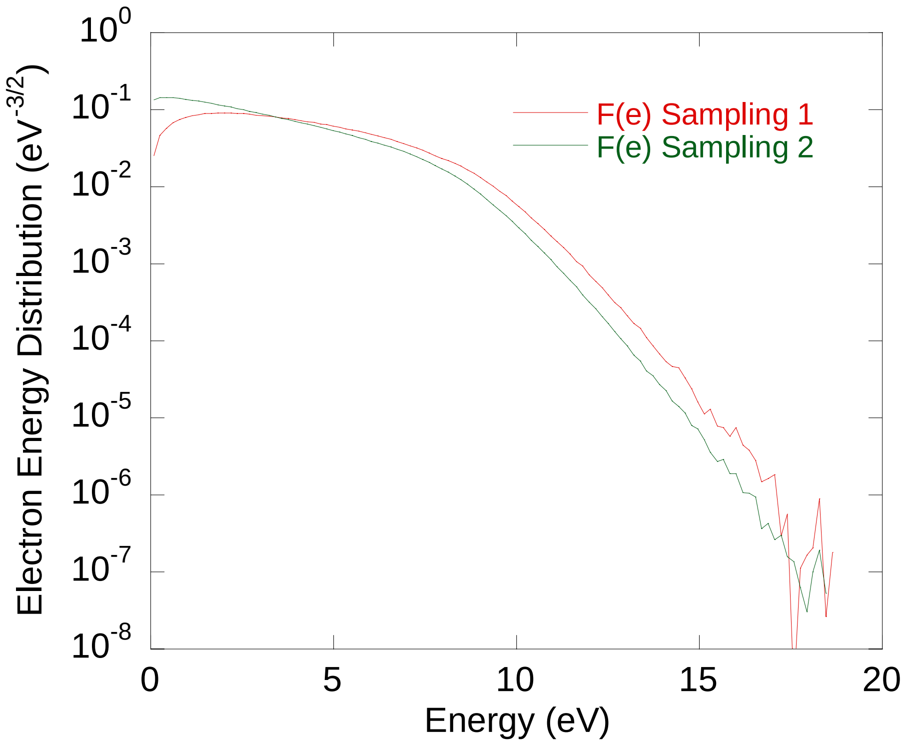
EXAMPLE: ELECTRON ENERGY DISTRIBUTION

- **Sampling method**
  - **1: Every Δt_{col}**
  - **2: Every Δt (constant) < Δt_{col}**
- **Rate Coefficients (cm^3/s)**
  - **Elastic 1.1 x 10^{-7}**
  - **Electronic 2.0 x 10^{-9}**
  - **Ionization 9.9 x 10^{-14}**
- **Number of Collisions:**
  - **Elastic 1.46 x 10^{7}**
  - **Electronic 2.21 x 10^{5}**
  - **Ionization 10**
  - **Null 5.93 x 10^{7}**

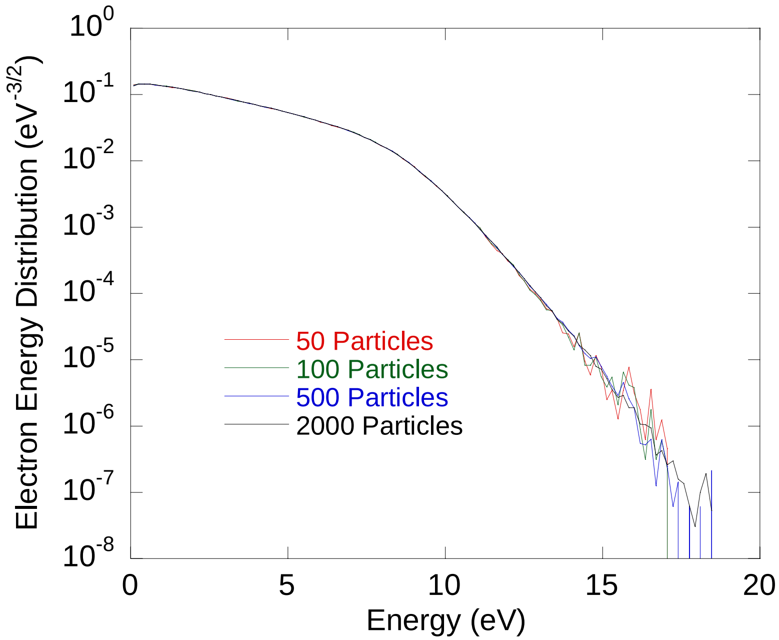


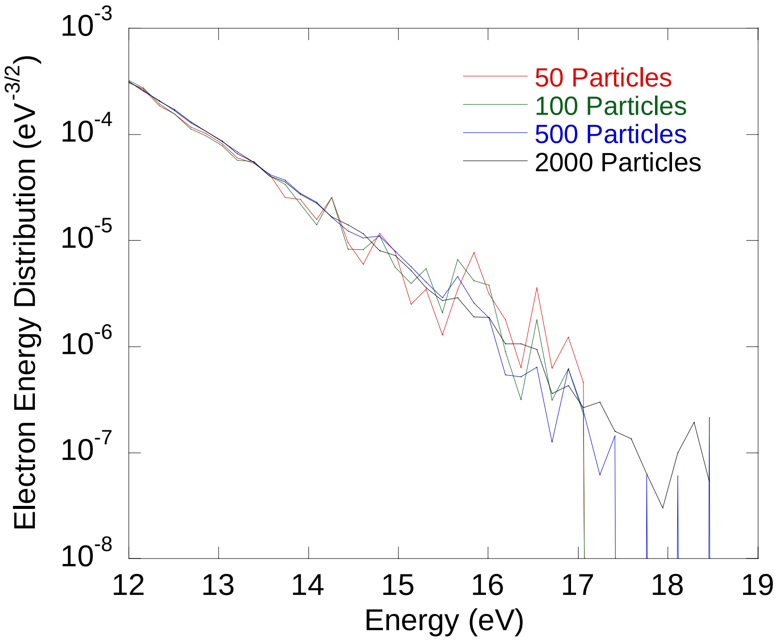
- **Lesson!!! Do NOT compute rate coefficients by counting collisions! Directly compute rate coefficients from EED.**

$$k(\vec{r},t)=\int f(\varepsilon,\vec{r},t)\left(\frac{2\varepsilon}{m_e}\right)^{1/2}\sigma(\varepsilon)\varepsilon^{1/2}d\varepsilon$$

EXAMPLE: ELECTRON ENERGY DISTRIBUTION

- **Required samplings are dictated by the tail of the EED. Rate coefficients for high threshold events are sensitive to the tail.**





Number of Particles	50	100	500	2000
Rate Coefs: Elastic	1.08×10^{-7}	1.08×10^{-7}	1.08×10^{-7}	1.08×10^{-7}
Electronic ($\Delta\varepsilon$ = 8 eV)	1.98×10^{-9}	1.99×10^{-9}	2.00×10^{-9}	1.99×10^{-9}
Ionization ($\Delta\varepsilon$ = 16 eV)	1.23×10^{-13}	6.51×10^{-14}	6.84×10^{-14}	9.94×10^{-14}
Samplings	2,953,842	5,899,608	29,327,876	117,332,716

EFFICIENCY ISSUES

- **Create look-up tables where-ever possible (memory and lookups are cheap, computations are expensive).**

- **Minimize null-collisions by having sub-intervals of energy range with different** $Max\left[\nu_{total}\left(\varepsilon\right)\right]$ **.**

- **Be cognizant of "pipelining" opportunities. Perform array operations with stencils to include-exclude indices for particles which are added-removed due to attachment, losses to walls or ionization.**

- **Take advantage of cyclic conditions to bin particles by phase as opposed to time.**

- **NEVER hardwire anything!! Define all cross sections, densities from "outside."**

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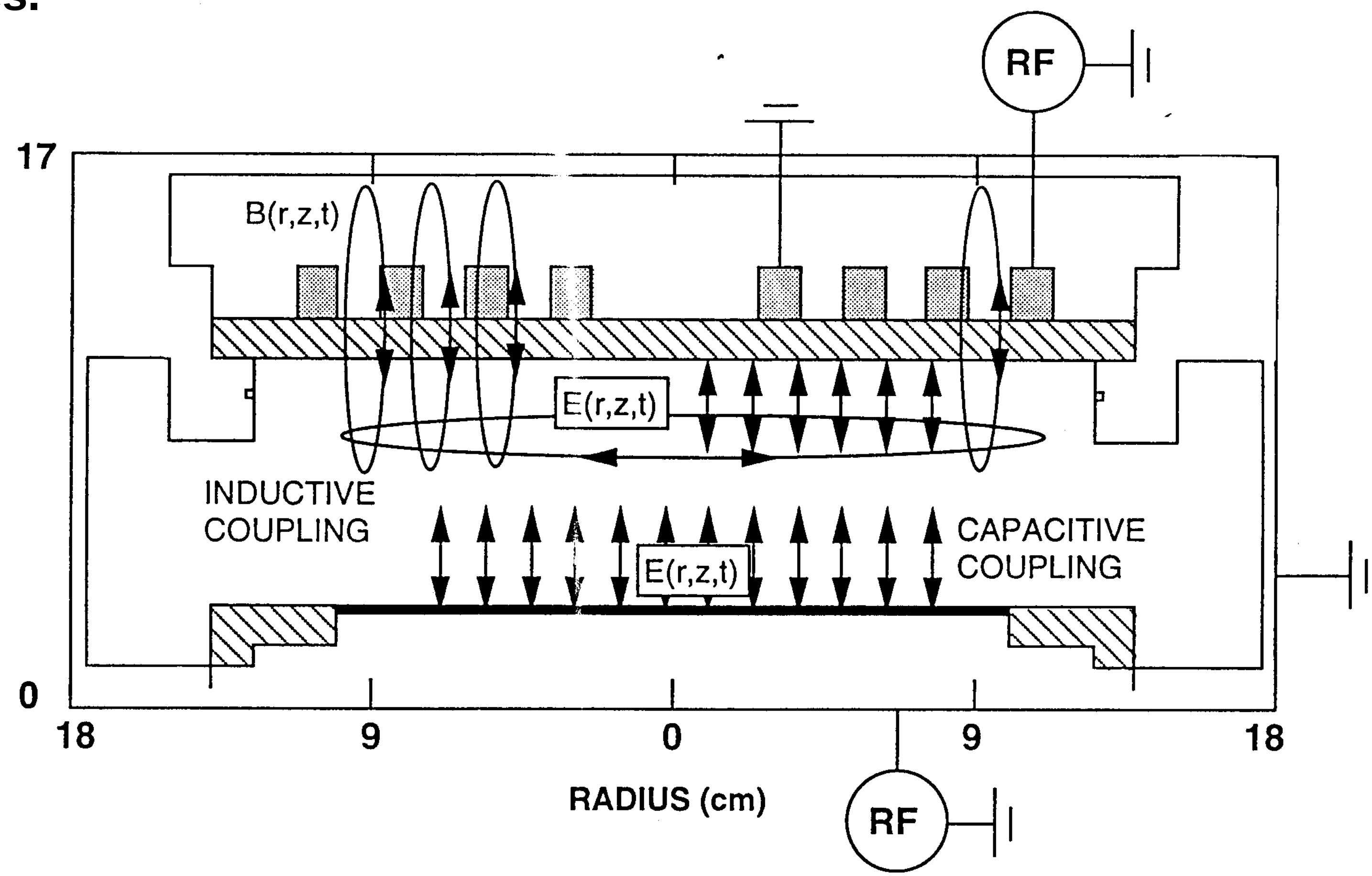
ADVANCED TOPICS

TYPICAL INDUCTIVELY COUPLED PLASMA FOR ETCHING

- **Power is coupled into the plasma by both inductive and capacitive routes.**



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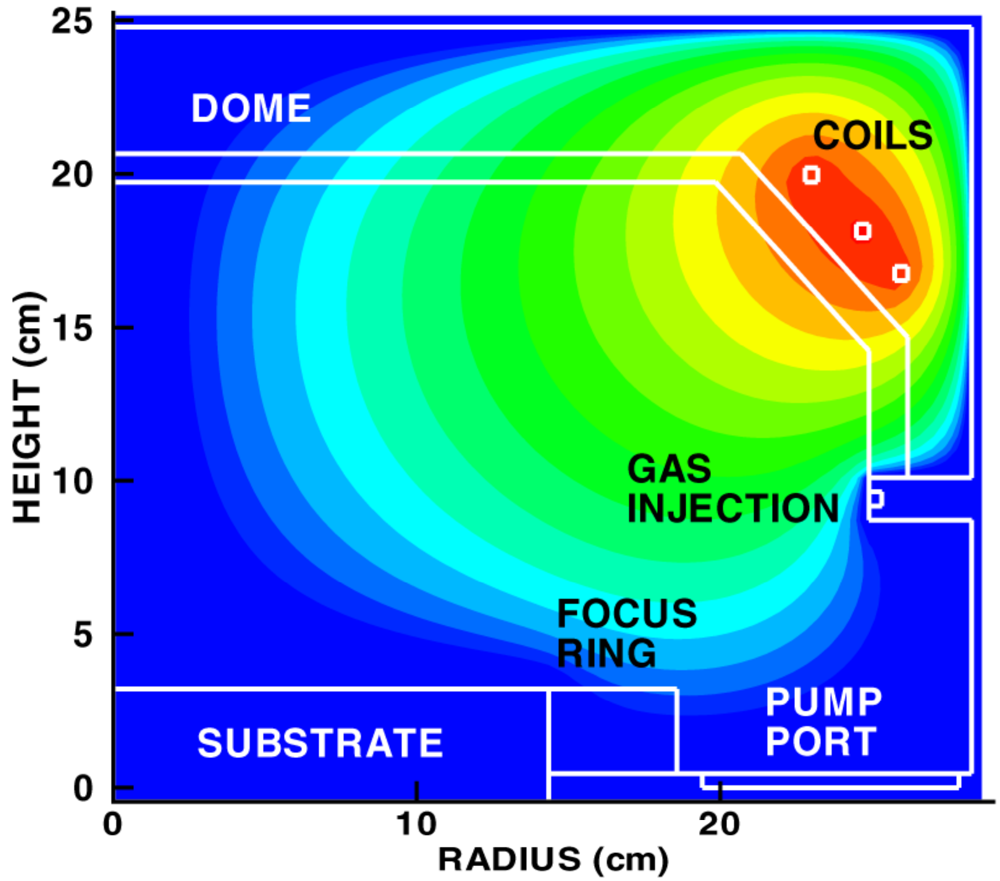
WALK THROUGH: Ar/Cl_2 PLASMA FOR p-Si ETCHING

- **The inductively coupled electromagnetic fields have a skin depth of 3-4 cm.**
- **Absorption of the fields produces power deposition in the plasma.**
- **Electric Field (max = 6.3 V/cm)**
  - **Ar/Cl_2 = 80/20**
  - **20 mTorr**
  - **1000 W ICP 2 MHz**
  - **250 V bias, 2 MHz (260 W)**



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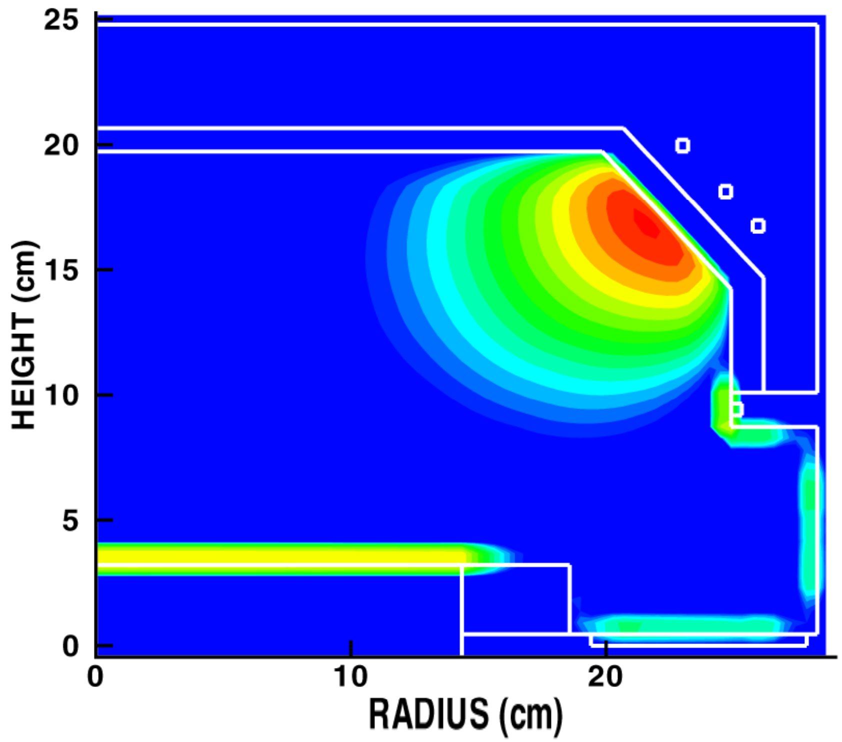
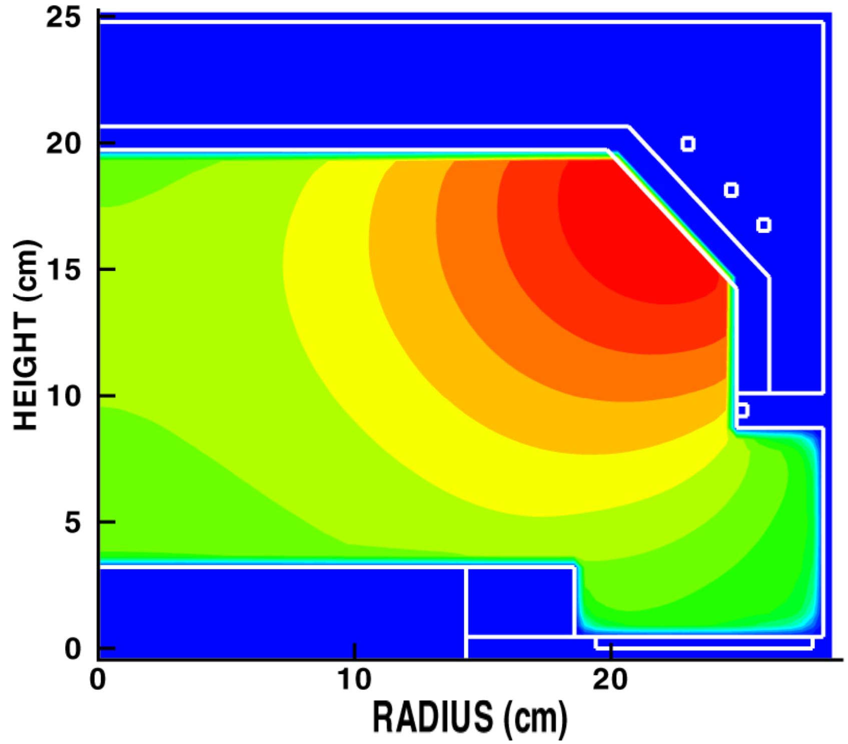
Ar/Cl_2 ICP: POWER AND ELECTRON TEMPERATURE

- **ICP Power heats electrons, capacitively coupled power dominantly accelerates ions.**





- **Power Deposition (max = 0.9 W/cm^3)**
- **Electron Temperature (max = 5 eV)**

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP 2 MHz, 250 V bias, 2 MHz (260 W)**

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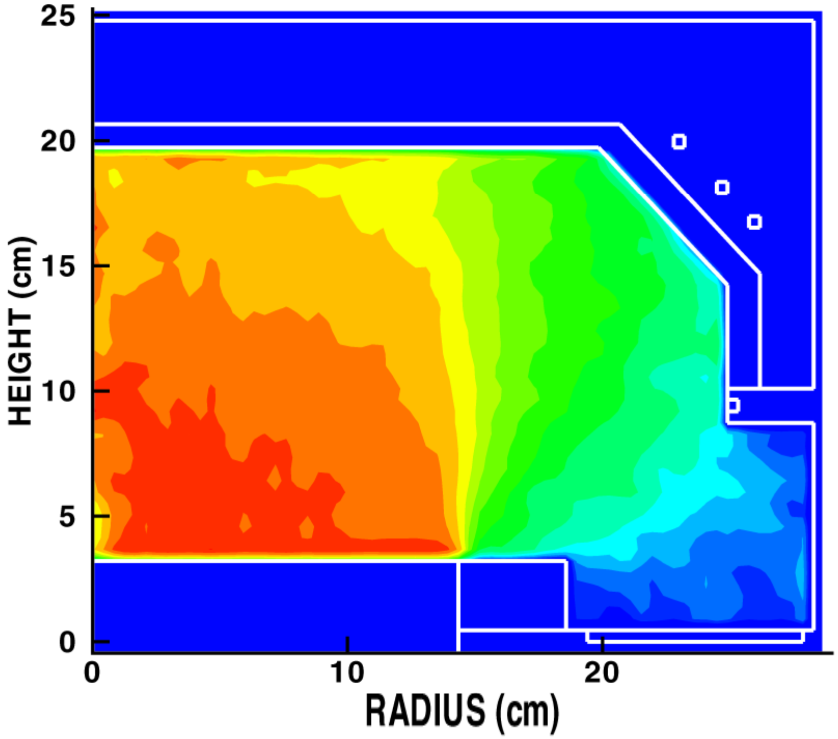
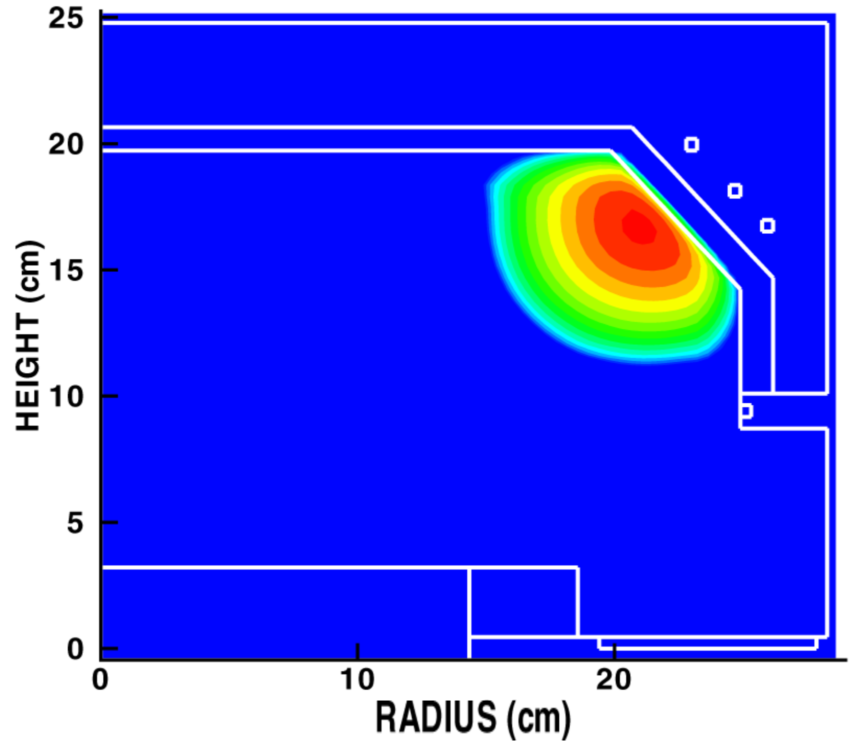
Ar/Cl_2 ICP: IONIZATION

- **Ionization is produced by bulk electrons and sheath accelerated secondary electrons.**



- **Beam Ionization**
(max = 1.3 x 10^{14} $cm^{-3}s^{-1}$)



- **Bulk Ionization**
(max = 5.4 x 10^{15} $cm^{-3}s^{-1}$)

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP 2 MHz, 250 V bias, 2 MHz (260 W)**

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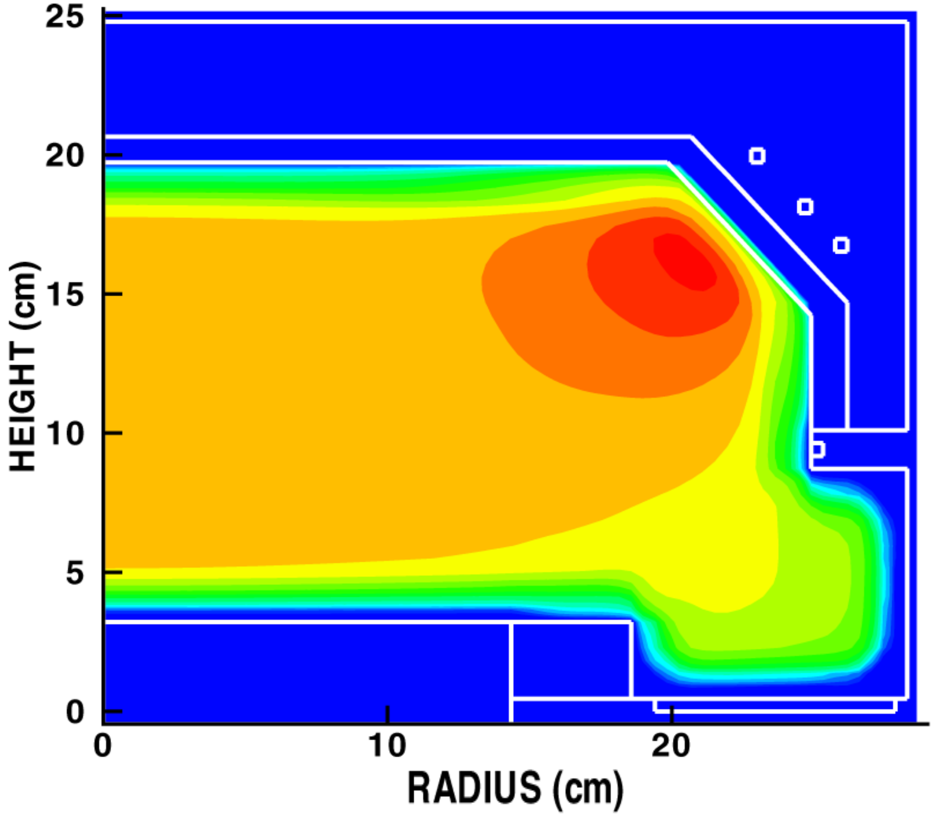
Ar/Cl_2 ICP: POSITIVE ION DENSITY

- **Diffusion from the remote plasma source produces uniform ion densities at the substrate.**



- **Positive Ion Density (max = 1.8 x 10^{11} cm^{-3})**

- **Ar/Cl_2 = 80/20, 20 mTorr, 1000 W ICP 2 MHz, 250 V bias, 2 MHz (260 W)**

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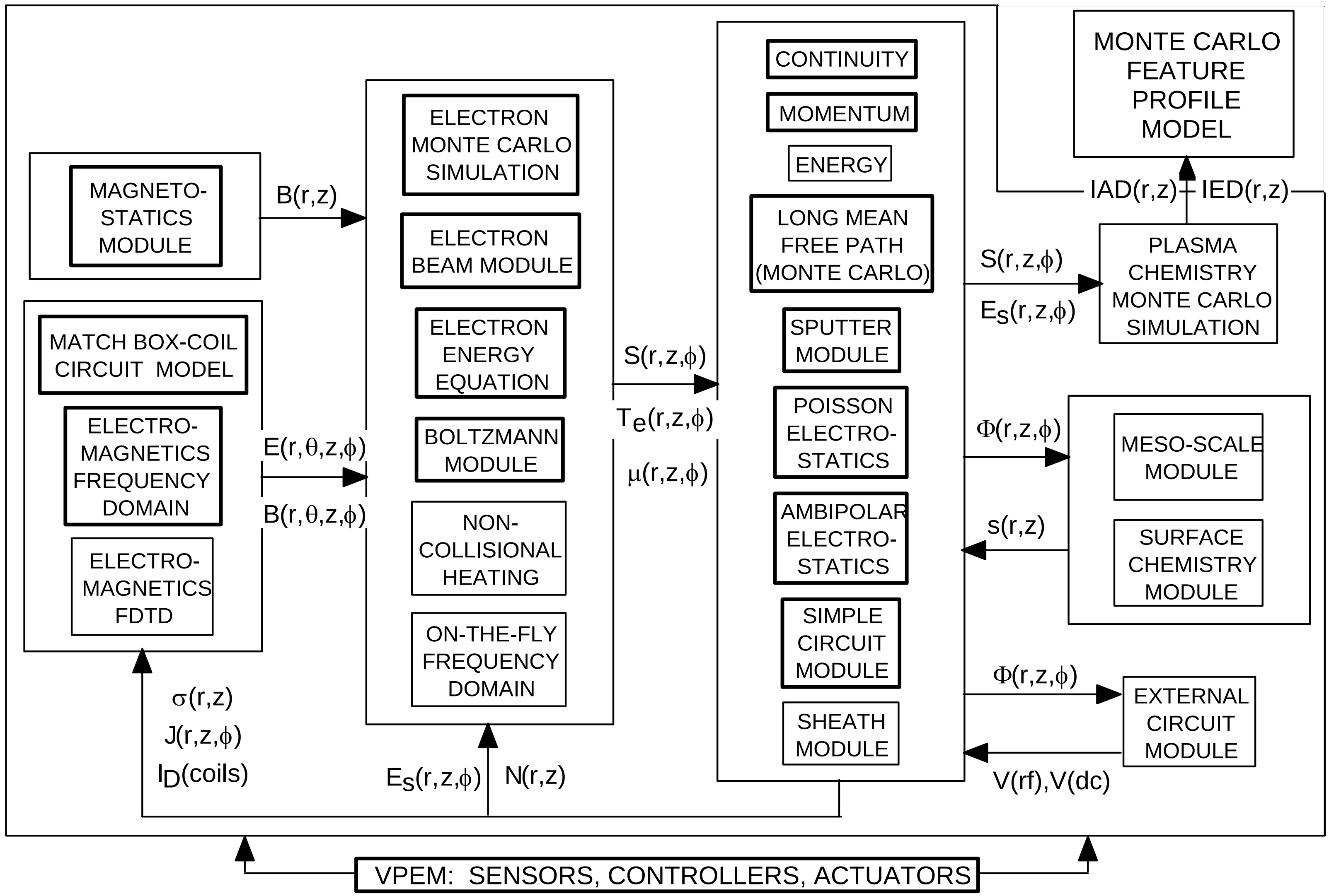
HYBRID PLASMA EQUIPMENT MODEL



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ELECTROMAGNETICS MODEL

- **The wave equation is solved in the frequency domain using sparse matrix techniques (2D,3D):**

$$-\nabla\left(\frac{1}{\mu}\nabla\cdot\overline{E}\right)+\nabla\cdot\left(\frac{1}{\mu}\nabla\overline{E}\right)=\frac{\partial^2\left(\varepsilon\overline{E}\right)}{\partial t^2}+\frac{\partial\left(\overline{\overline{\sigma}}\cdot\overline{E}+\overline{J}\right)}{\partial t}$$

$$\vec{E}(\vec{r},t)=\vec{E}'(\vec{r})\exp(-i(\omega t+\varphi(\vec{r})))$$

- **Conductivities are tensor quantities (2D,3D):**

$$\overline{\overline{\sigma}}=\sigma_o\frac{m\nu_m}{q\alpha}\frac{1}{\left(\alpha^2+\left|\vec{B}\right|^2\right)}\begin{pmatrix}\alpha^2+B_r^2 & \alpha B_z+B_rB_\theta & -\alpha B_\theta+B_rB_z\\ -\alpha B_z+B_rB_\theta & \alpha^2+B_\theta^2 & \alpha B_r+B_\theta B_z\\ -\alpha B_\theta+B_rB_z & -\alpha B_r+B_\theta B_z & \alpha^2+B_z^2\end{pmatrix}$$

$$\vec{j}=\overline{\overline{\sigma}}\cdot\vec{E}\qquad\qquad \alpha=\frac{\left(i\omega+\nu_m\right)}{q/m},\quad \sigma_o=\frac{q^2n_e}{m\nu_m}$$

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ELECTROMAGNETICS MODEL (cont.)

- **The electrostatic term in the wave equation is addressed using a perturbation to the electron density (2D).**

$$\nabla \cdot \overline{E} = \frac{\rho}{\varepsilon} = \frac{q\Delta n_e}{\varepsilon}, \quad \Delta n_e = -\nabla \cdot \left(\frac{\overline{\overline{\sigma}} \cdot \overline{E}}{q} \right) / \left(\frac{1}{\tau} + i\omega \right)$$

- **Conduction currents can be kinetically derived from the Electron Monte Carlo Simulation to account for non-collisional effects (2D).**

$$\mathrm{J}_{\mathrm{e}}(\vec{r},t) = J_o(\vec{r})\exp(i(\omega t + \phi_v(\vec{r}))) = -qn_e(\vec{r})\vec{v}_e(\vec{r})\exp\left(i\left(\omega t + \vec{\phi}_v(\vec{r})\right)\right)$$

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ELECTRON ENERGY TRANSPORT

- **Continuum (2D,3D):**

$$\partial\left(\frac{3}{2}n_e kT_e\right)/\partial t = S(T_e) - L(T_e) - \nabla\cdot\left(\frac{5}{2}\Phi kT_e - \overline{\overline{\kappa}}(T_e)\cdot\nabla T_e\right) + S_{EB}$$

where	**$S(T_e)$**	**=**	**Power deposition from electric fields**
	$L(T_e)$	**=**	**Electron power loss due to collisions**
	Φ	**=**	**Electron flux**
	$\kappa(T_e)$	**=**	**Electron thermal conductivity tensor**
	S_{EB}	**=**	**Power source source from beam electrons**

- **Power deposition has contributions from wave and electrostatic heating.**

- **Kinetic (2D,3D): A Monte Carlo Simulation is used to derive** $f(\varepsilon,\vec{r},t)$ **including electron-electron collisions using electromagnetic fields from the EMM and electrostatic fields from the FKM.**

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PLASMA CHEMISTRY, TRANSPORT AND ELECTROSTATICS

- **Continuity, momentum and energy equations are solved for each species (with jump conditions at boundaries) (2D,3D).**

$$\frac{\partial N_i}{\partial t} = -\nabla \cdot (N_i \vec{\mathrm{v}}_i) + S_i$$

$$\frac{\partial (N_i \vec{v}_i)}{\partial t} = \frac{1}{m_i} \nabla (k N_i T_i) - \nabla \cdot (N_i \vec{v}_i \vec{v}_i) + \frac{q_i N_i}{m_i} \left(\vec{E} + \vec{v}_i \times \vec{B} \right) - \nabla \cdot \overline{\mu}_i - \sum_j \frac{m_j}{m_i + m_j} N_i N_j (\vec{v}_i - \vec{v}_j) \nu_{ij}$$

$$\frac{\partial (N_i \varepsilon_i)}{\partial t} + \nabla \cdot \mathrm{Q}_i + P_i \nabla \cdot \mathrm{U}_i + \nabla \cdot (N_i \mathrm{U}_i \varepsilon_i) = \frac{N_i q_i^2 \nu_i}{m_i (\nu_i^2 + \omega^2)} E^2 + \frac{N_i q_i^2}{m_i \nu_i} E_s^2 + \sum_j 3 \frac{m_{ij}}{m_i + m_j} N_i N_j R_{ij} k_B (T_j - T_i) \pm \sum_j 3 N_i N_j R_{ij} k_B T_j$$

- **Implicit solution of Poisson's equation (2D,3D):**

$$\nabla \cdot \varepsilon \nabla \Phi (t + \Delta t) = -\left(\rho_s + \sum_i q_i N_i - \Delta \mathrm{t} \cdot \sum_{\mathrm{i}} \left(\mathrm{q}_{\mathrm{i}} \nabla \cdot \vec{\phi}_i \right) \right)$$

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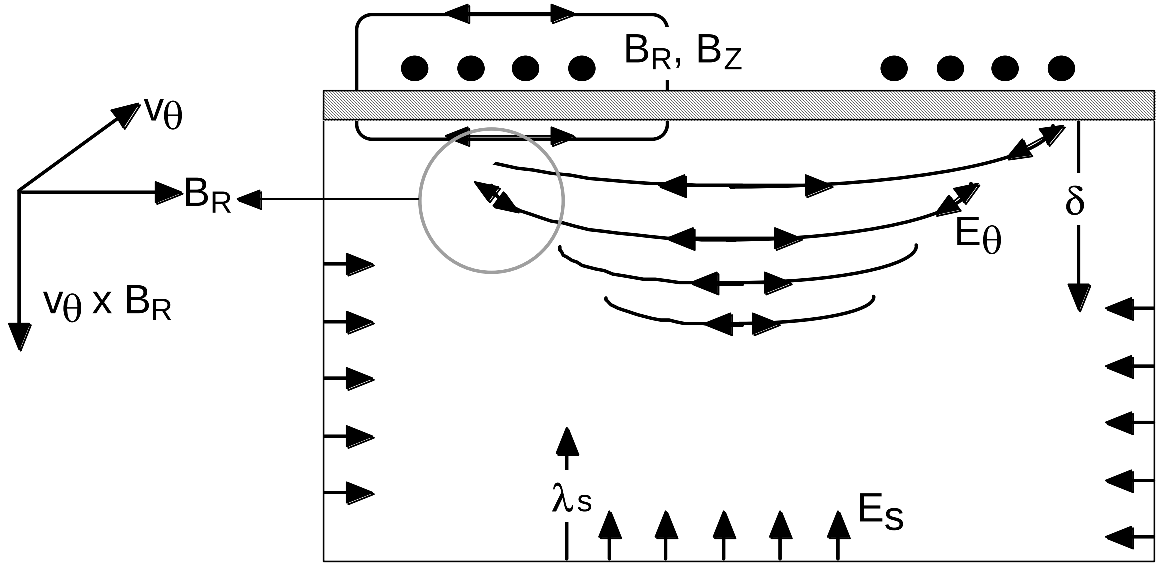
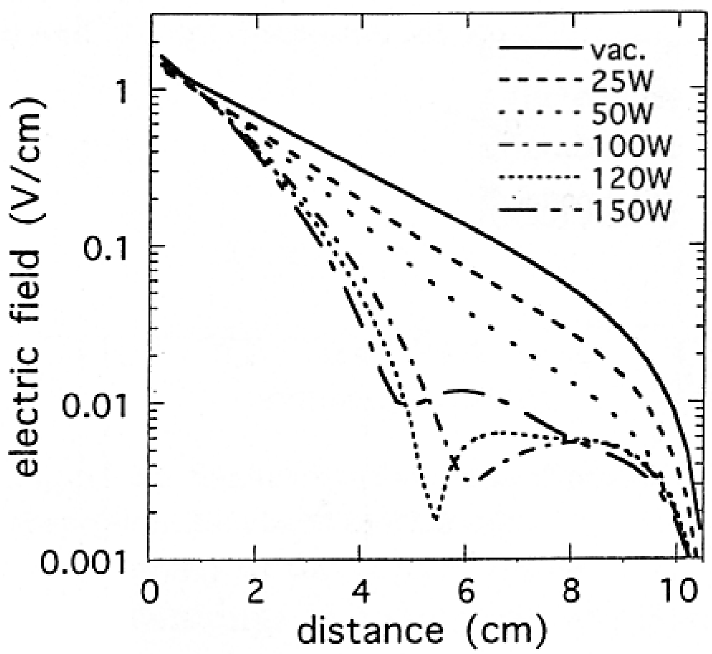
FORCES ON ELECTRONS IN ICPs



- **Inductive electric field provides azimuthal acceleration; penetrates** $\delta = \left(m_e / \left(e^2 \mu_o n_e\right)\right)^{1/2}$ **(1-3 cm)**
- **Electrostatic (capacitive); penetrates** $\lambda_S \approx 10\lambda_D,\ \lambda_D = \left(kT_e / \left(8\pi n_e e^2\right)\right)^{1/2}$ **(100s μm to mm)**
- **Non-linear Lorentz Force** $\vec{F} = v_\theta \times \vec{B}_{rf}$

ANAMOLOUS SKIN EFFECT AND POWER DEPOSITION



- Ref: V. Godyak, "Electron Kinetics of Glow Discharges"

- **Collisional heating:**

$$\lambda_{mfp} < \delta_{skin}, \quad \vec{J}_e(\vec{r},t) = \sigma(\vec{r},t)\vec{E}(\vec{r},t)$$

- **Anomalous skin effect:**

$$\lambda_{mfp} > \delta_{skin}$$

$$\vec{J}_e(\vec{r},t) = \iint \sigma(\vec{r},\vec{r}\,',t,t')\vec{E}(\vec{r}\,',t')d\vec{r}\,'dt'$$

$$\vec{F} = \vec{v} \times \vec{B}$$

- **Electrons receive (positive) and deliver (negative) power from/to the E-field.**
- **E-field is non-monotonic.**

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COLLISIONLESS TRANSPORT ELECTRIC FIELDS

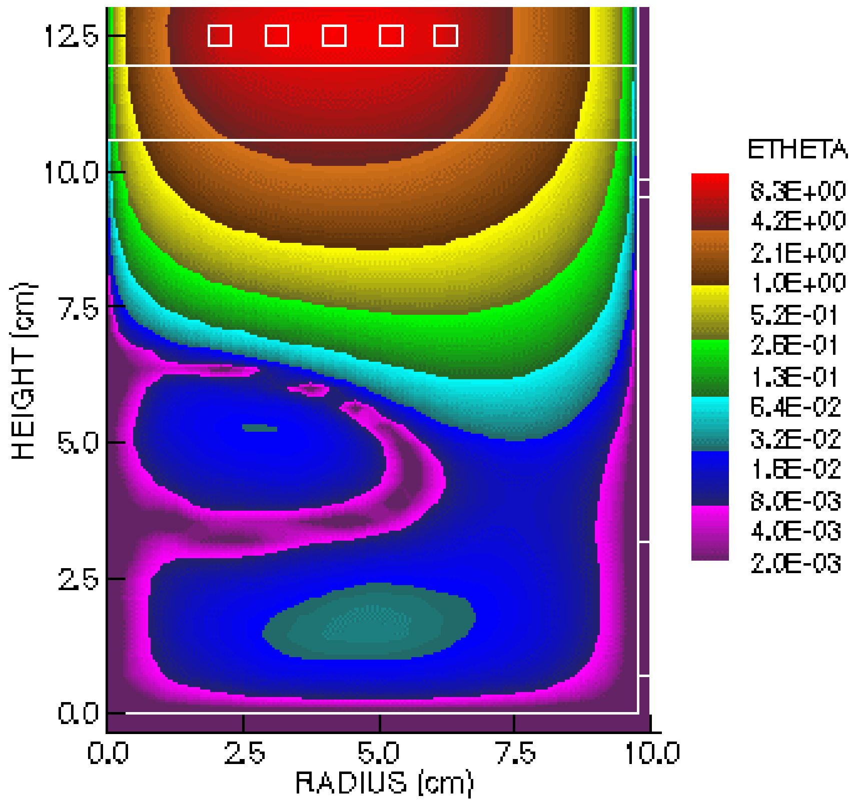
- **We capture these affects by kinetically deriving electron current.**

$$\oint \vec{j}(\vec{r})\exp\left(i\omega(t-t_o)\right)\cdot dA = \sum_k q_k \vec{v}_k(\vec{r})\exp\left(i\omega(t_k - t_o)\right)$$

- **E_θ during the rf cycle exhibits extrema and nodes resulting from this non-collisional transport.**

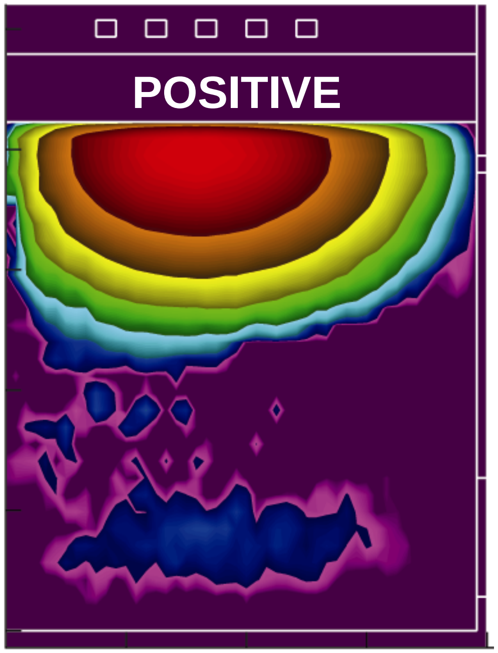
- **"Sheets" of electrons with different phases provide current sources interfering or reinforcing the electric field for the next sheet.**

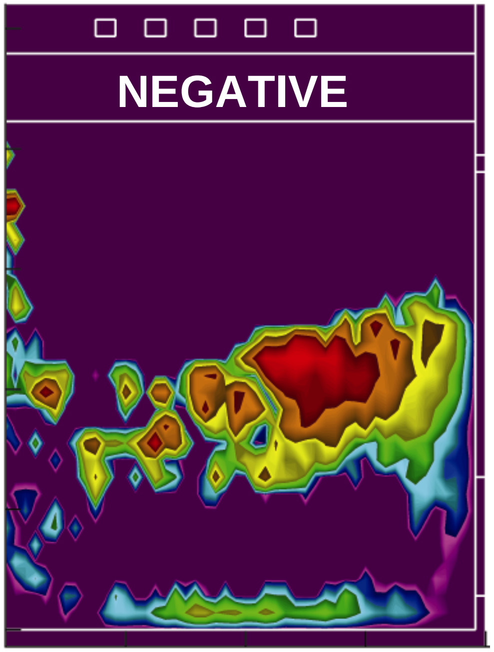
- **Axial transport results from $\vec{v}\times\vec{B}_{rf}$ forces.**



ANIMATION SLIDE

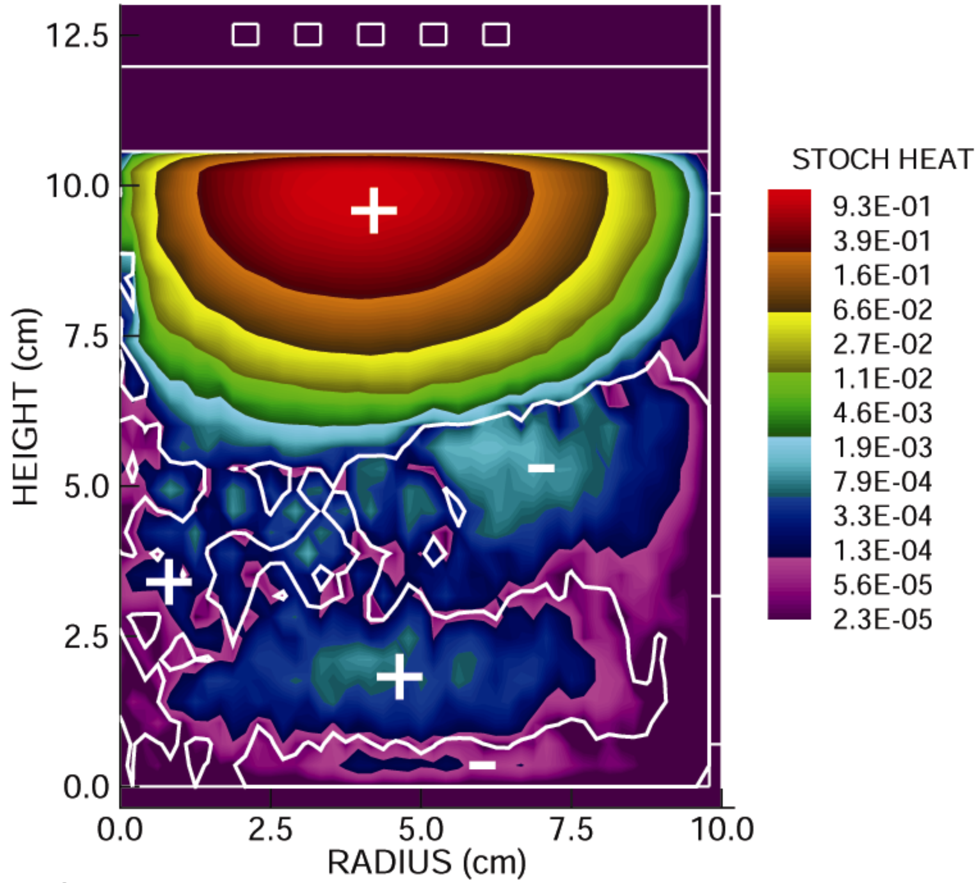
- **Ar, 10 mTorr, 7 MHz, 100 W**





POWER DEPOSITION: POSITIVE AND NEGATIVE

- **The end result is regions of positive and negative power deposition.**



- **Ar, 10 mTorr, 7 MHz, 100 W**

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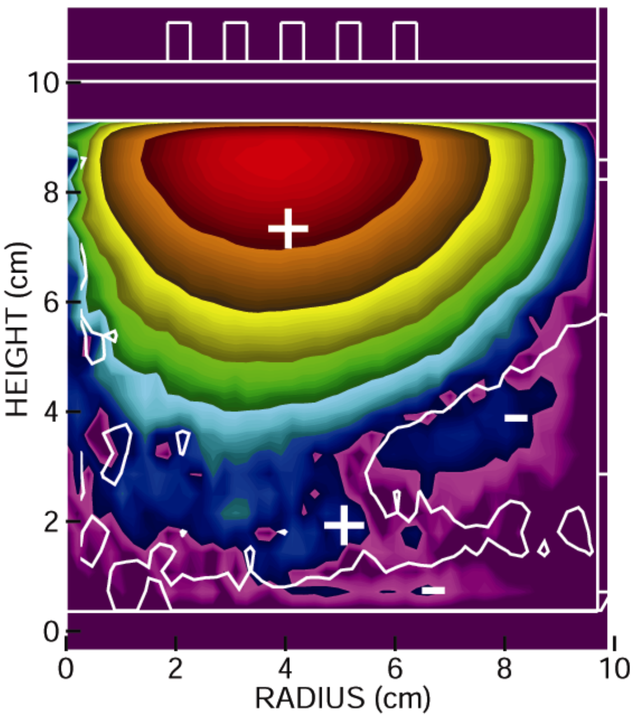
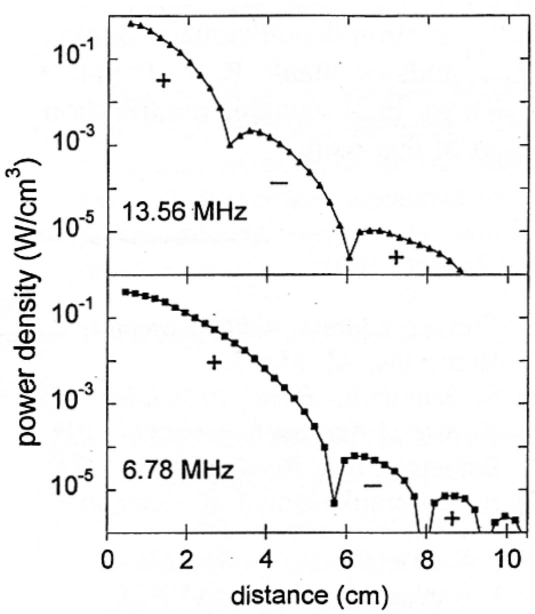
POWER DEPOSITION vs FREQUENCY

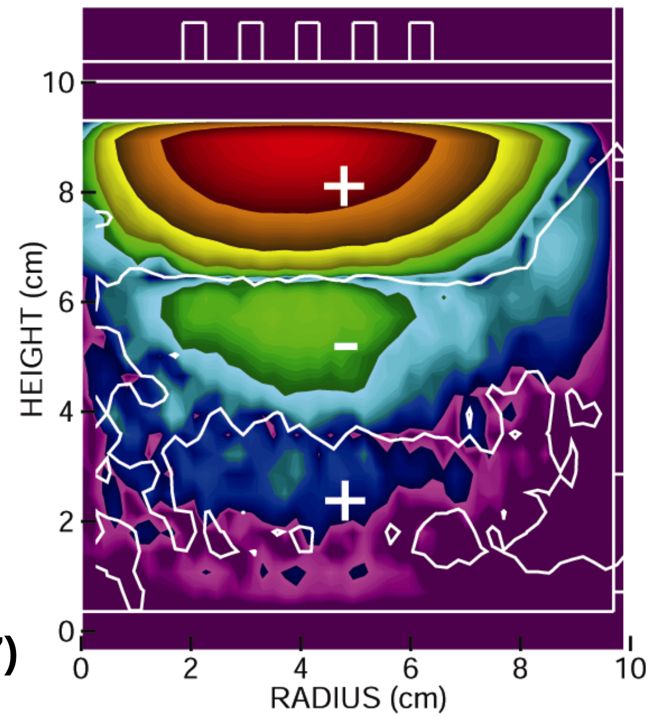
- The shorter skin depth at high frequency produces more layers of negative power deposition of larger magnitude.



- 6.7 MHz
(5x10^{-5} – 1.4 W/cm^3)



- Ref: Godyak, PRL (1997)
- Ar, 10 mTorr, 200 W



- 13.4 MHz
(8x10^{-5} – 2.2 W/cm^3)

MIN MAX

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TIME DEPENDENCE OF EEDs: FOURIER ANALYSIS

- **To obtain time dependent EEDs, Fourier transforms are performed "on-the-fly" in the Electron Monte Carlo Simulation.**

- **As electron trajectories are integrated, complex Fourier coefficients and weightings are incremented by.**

$$\Delta\Psi_n\left(\varepsilon_i,\vec{r}_k\right)=\sum_j w_j \Delta t_j \exp\left(in\omega t_j\right)\delta((\varepsilon_i \pm \tfrac{1}{2}\Delta\varepsilon_i)-\varepsilon_j)\sum_k \delta((\vec{r}_{l+k} \pm \tfrac{1}{2}\Delta\vec{r}_{l+k})-\vec{r}_j),$$

$$\Delta W_{jk} = \sum_j w_j \Delta t_j \sum_k \delta((\vec{r}_{l+k} \pm \tfrac{1}{2}\Delta\vec{r}_{l+k})-\vec{r}_j)$$

- **The Fourier coefficients are then obtained from:**

$$A_n(\varepsilon_i,\vec{r}_k) = \left|\frac{\Psi_n(\varepsilon_i,\vec{r}_k)}{W_{ik}}\right|,\ \ \phi_n(\varepsilon_i,\vec{r}_k) = \tan^{-1}\left(\frac{\mathrm{Im}[\Psi_n(\varepsilon_i,\vec{r}_k)]}{\mathrm{Re}[\Psi_n(\varepsilon_i,\vec{r}_k)]}\right)$$

TIME DEPENDENCE OF EEDs: FOURIER ANALYSIS

- **The time dependence of the nth harmonic of the EED is then reconstructed**

$$f_n(\varepsilon,\vec{r},t) = A_n(\varepsilon,\vec{r})\sin\left[\omega nt + \phi_n(\varepsilon,\vec{r})\right]$$

- **…and the total time dependence of the electron distribution function is obtain from summation of the harmonics:**

$$f(\varepsilon,\vec{r},t) = \sum_{n=0}^{N} f_n(\varepsilon,\vec{r},t)$$

….where f_0 is the time averaged distribution function.

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EXCITATION RATES: "ON THE FLY"

- **In a similar manner, Fourier components of excitation rates can be obtained directly from the Electron MCS**

- **For the n^th harmonic of the m^th process,**

$$k'_{nml} \rightarrow k'_{nml} + \sum_j w_j \sigma_m(\varepsilon_j)\upsilon_j \exp\left(in\omega t\right)\sum_k \delta((\vec{r}_{l+k} \pm \tfrac{1}{2}\Delta\vec{r}_{l+k}) - \vec{r}_j)$$

- **The resulting Fourier coefficients then reconstruct the time dependence of electron impact source functions.**

$$S_{ml}(t) = [e]_l N_{ml} \sum_{n=0}^{n_m} \left|k_{nml}\right| \sin(n\omega t + \phi_{nml}),$$

$$\phi_{nml} = \tan^{-1}\frac{\mathrm{Im}(k_{nml})}{\mathrm{Re}(k_{nml})}$$

ALGORITHM FOR E-E COLLISIONS

- **The basis of the algorithm for e-e collisions is “particle-mesh”.**
- **Statistics on the EEDs are collected according to spatial location.**
- **A collision target is randomly selected from the EED at that location and a random direction is assigned for the target’s velocity.**
- **The relative speed between the electron and its target electron is used to determine the probability for an e-e collision**

$$P_{ee} = n_e(\vec{r}) \cdot \sigma_{ee}(v) \cdot v \cdot \Delta t, \quad v = \left|\vec{v}_{e1} - \vec{v}_{e2}\right|$$

$$\sigma_{ee}(v) = 4\pi b_o^2 \left[1 + \ln\left(\frac{\lambda_D}{b_o}\right)\right], \quad b_o = \frac{q^2 / 4\pi\varepsilon_o}{\tfrac{1}{2} m_e v^2}$$

- **If a collision occurs, classical collision dynamics determine the change in momentum of the electron.**
- **The consequences of e-e collisions on the targets are obtained by continuously updating the stored EEDs.**

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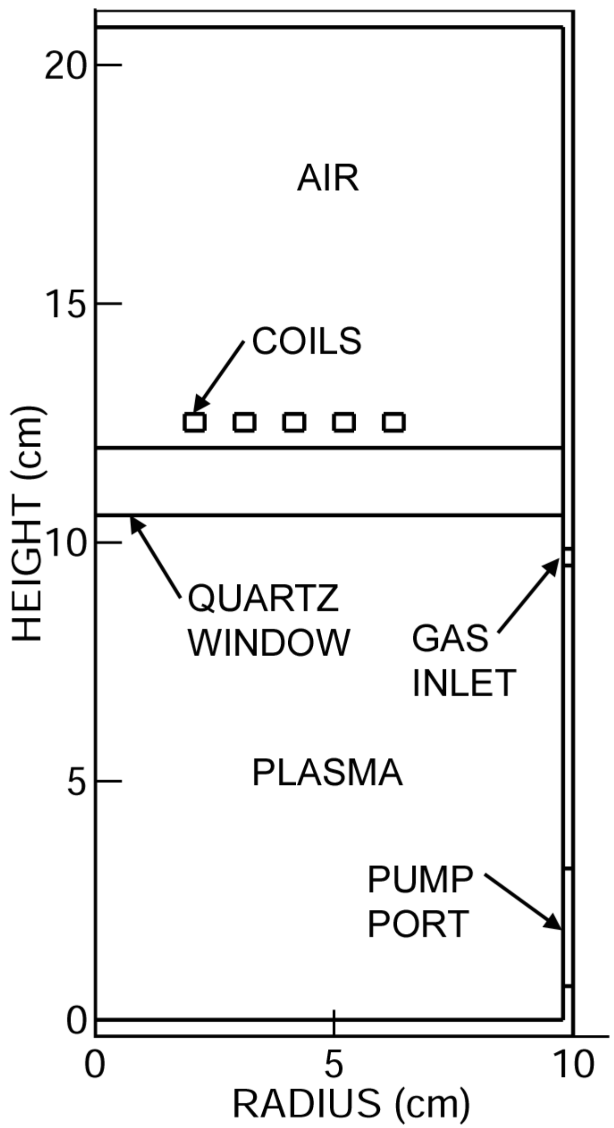
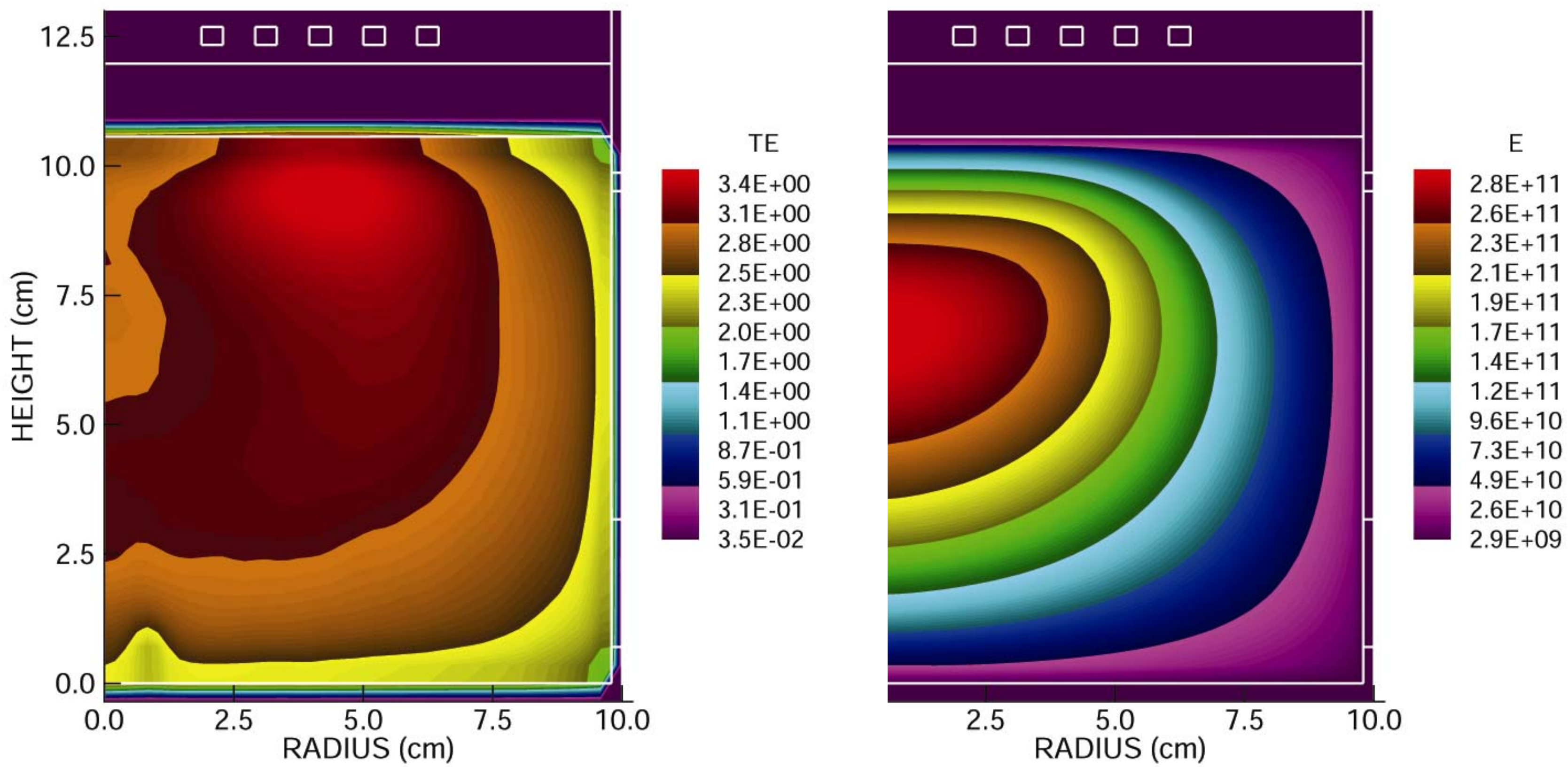
ICP CELL FOR INVESTIGATION



- **The experimental cell is an ICP reactor with a Faraday shield to minimize capacitive coupling.**

TYPICAL CONDITIONS: Ar, 10 mTorr, 200 W, 7 MHz



- **On axis peak in [e] occurs in spite of off-axis power deposition and off-axis peak in electron temperature.**

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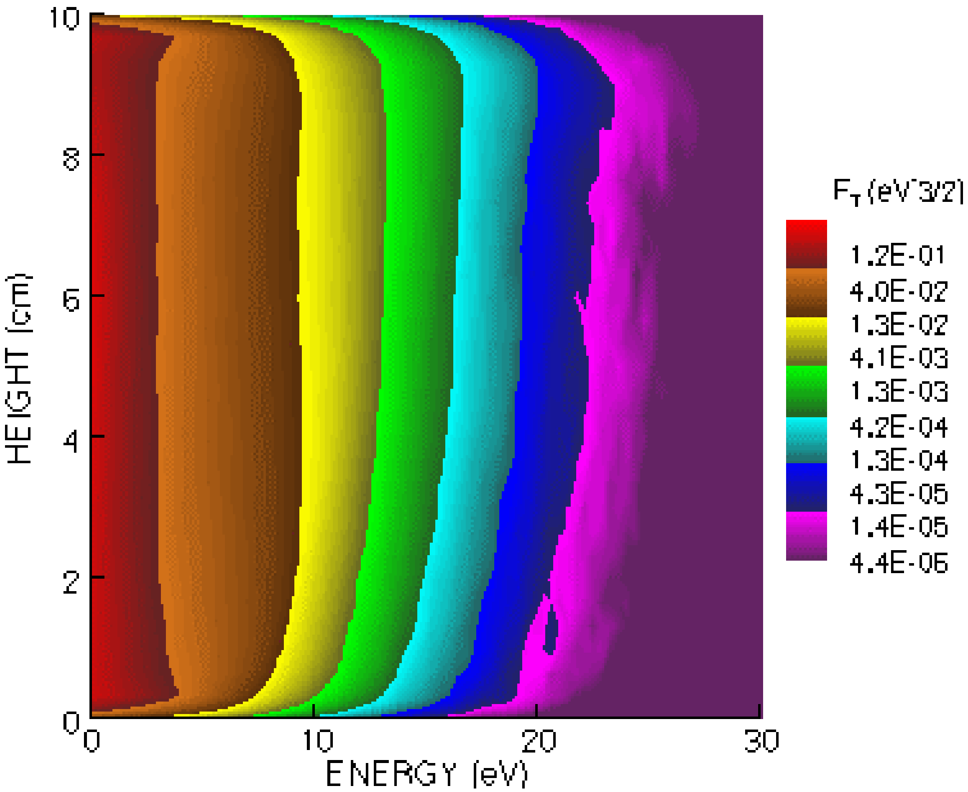
TIME DEPENDENCE OF THE EED

- **Time variation of the EED is mostly at higher energies where electrons are more collisional.**
- **Dynamics are dominantly in the electromagnetic skin depth where both collisional and non-linear Lorentz Forces) peak.**
- **The second harmonic dominates these dynamics.**



- **Ar, 10 mTorr, 100 W, 7 MHz, r = 4 cm**

ANIMATION SLIDE

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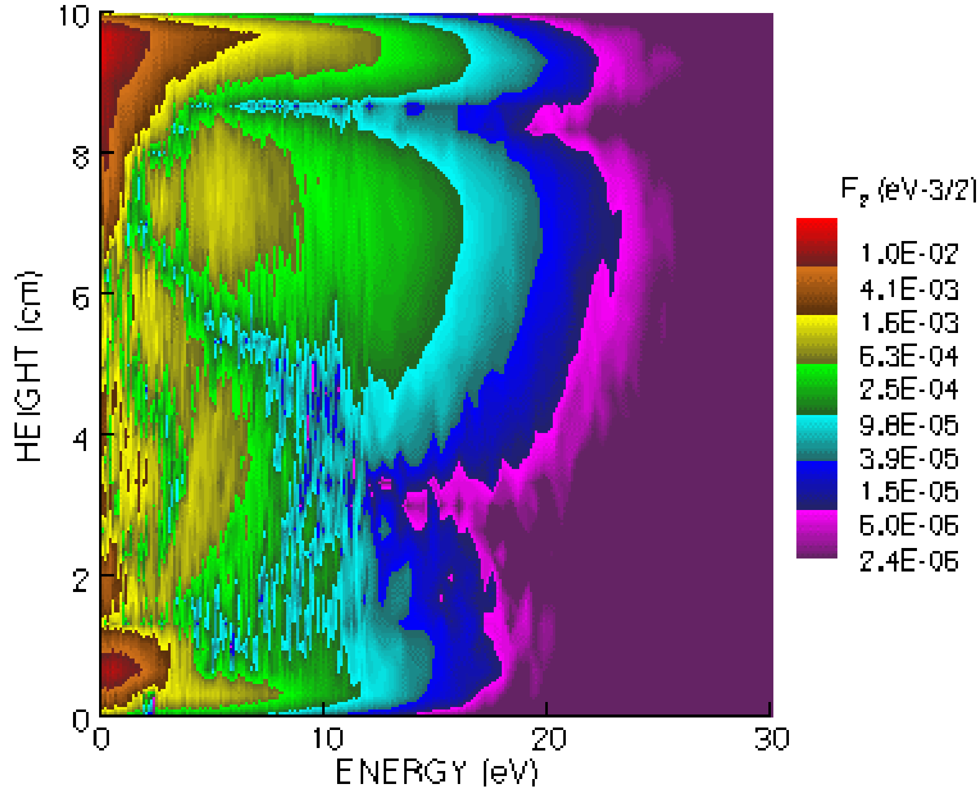
TIME DEPENDENCE OF THE EED: 2nd HARMONIC

- Electrons in skin depth quickly increase in energy and are "launched" into the bulk plasma.
- Undergoing collisions while traversing the reactor, they degrade in energy.
- Those surviving "climb" the opposite sheath, exchanging kinetic for potential energy.
- Several "pulses" are in transit simultaneously.



- Amplitude of 2nd Harmonic

ANIMATION SLIDE

- Ar, 10 mTorr, 100 W, 7 MHz, r = 4 cm

HARMONICS IN ICP

- To investigate harmonics an Ar/N_2 gas mixture was selected as having low and high threshold processes.

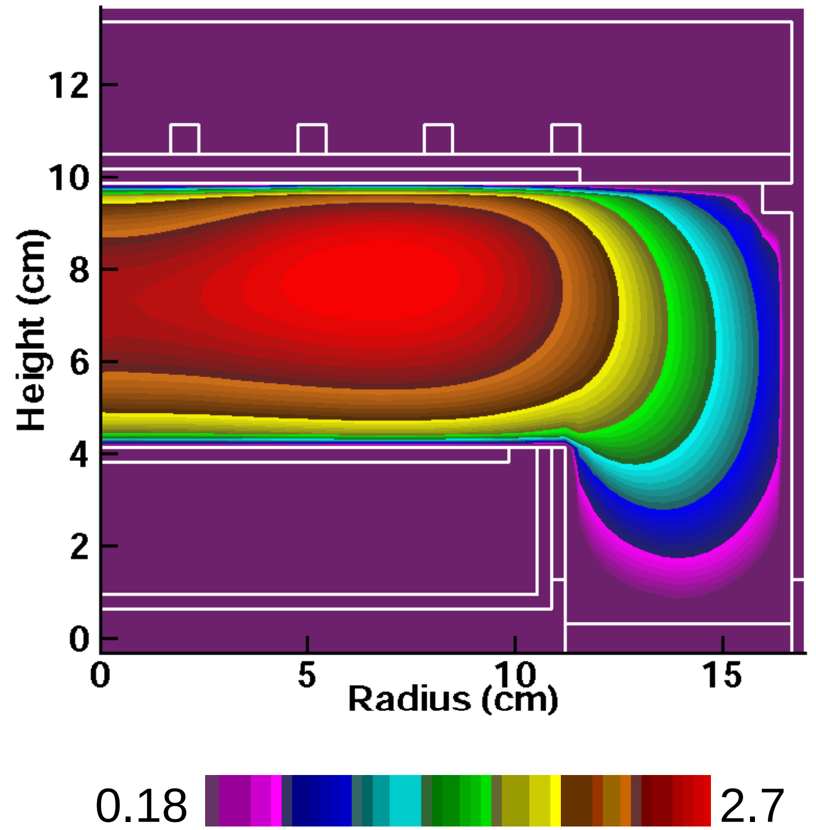
- $e^- + Ar \rightarrow Ar^+ + e^- + e^-$, $\Delta\varepsilon = 16$ eV

  High threshold reactions capture modulation in the tail of the EED.

- $e^- + N_2 \rightarrow N_2\,(vib) + e^-$, $\Delta\varepsilon = 0.29$ eV

  Low threshold reactions capture modulation of the bulk of the EED.

- Base case conditions:
  - Pressure: 5 mTorr
  - Frequency: 13.56 MHz
  - Ar / N_2: 90 / 10
  - Power : 650 W



Electron density (10^{11} cm^{-3})

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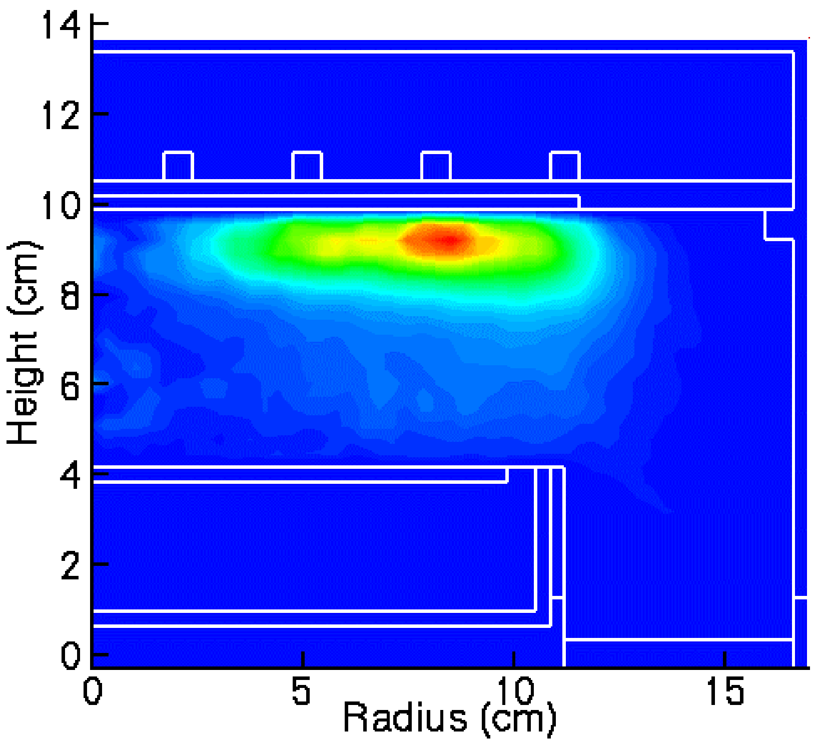
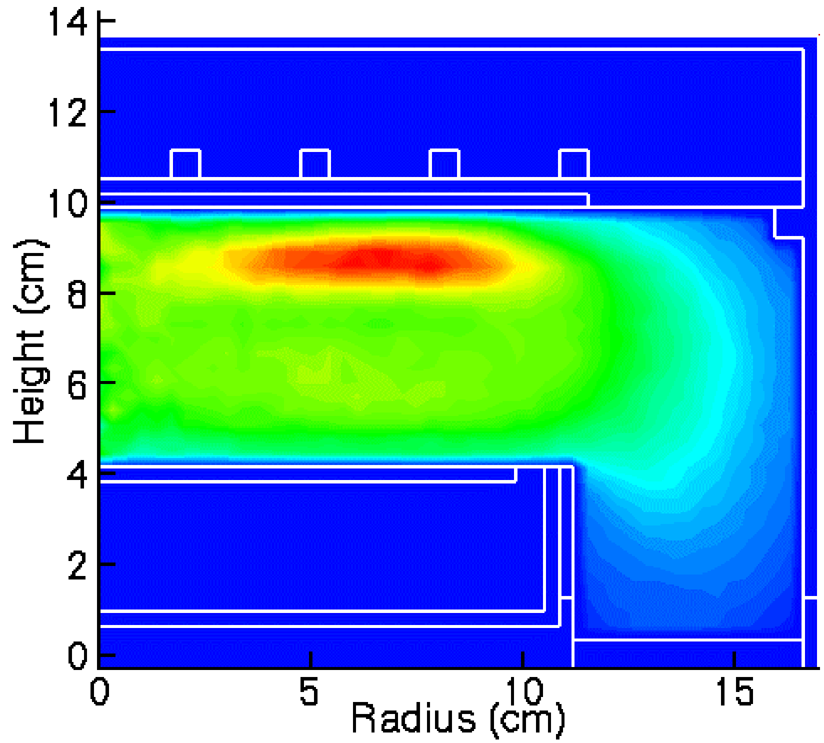
SOURCES FUNCTION vs TIME: THRESHOLD

- **Ionization of Ar has more modulation than vibrational excitation of N_2 due to modulation of the tail of the EED.**

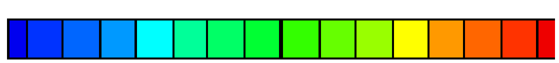


• Ionization of Ar
$6 \times 10^{14} - 3 \times 10^{16}$ $cm^{-3}s^{-1}$



• Excitation of $N_2(v)$
$1.4 \times 10^{14} - 8 \times 10^{15}$ $cm^{-3}s^{-1}$

ANIMATION SLIDE

MIN  **MAX**

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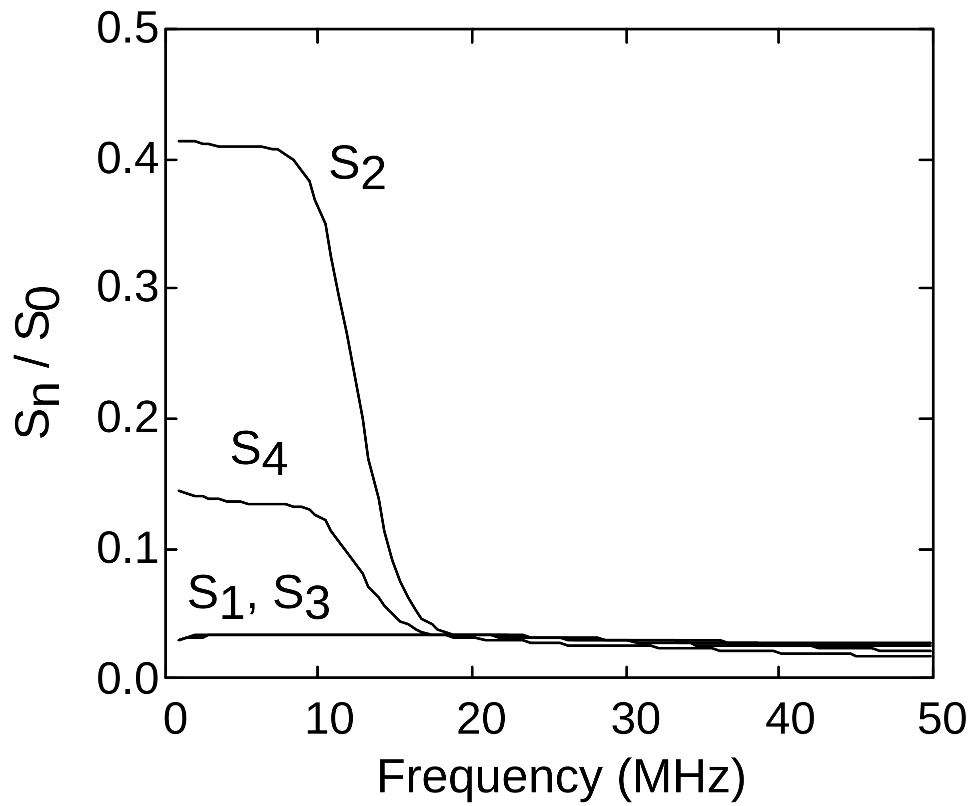
HARMONICS OF Ar IONIZATION: FREQUENCY

- **At large ω, both υ_m/ω and $1/(\upsilon_m\omega)$ are small, and so both collisional and NLF harmonics are small.**

- **At small ω, both υ_m/ω and $1/(\upsilon_m\omega)$ are large. Both collisional and NLF contribute to harmonics.**



- **Harmonic Amplitude/Time Average**

- **Ar/N_2=90/10, 5 mTorr**

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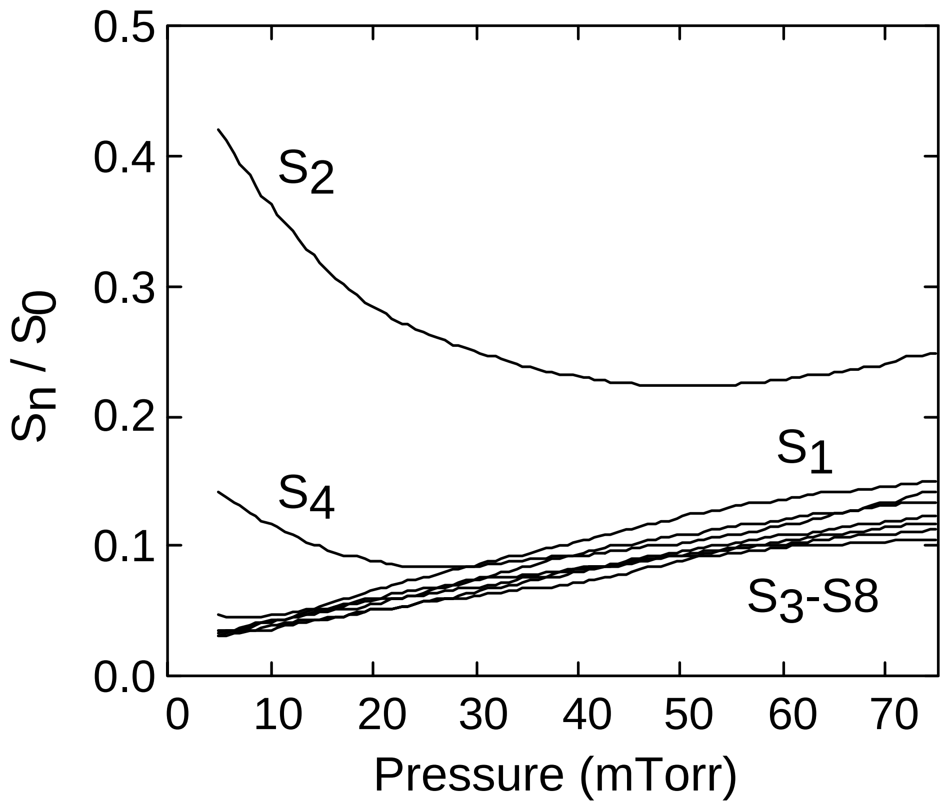
HARMONICS OF Ar IONIZATION: PRESSURE

- **At large P, υ_m/ω is large and $1/(\upsilon_m\omega)$ is small. Harmonics result from collisional (or linear) processes.**

- **At small P, υ_m/ω is small and $1/(\upsilon_m\omega)$ are large. Harmonics likely result from NLF.**



- **Harmonic Amplitude/Time Average**

- **Ar/N_2=90/10, 13.56 MHz**

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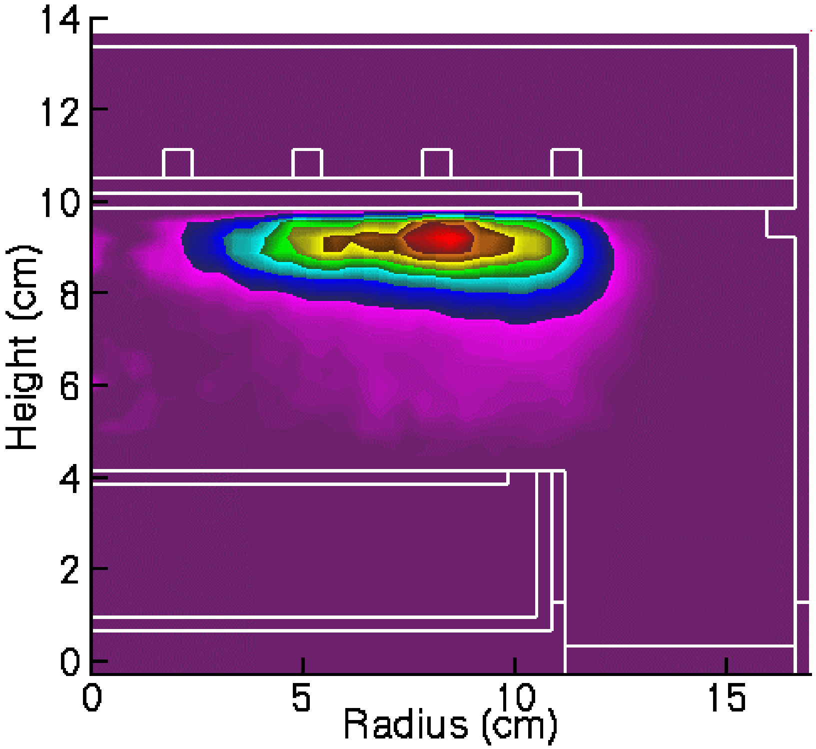
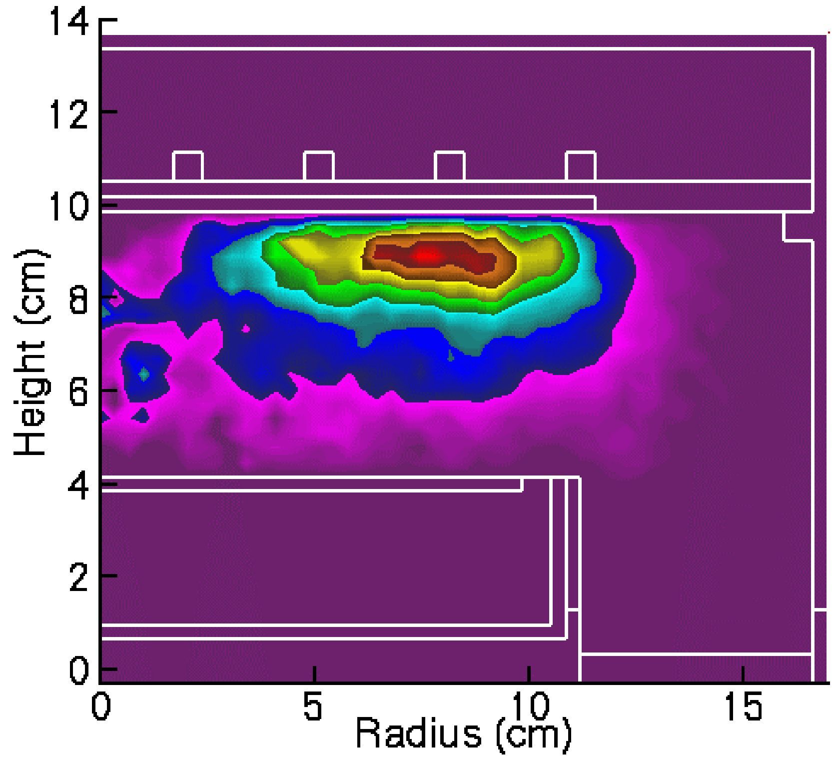
TIME DEPENDENCE OF Ar IONIZATION: PRESSURE

- Although B_{rf} may be nearly the same, at large P, v_θ and mean-free-paths are smaller, leading to lower harmonic amplitudes.



- **5 mTorr**

6×10^{14} – 3×10^{16} cm^{-3}s^{-1}



- **20 mTorr**

1.5×10^{14} – 1.7×10^{16} cm^{-3}s^{-1}

ANIMATION SLIDE

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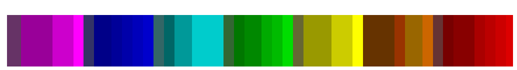
MIN  **MAX**

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