Modeling and Simulation of Plasma Based Applications in the Microwave and RF Frequency Range

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What is a plasma?

What is a plasma?

- Often referred to as “The fourth state of matter”
    - Solid – Liquid – Gas – Plasma
- Consists of:
    - Neutrals
    - Ions and electrons
- Can be created by:
    - Superheating a gas (thermal plasma)
    - Using EM fields to heat the charged particles (non-thermal plasma)

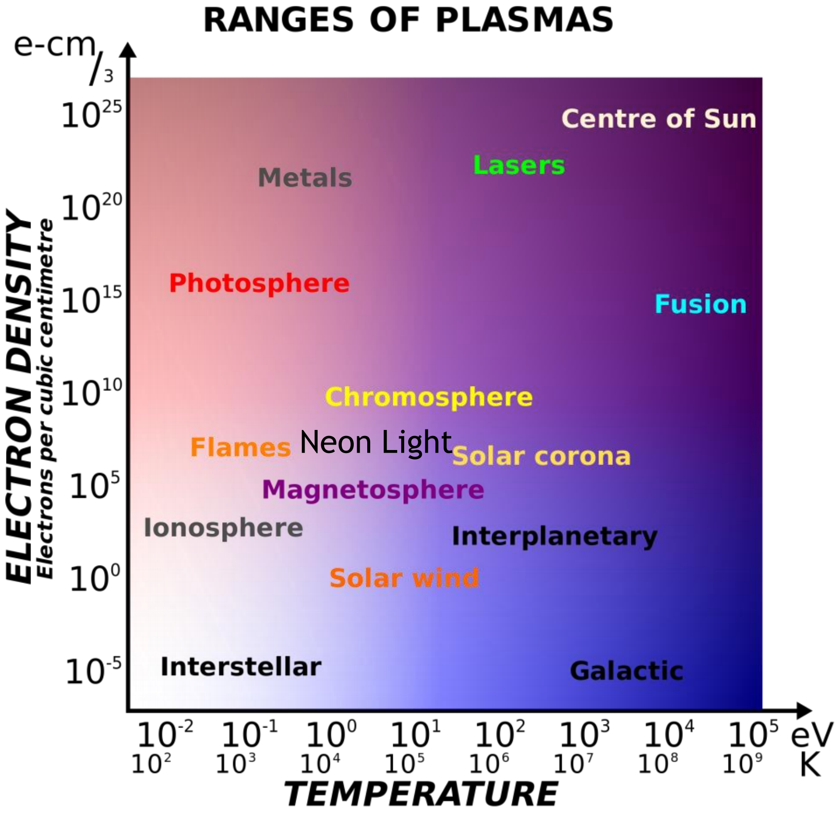
What is a plasma?

- Collective behavior
  - Due to long-range Coulomb forces

- Quasi-Neutral
  - Electrostatic forces will quickly expel any charge surplus

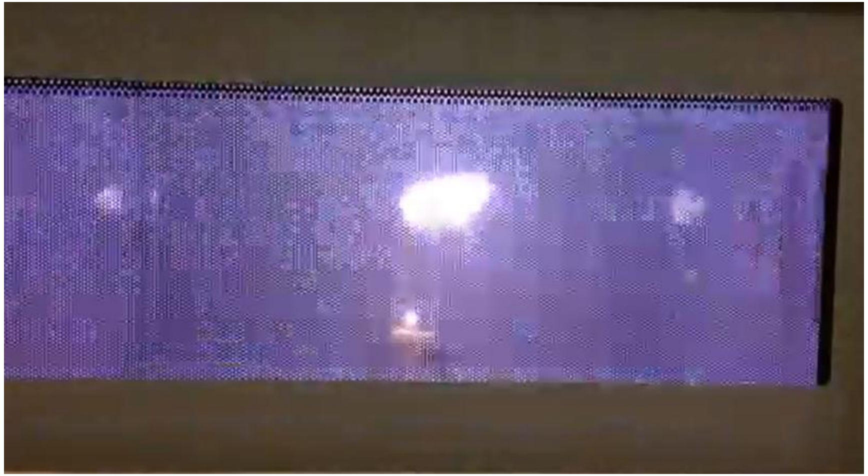
Plasma Outside of the Laboratory

"99.999% of the visible universe is plasma. We just happen to live in the remaining 0.001%"



What makes it so interesting?

Light Generation



- De-Excitation (Electron transitions, e.g. Rydberg/Lyman)
- Recombination

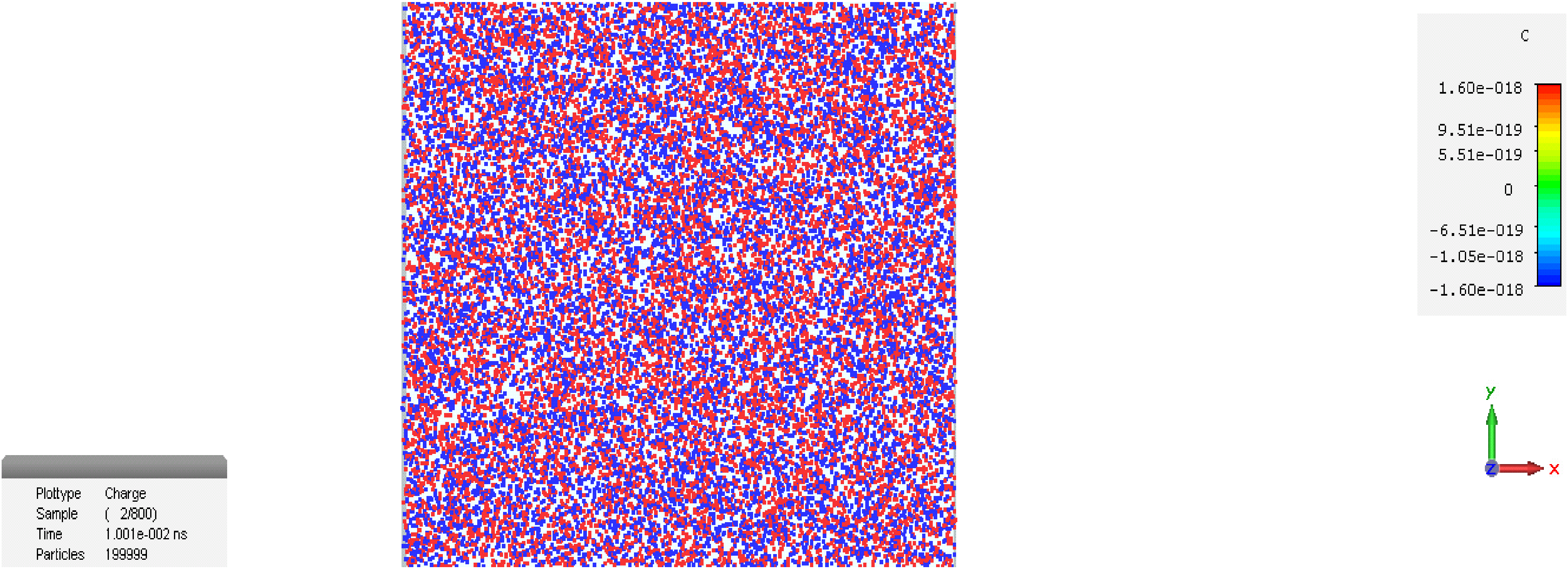
Plasma Frequency

- $\omega_{pe} = \sqrt{\frac{n_e e^2}{m_e \varepsilon_0}}$
- Waves below this frequency are reflected. Waves above this frequency can pass through the plasma
- Space vehicle re-entry

Plasma Sheath

- Sheath formation
  - Assume quasi-neutral plasma in touch with metal
  - More electrons than ions will hit wall due to mobility
  - Negative charge builds up on wall
  - Ions near wall will be accelerated towards wall
  - Result is a sheath of electron depletion between plasma bulk and metal wall

Plasma Sheath Formation



Plottype Charge
Sample (2/800)
Time 1.001e-002 ns
Particles 199999

Plasma Sheath: Applications

- Plasma etching

- Ion sources

Why simulate it?

Why Simulation?

- Difficult to access/reproduce
    - Space plasmas: Very low densities, large plasma dimensions
    - Solar plasmas: Extremely high densities and temperatures
- Difficult to measure
    - Probes are intrusive and can distort the plasma
    - (Relatively) short time scales

- Spectroscopy?
    - Often only integrated values, not spatially resolved
    - Windows in reactor are often undesirable

Why Simulation?

- Simulation yields
    - Spatially resolved results
    - Temporally resolved results
    - Without disturbing the plasma

- Reproducibility
    - Limitation: Monte-Carlo, degenerated systems

Basic Physics behind Simulation

- Maxwell's equation for EM fields

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

- Particle movement according to Newton

$$\vec{F} = m\vec{a}$$

Basic Physics behind Simulation

- Collisions:
  - Elastic collisions
  - Inelastic collisions
    - Ionization/Recombination
    - Excitation/De-Excitation
    - Disassociation
    - Molecular chemistry
    - …

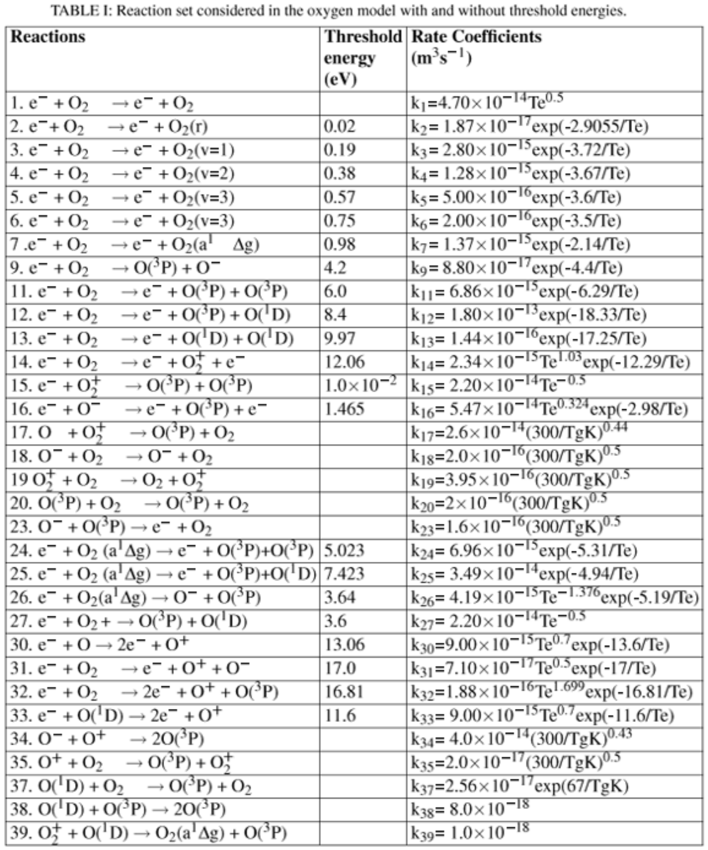


TABLE I: Reaction set considered in the oxygen model with and without threshold energies.

Reactions	**Threshold energy (eV)**	**Rate Coefficients (m^3s^{-1})**
1. $e^- + O_2 \rightarrow e^- + O_2$		$k_1 = 4.70 \times 10^{-14} Te^{0.5}$
2. $e^- + O_2 \rightarrow e^- + O_2(r)$	0.02	$k_2 = 1.87 \times 10^{-17} \exp(-2.9055/Te)$
3. $e^- + O_2 \rightarrow e^- + O_2(v=1)$	0.19	$k_3 = 2.80 \times 10^{-15} \exp(-3.72/Te)$
4. $e^- + O_2 \rightarrow e^- + O_2(v=2)$	0.38	$k_4 = 1.28 \times 10^{-15} \exp(-3.67/Te)$
5. $e^- + O_2 \rightarrow e^- + O_2(v=3)$	0.57	$k_5 = 5.00 \times 10^{-16} \exp(-3.6/Te)$
6. $e^- + O_2 \rightarrow e^- + O_2(v=3)$	0.75	$k_6 = 2.00 \times 10^{-16} \exp(-3.5/Te)$
7 .$e^- + O_2 \rightarrow e^- + O_2(a^1 \Delta g)$	0.98	$k_7 = 1.37 \times 10^{-15} \exp(-2.14/Te)$
9. $e^- + O_2 \rightarrow O(^3P) + O^-$	4.2	$k_9 = 8.80 \times 10^{-17} \exp(-4.4/Te)$
11. $e^- + O_2 \rightarrow e^- + O(^3P) + O(^3P)$	6.0	$k_{11} = 6.86 \times 10^{-15} \exp(-6.29/Te)$
12. $e^- + O_2 \rightarrow e^- + O(^3P) + O(^1D)$	8.4	$k_{12} = 1.80 \times 10^{-13} \exp(-18.33/Te)$
13. $e^- + O_2 \rightarrow e^- + O(^1D) + O(^1D)$	9.97	$k_{13} = 1.44 \times 10^{-16} \exp(-17.25/Te)$
14. $e^- + O_2 \rightarrow e^- + O_2^+ + e^-$	12.06	$k_{14} = 2.34 \times 10^{-15} Te^{1.03} \exp(-12.29/Te)$
15. $e^- + O_2^+ \rightarrow O(^3P) + O(^3P)$	1.0×10^{-2}	$k_{15} = 2.20 \times 10^{-14} Te^{-0.5}$
16. $e^- + O^- \rightarrow e^- + O(^3P) + e^-$	1.465	$k_{16} = 5.47 \times 10^{-14} Te^{0.324} \exp(-2.98/Te)$
17. $O + O_2^+ \rightarrow O(^3P) + O_2$		$k_{17} = 2.6 \times 10^{-14} (300/TgK)^{0.44}$
18. $O^- + O_2 \rightarrow O^- + O_2$		$k_{18} = 2.0 \times 10^{-16} (300/TgK)^{0.5}$
19 $O_2^+ + O_2 \rightarrow O_2 + O_2^+$		$k_{19} = 3.95 \times 10^{-16} (300/TgK)^{0.5}$
20. $O(^3P) + O_2 \rightarrow O(^3P) + O_2$		$k_{20} = 2 \times 10^{-16} (300/TgK)^{0.5}$
23. $O^- + O(^3P) \rightarrow e^- + O_2$		$k_{23} = 1.6 \times 10^{-16} (300/TgK)^{0.5}$
24. $e^- + O_2 (a^1\Delta g) \rightarrow e^- + O(^3P) + O(^3P)$	5.023	$k_{24} = 6.96 \times 10^{-15} \exp(-5.31/Te)$
25. $e^- + O_2 (a^1\Delta g) \rightarrow e^- + O(^3P) + O(^1D)$	7.423	$k_{25} = 3.49 \times 10^{-14} \exp(-4.94/Te)$
26. $e^- + O_2(a^1\Delta g) \rightarrow O^- + O(^3P)$	3.64	$k_{26} = 4.19 \times 10^{-15} Te^{-1.376} \exp(-5.19/Te)$
27. $e^- + O_2 + \rightarrow O(^3P) + O(^1D)$	3.6	$k_{27} = 2.20 \times 10^{-14} Te^{-0.5}$
30. $e^- + O \rightarrow 2e^- + O^+$	13.06	$k_{30} = 9.00 \times 10^{-15} Te^{0.7} \exp(-13.6/Te)$
31. $e^- + O_2 \rightarrow e^- + O^+ + O^-$	17.0	$k_{31} = 7.10 \times 10^{-17} Te^{0.5} \exp(-17/Te)$
32. $e^- + O_2 \rightarrow 2e^- + O^+ + O(^3P)$	16.81	$k_{32} = 1.88 \times 10^{-16} Te^{1.699} \exp(-16.81/Te)$
33. $e^- + O(^1D) \rightarrow 2e^- + O^+$	11.6	$k_{33} = 9.00 \times 10^{-15} Te^{0.7} \exp(-11.6/Te)$
34. $O^- + O^+ \rightarrow 2O(^3P)$		$k_{34} = 4.0 \times 10^{-14} (300/TgK)^{0.43}$
35. $O^+ + O_2 \rightarrow O(^3P) + O_2^+$		$k_{35} = 2.0 \times 10^{-17} (300/TgK)^{0.5}$
37. $O(^1D) + O_2 \rightarrow O(^3P) + O_2$		$k_{37} = 2.56 \times 10^{-17} \exp(67/TgK)$
38. $O(^1D) + O(^3P) \rightarrow 2O(^3P)$		$k_{38} = 8.0 \times 10^{-18}$
39. $O_2^+ + O(^1D) \rightarrow O_2(a^1\Delta g) + O(^3P)$		$k_{39} = 1.0 \times 10^{-18}$

G. Roberson et al., *Global model simulations of low-pressure oxygen discharges*, Braz. J. Phys. vol.37, http://dx.doi.org/10.1590/S0103-97332007000300019

Kinetic Models

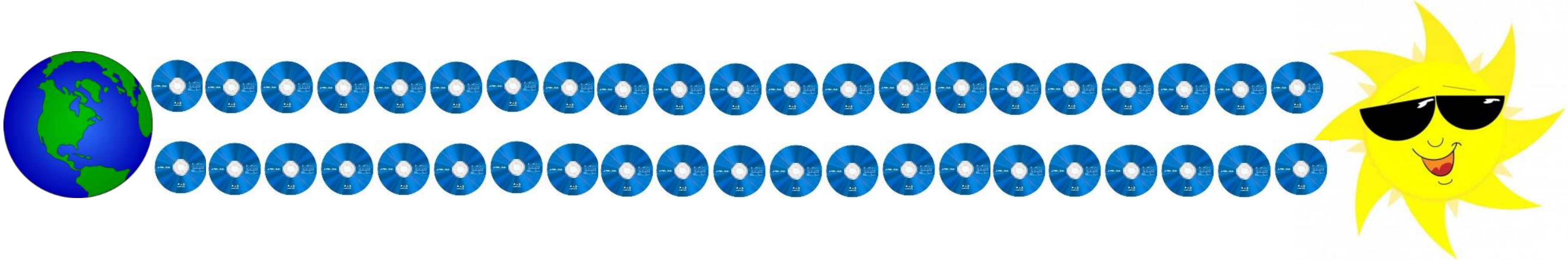
Approach 1: Kinetic Modeling

- Full Physics (Maxwell + Newton + collisions)
- All results of interest can be extracted
- Applicable to all plasmas
- Three options:
  - Direct: N particles with all states, external forces
  - Particle distribution functions: Solving the Boltzmann equation
  - Particle-In-Cell (PIC)

Explicit Modeling of Particles

- Maxwell + Newton + collisions for each particle

- Problem:
  - 1 mol of gas at 1 point in time, 6 unknowns per particle
  - About 13.4 YB (=1.34E13 TB)



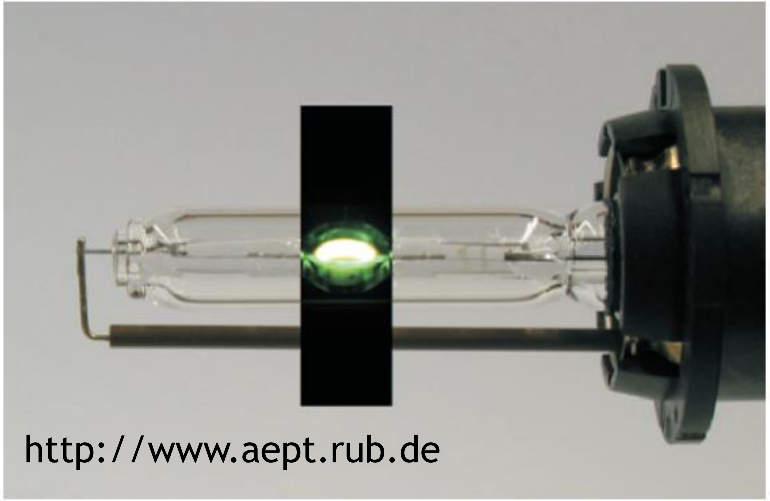
Solving the Boltzmann Equation

- Instead of considering every particle as an individual, define a distribution function f(**x**, **v**, t) for each species
- The Boltzmann equation describes how the distribution function evolves over time:

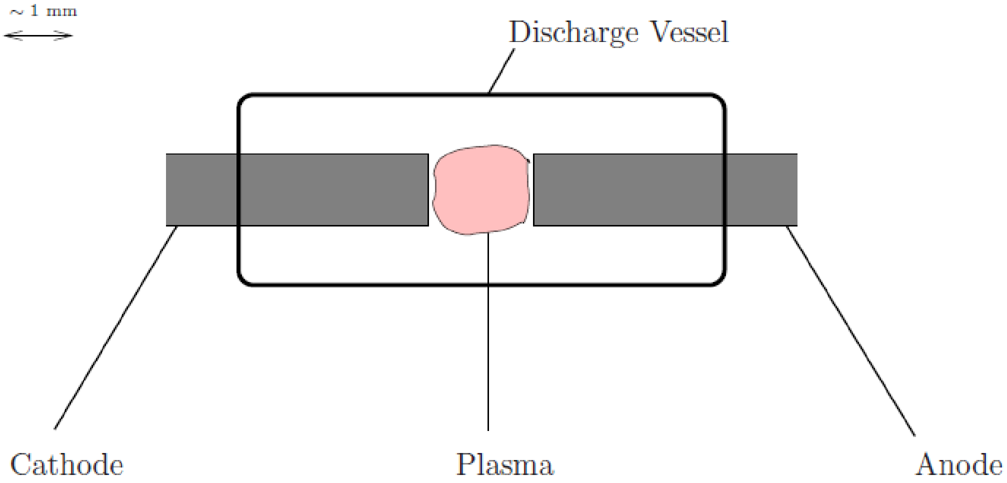
$$\frac{\mathrm{d}f(\vec{x},\vec{v},t)}{\mathrm{d}t} = f_c$$

Simple enough – or is it? Let’s apply it to a simple case!

The Near-Cathode Region in HIDs

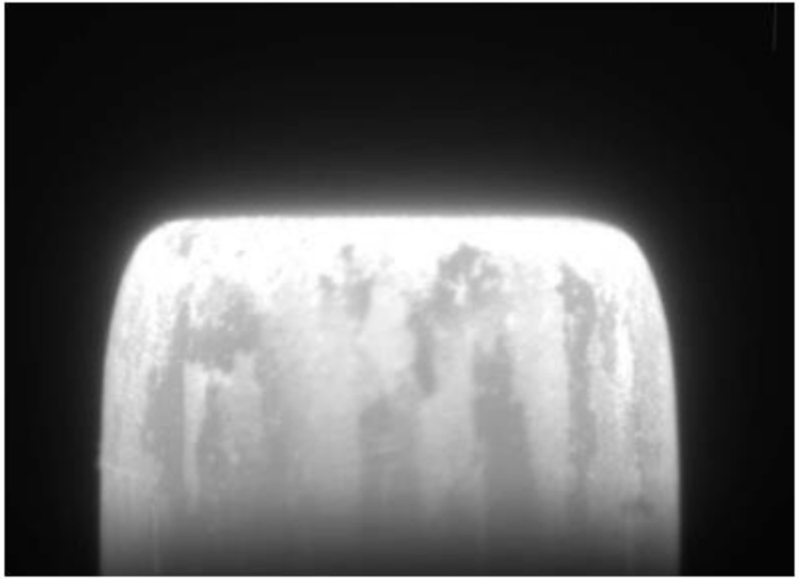

http://www.aept.rub.de

D-Lamp for automotive headlights

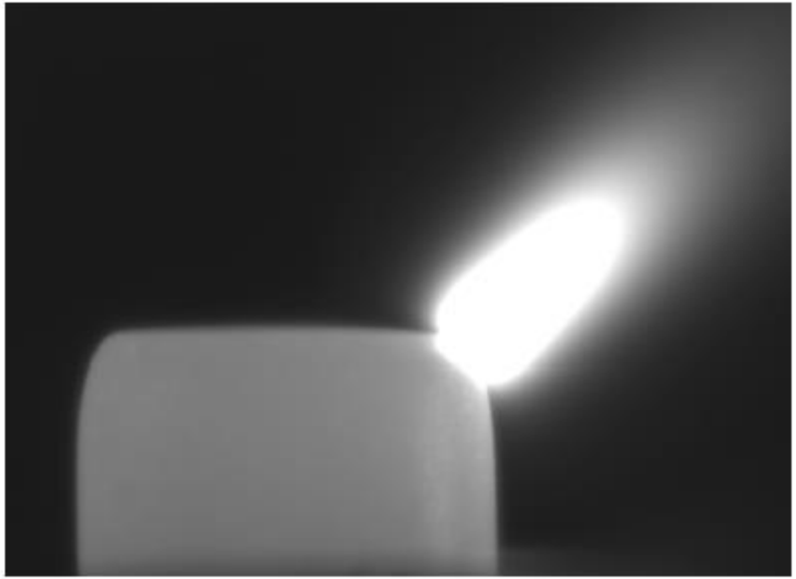


Different Spot Attachments

Diffuse Mode

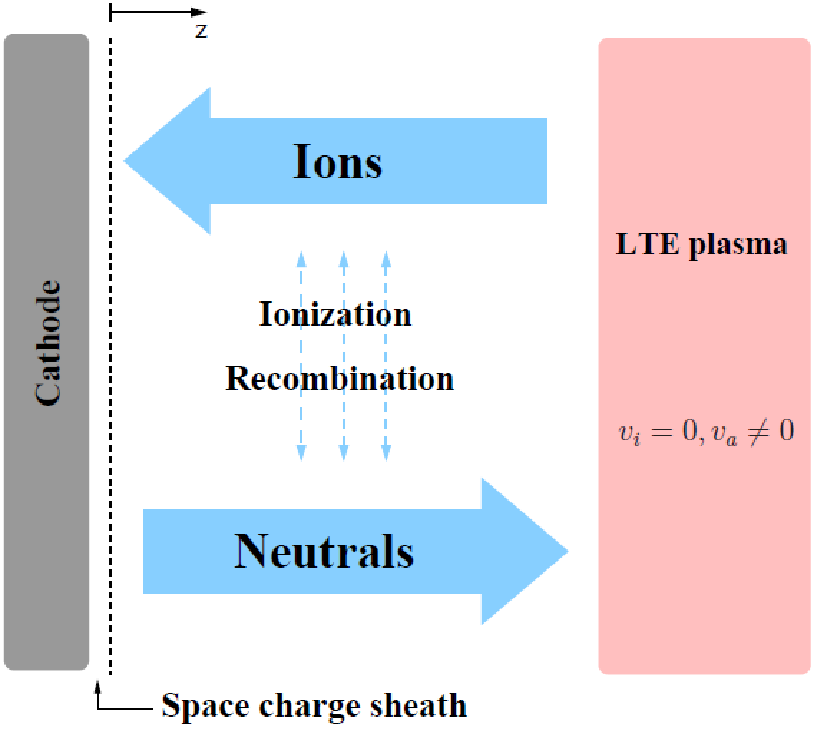


Spot Mode



S. Lichtenberg et al., J. Phys. D: Appl. Phys. **35** (2002) 1648–1656

Solving the Boltzmann Equation



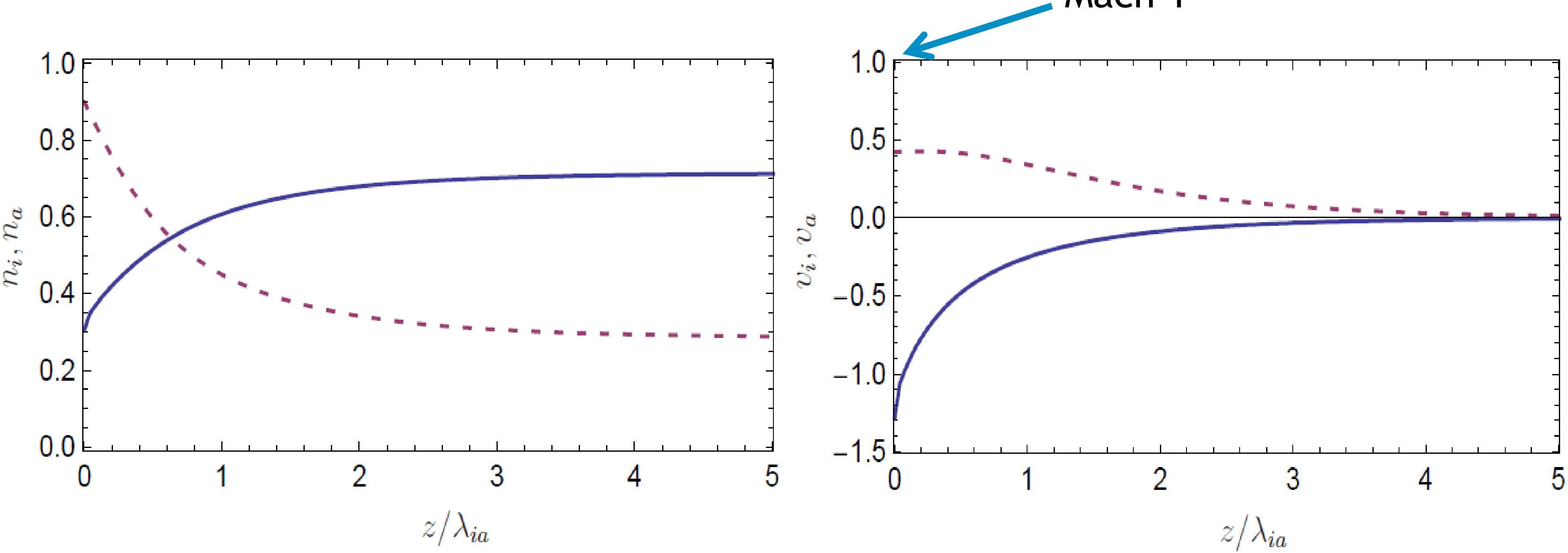
$$
\begin{aligned}
& v_\parallel \frac{\partial f_i}{\partial z} - \frac{\beta}{n_i}\frac{\mathrm{d}n_i}{\mathrm{d}z}\frac{\partial f_i}{\partial v_\parallel} \\
& = n_i f_a - \gamma(1+\gamma)n_i^2 f_i + \tilde{\nu}_1\left(3f_i + \boldsymbol{v}\cdot\nabla_{\boldsymbol{v}} f_i + \nabla_{\boldsymbol{v}}^2 f_i\right) \\
& \quad + \int_{\Omega'}\int_{\Omega}\int_{g'} g'^3 \Bigg[\alpha_{ii}\left(f_i\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}+\frac{g'\boldsymbol{e}'}{2}\right) f_i\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}-\frac{g'\boldsymbol{e}'}{2}\right) - f_i(\boldsymbol{v})f_i(\boldsymbol{v}-g'\boldsymbol{e}')\right) \\
& \qquad + \alpha_{ia}\left(f_i\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}+\frac{g'\boldsymbol{e}'}{2}\right) f_a\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}-\frac{g'\boldsymbol{e}'}{2}\right) - f_i(\boldsymbol{v})f_a(\boldsymbol{v}-g'\boldsymbol{e}')\right)\Bigg] \\
& \qquad \times \mathrm{d}g'\mathrm{d}\Omega\mathrm{d}\Omega'
\end{aligned}
\tag{4.50}
$$

$$\frac{\mathrm{d}f(\vec{x},\vec{v},t)}{\mathrm{d}t} = f_c$$

$$
\begin{aligned}
& v_\parallel \frac{\partial f_a}{\partial z} \\
& = -n_i f_a + \gamma(1+\gamma)n_i^2 f_i + \tilde{\nu}_1\left(3f_a + \boldsymbol{v}\cdot\nabla_{\boldsymbol{v}} f_a + \nabla_{\boldsymbol{v}}^2 f_a\right) \\
& \quad + \int_{\Omega'}\int_{\Omega}\int_{g'} g'^3 \Bigg[\alpha_{aa}\left(f_a\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}+\frac{g'\boldsymbol{e}'}{2}\right) f_a\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}-\frac{g'\boldsymbol{e}'}{2}\right) - f_a(\boldsymbol{v})f_a(\boldsymbol{v}-g'\boldsymbol{e}')\right) \\
& \qquad + \alpha_{ai}\left(f_a\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}+\frac{g'\boldsymbol{e}'}{2}\right) f_i\left(\boldsymbol{v}-\frac{g'\boldsymbol{e}}{2}-\frac{g'\boldsymbol{e}'}{2}\right) - f_a(\boldsymbol{v})f_i(\boldsymbol{v}-g'\boldsymbol{e}')\right)\Bigg] \\
& \qquad \times \mathrm{d}g'\mathrm{d}\Omega\mathrm{d}\Omega'
\end{aligned}
\tag{4.51}
$$

F H Scharf, *Fluid Dynamic and Kinetic Modeling of the Near-Cathode Region in Thermal Plasmas*, Logos 2009

Solve for Density and Velocity

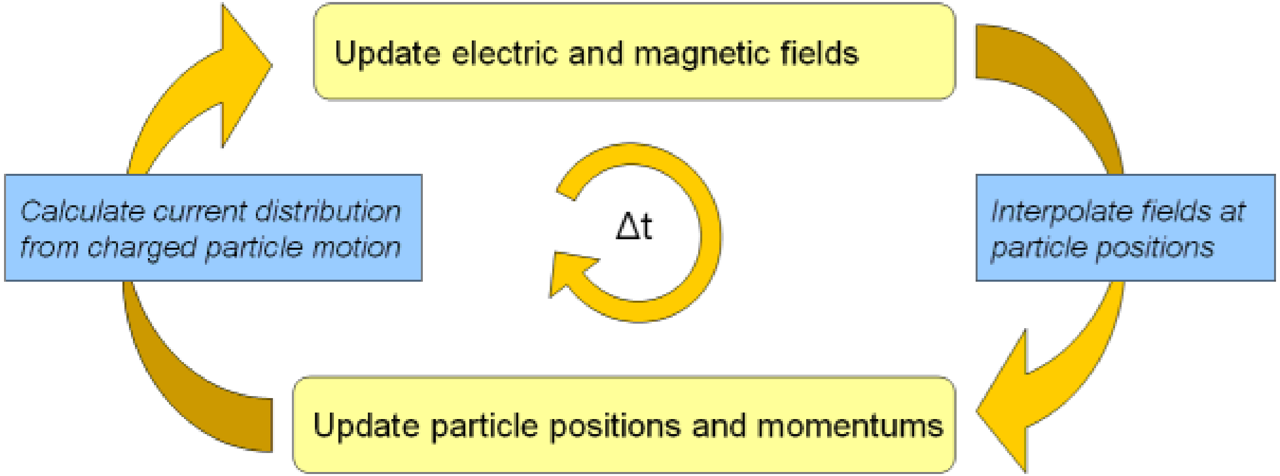


Solid: Ions

Dashed: Neutral particles

Particle-In-Cell

- Use a computer to create an ensemble of particles



Update electric and magnetic fields

Calculate current distribution from charged particle motion

Δt

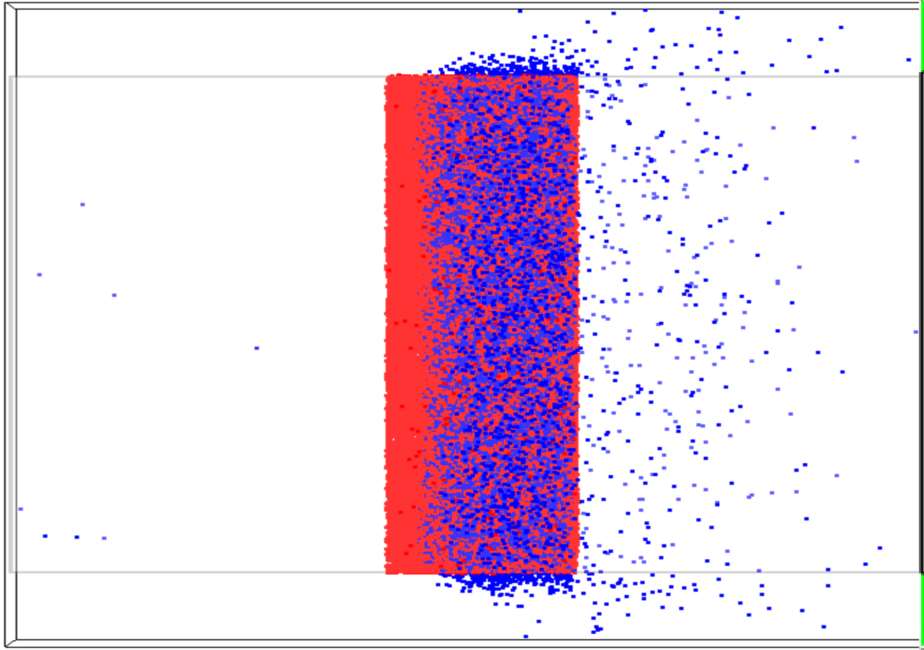
Interpolate fields at particle positions

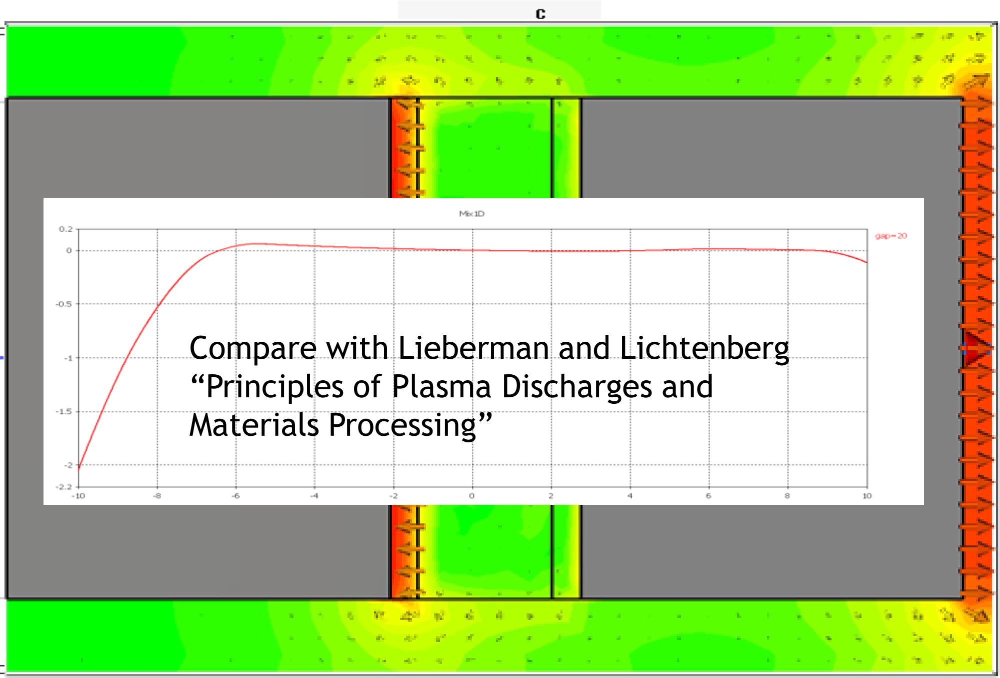
Update particle positions and momentums

- If the number of particles in the ensemble is large enough, the behavior or the ensemble will approach the real behavior
- Collisions are typically considered stochastically (PIC-MC)

RF Sheath of Argon Plasma

- 350,000 macro particles (ratio 10:1)

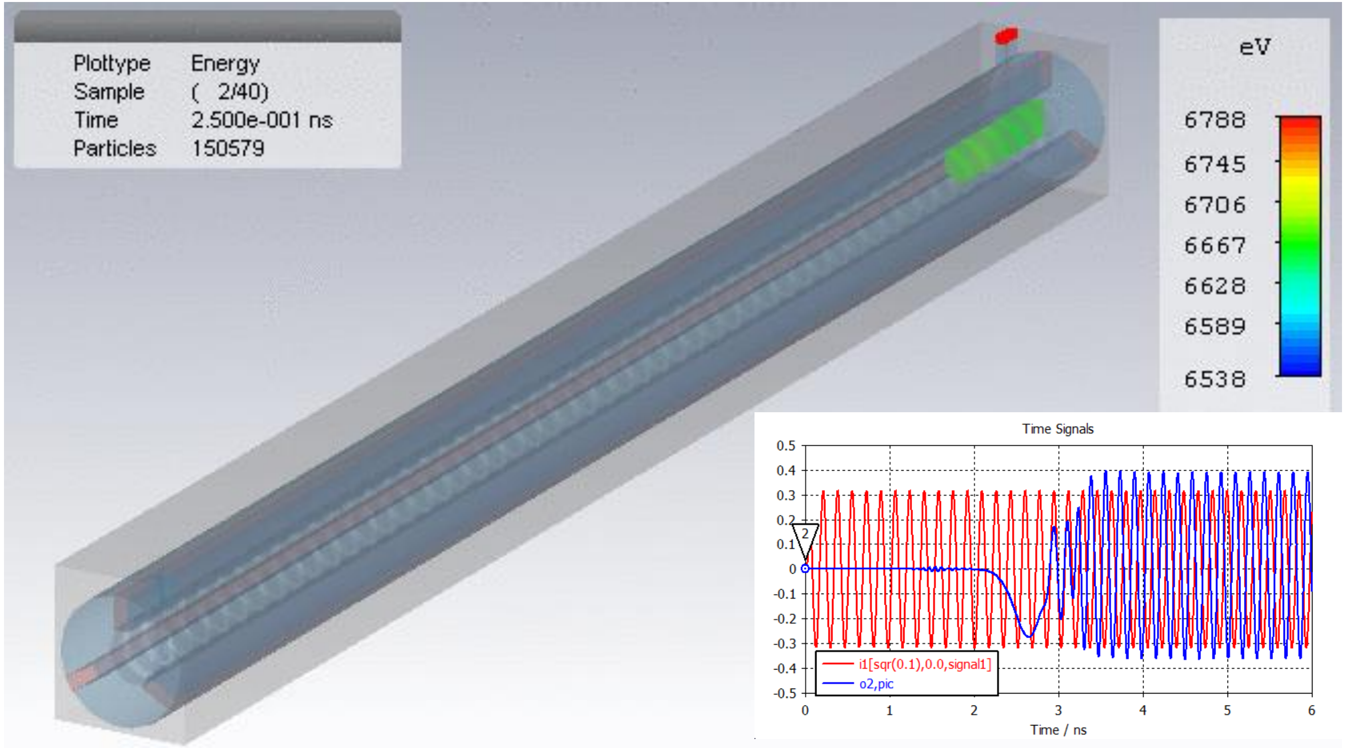




Compare with Lieberman and Lichtenberg “Principles of Plasma Discharges and Materials Processing”

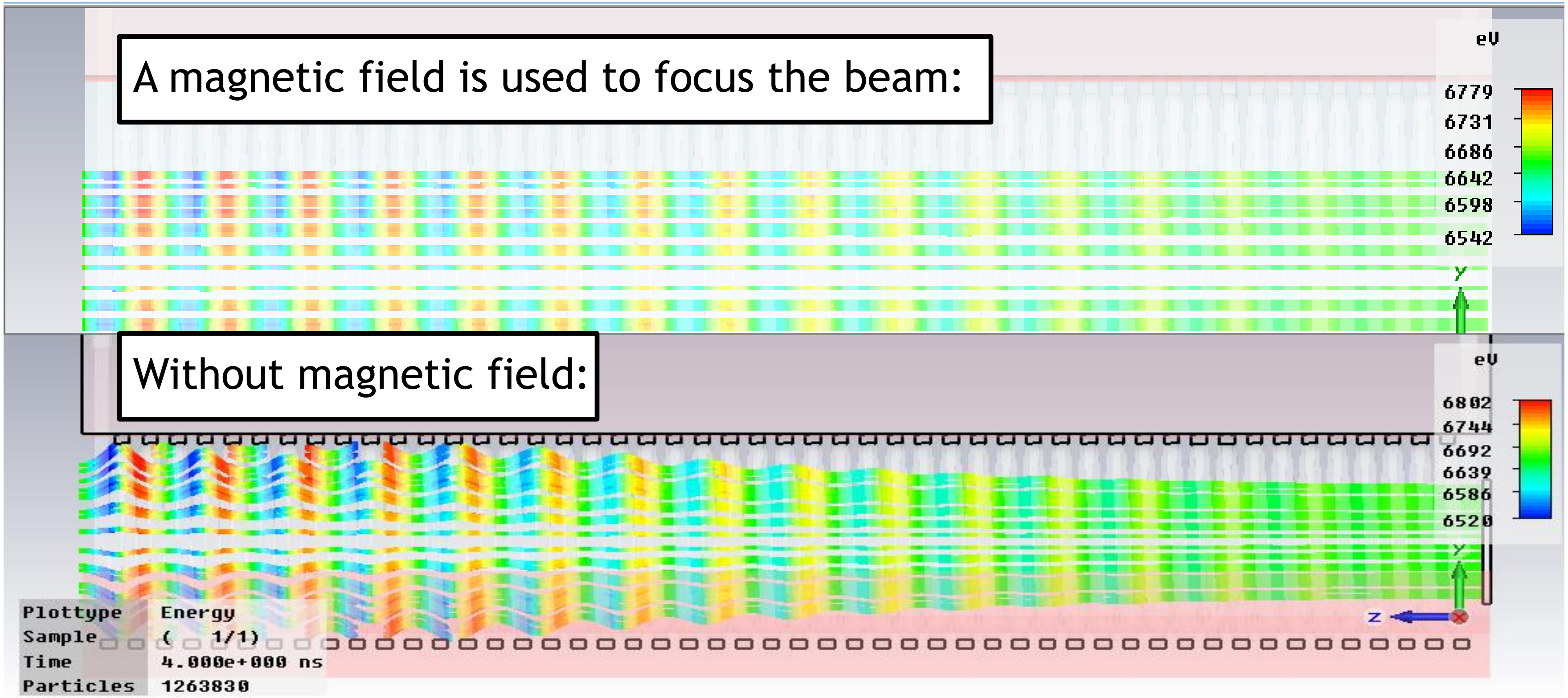
Traveling Wave Tube (TWT)

Traveling Wave Tube (TWT) devices can be used as amplifiers:



Plottype Energy
Sample (2/40)
Time 2.500e-001 ns
Particles 150579

Traveling Wave Tube (TWT)



A magnetic field is used to focus the beam:

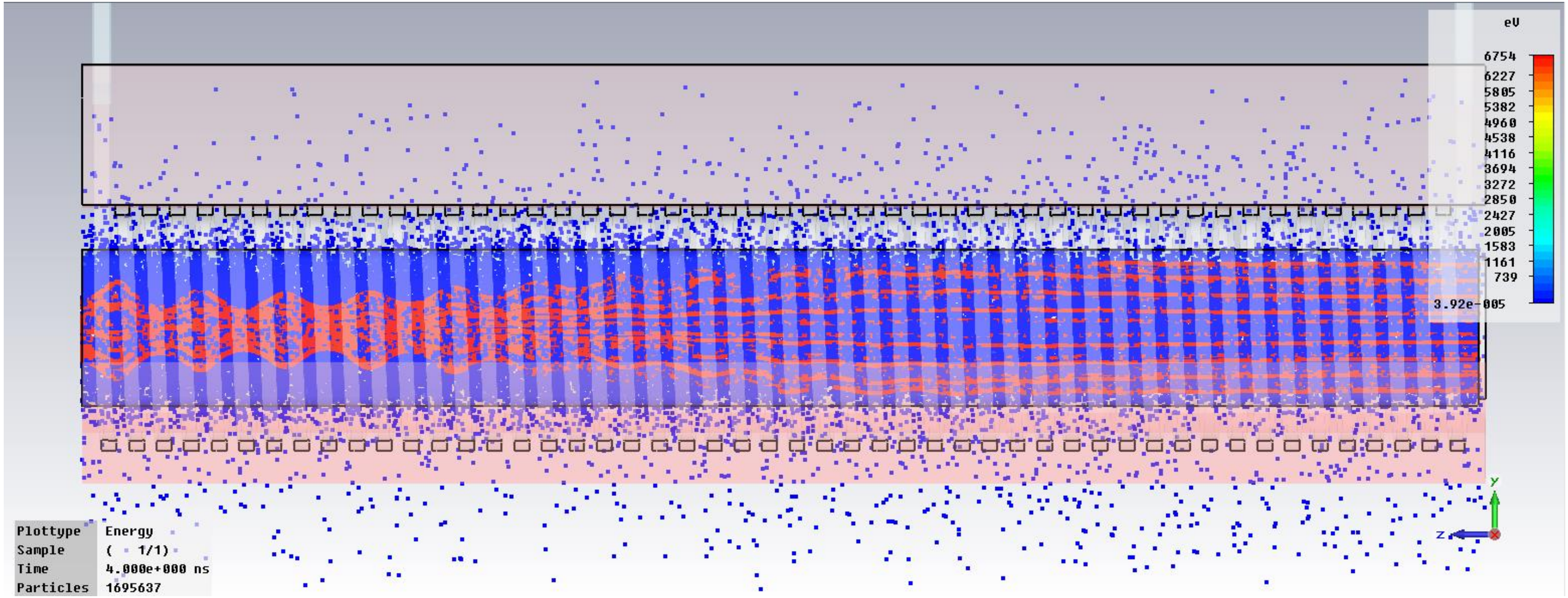
Without magnetic field:

Plottype Energy
Sample (1/1)
Time 4.000e+000 ns
Particles 1263830

Magnets/coils can be heavy, can we do this without magnetic field?

Example: Pasotron

- A plasma can be used to focus the electron beam:



Plottype Energy
Sample (1/1)
Time 4.000e+000 ns
Particles 1695637

Red: High energy electrons in beam Blue: Low energy electrons in plasma

Fluid Dynamic Models

Approach 2: Fluid dynamic model

- Each species is treated as a fluid
  - Implies strong interaction between particles of same kind

- Magneto Hydro Dynamics (MHD):
  Maxwell’s equations + Navier-Stokes

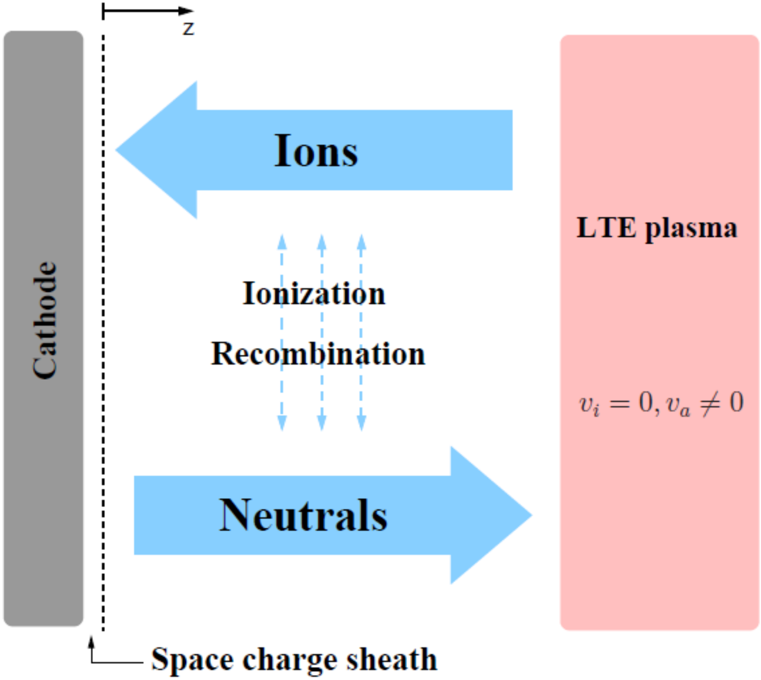
- Collisions treated by collision coefficients

Approach 2: Fluid dynamic model

- Good for high densities
- Breaks down for low densities, particularly in the sheath region
- Knudsen number: $\mathrm{Kn} = \lambda / L$
- Fluid approximation is good if Kn << 1

- Surprisingly robust, due to conservation of mass, momentum, energy

Solving the Fluid Dynamic Equations



z

Cathode

Ions

Ionization

Recombination

Neutrals

LTE plasma

$v_i = 0, v_a \neq 0$

Space charge sheath

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}z}(n_i v_i) &= k_i n_i n_a - k_r n_i^3 \\
\frac{\mathrm{d}}{\mathrm{d}z}(n_a v_a) &= -k_i n_i n_a + k_r n_i^3 \\
\frac{\mathrm{d}}{\mathrm{d}z}(n_i m_i v_i^2) &= -(T_h + T_e)\frac{\mathrm{d}n_i}{\mathrm{d}z} - n_i n_a k_{cx} m_i (v_i - v_a) + k_i n_i n_a m_i v_a - k_r n_i^3 m_i v_i \\
\frac{\mathrm{d}}{\mathrm{d}z}(n_a m_i v_a^2) &= -T_h \frac{\mathrm{d}n_a}{\mathrm{d}z} + n_i n_a k_{cx} m_i (v_i - v_a) - k_i n_i n_a m_i v_a + k_r n_i^3 m_i v_i
\end{aligned}
$$

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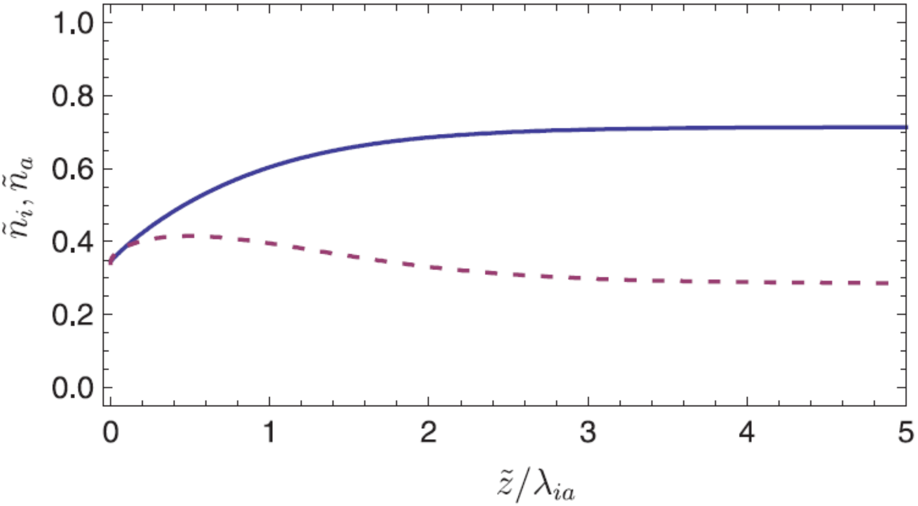
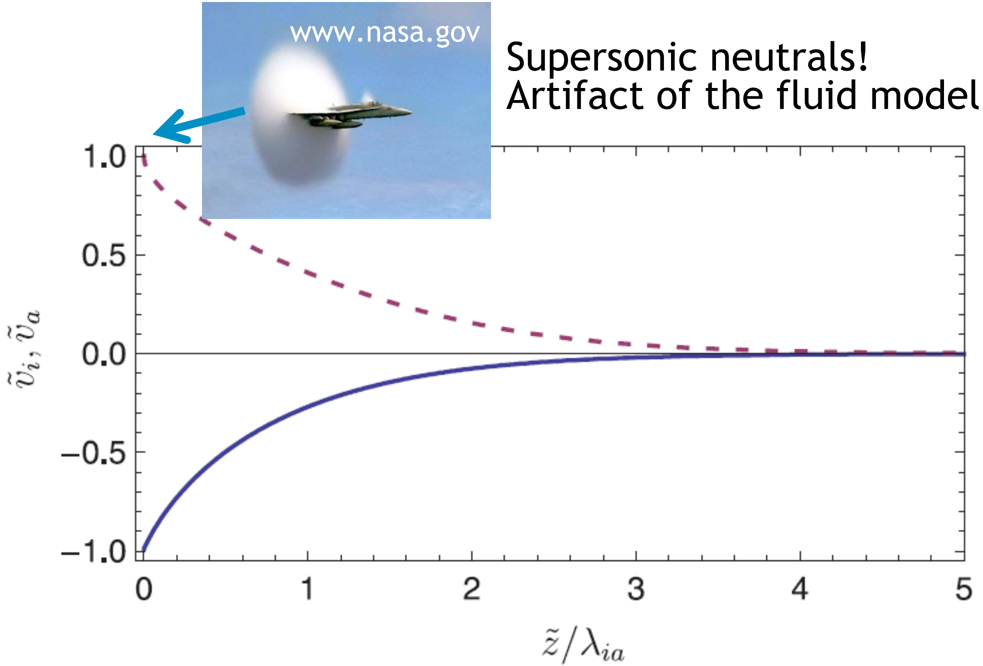
[2] F H Scharf and R P Brinkmann, *J. Phys. D: Appl. Phys.* **41** (2008) 185206

Solve for Density and Velocity





Supersonic neutrals!
Artifact of the fluid model

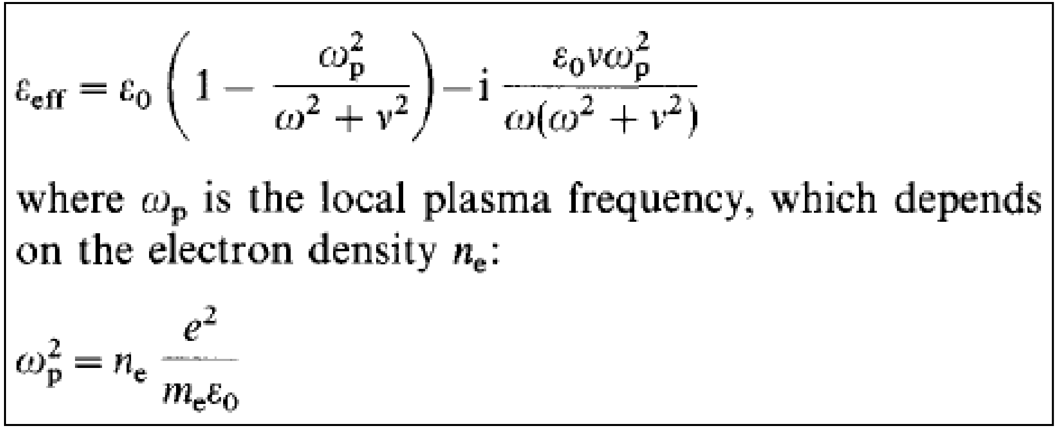
Solid: Ions

Dashed: Neutral particles

Global Models

Approach 3: Global model

- Plasma treated as stationary medium with a given permittivity
- Stationary ions, mobile electrons
    - Cold plasma approximation/Drude model



$$\varepsilon_{\mathrm{eff}} = \varepsilon_0 \left(1 - \frac{\omega_{\mathrm{p}}^2}{\omega^2 + \nu^2} \right) - \mathrm{i}\, \frac{\varepsilon_0 \nu \omega_{\mathrm{p}}^2}{\omega(\omega^2 + \nu^2)}$$

where ω_{p} is the local plasma frequency, which depends on the electron density n_{e}:

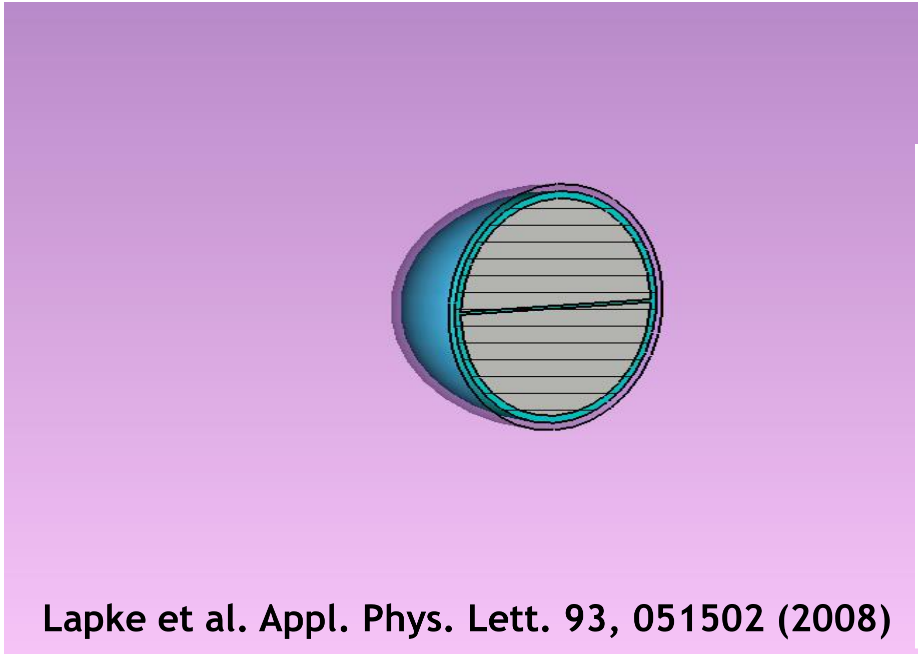
$$\omega_{\mathrm{p}}^2 = n_{\mathrm{e}} \frac{e^2}{m_{\mathrm{e}} \varepsilon_0}$$

Approach 3: Global model

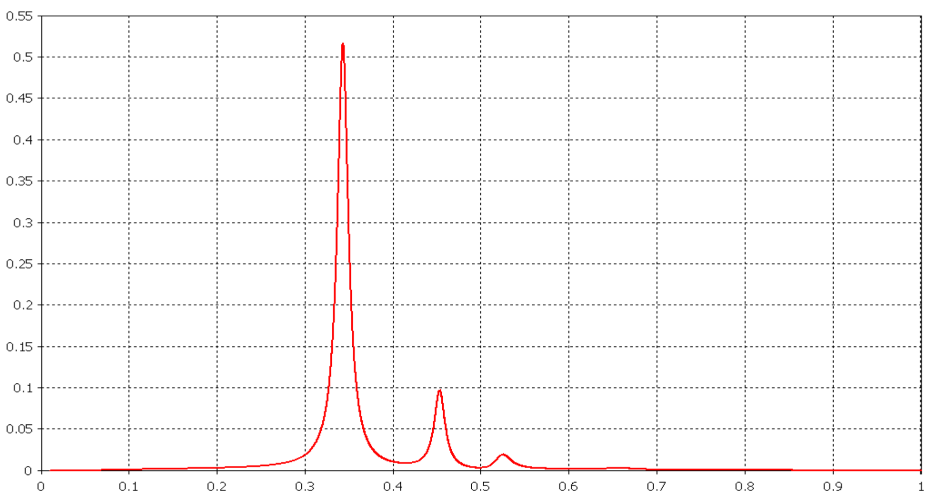
- Requires ab initio knowledge about plasma
- Can only describe the effect of the plasma on EM, not the behavior of the plasma itself.
- Maxwell’s equations only
- Fast!

Multipole Resonance Probe (MPRP)

- The MPRP is a non-intrusive measuring device
- Plasma parameters can be determined from power absorption spectrum

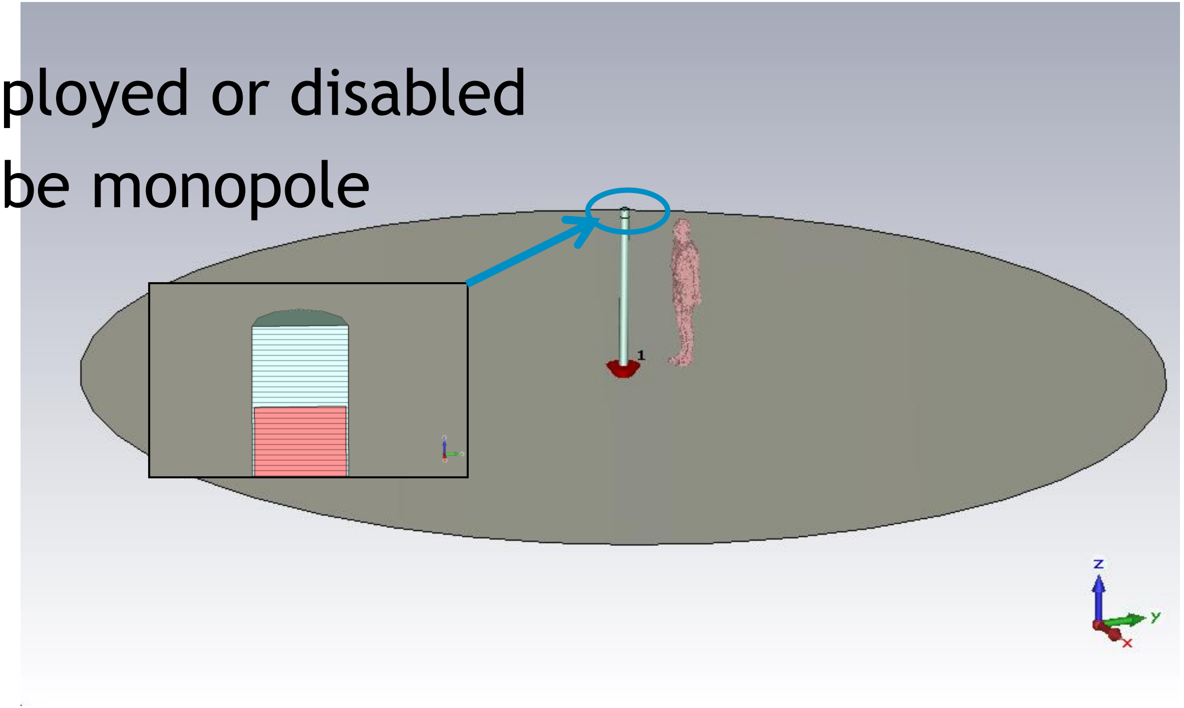


Lapke et al. Appl. Phys. Lett. 93, 051502 (2008)

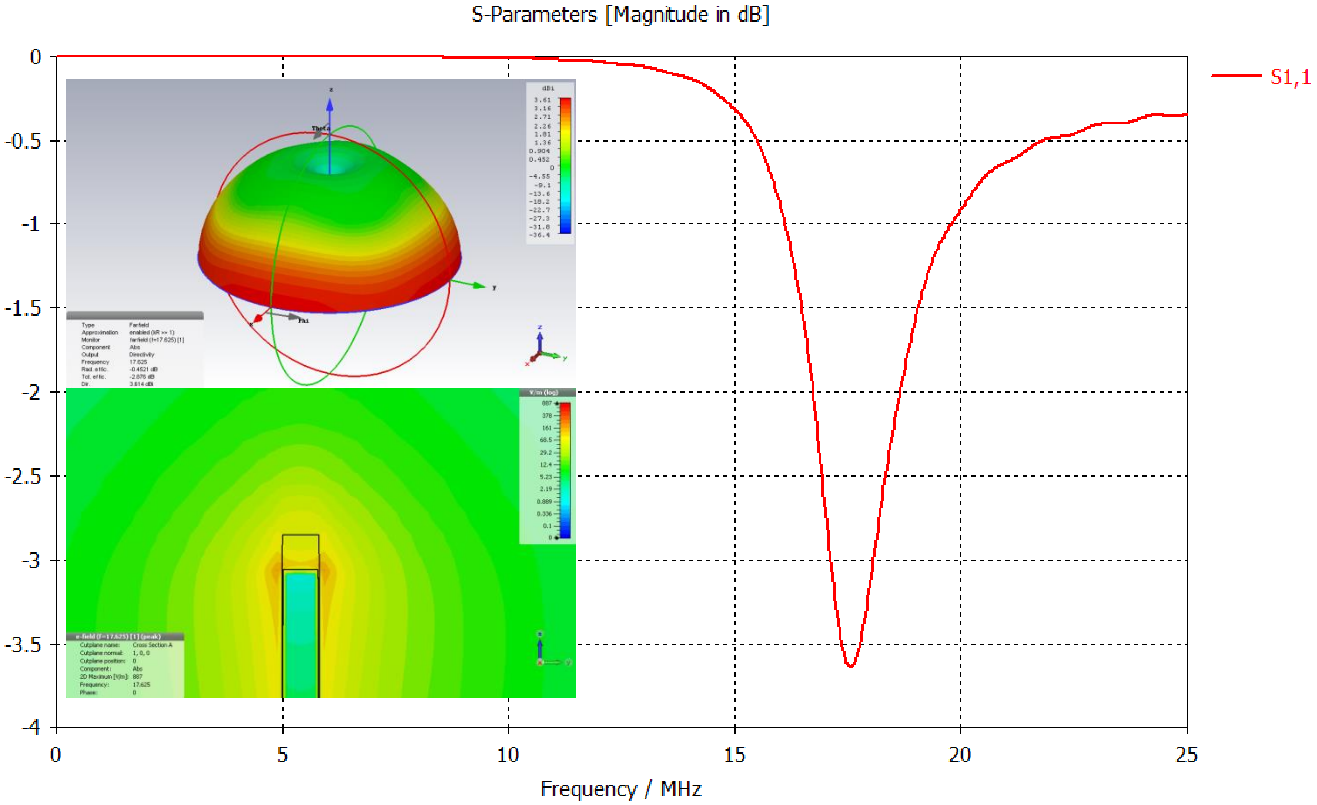


Plasma Antenna

- Plasma is a conducting medium and can act as an antenna
- Can be quickly deployed or disabled
- Example: Neon tube monopole



Neon Tube Monopole

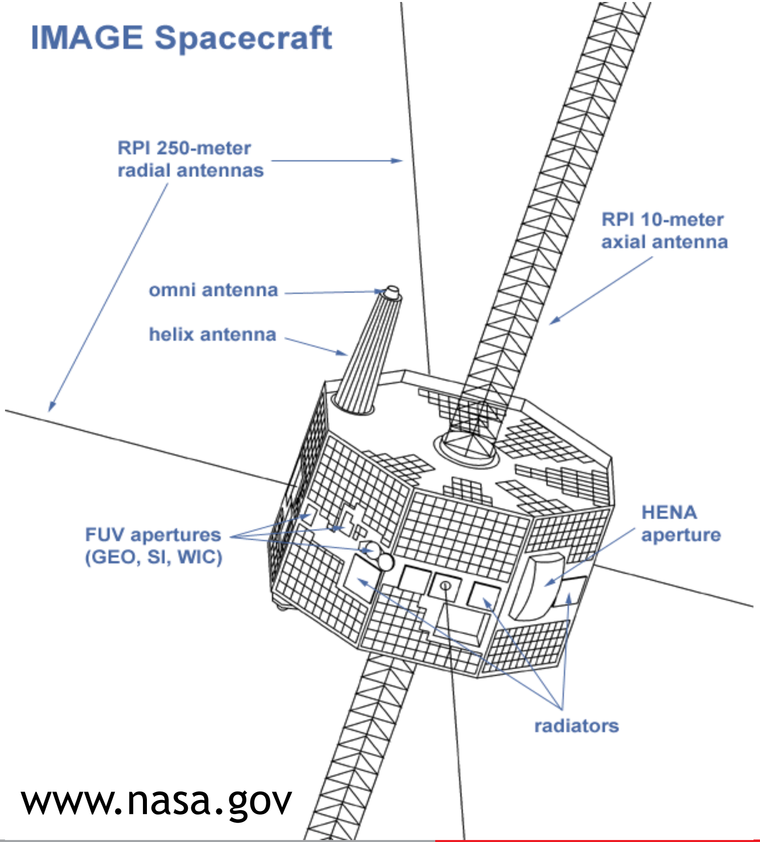


Type Farfield
Approximation enabled (kR >> 1)
Monitor farfield (f=17.625) [1]
Component Abs
Output Directivity
Frequency 17.625
Rad. effic. -0.4521 dB
Tot. effic. -2.876 dB
Dir. 3.614 dBi

e-field (f=17.625) [1] (peak)
Cutplane name: Cross Section A
Cutplane normal: 1, 0, 0
Cutplane position: 0
Component: Abs
2D Maximum [V/m]: 887
Frequency: 17.625
Phase: 0

NASA IMAGE RPI in Magnetosphere

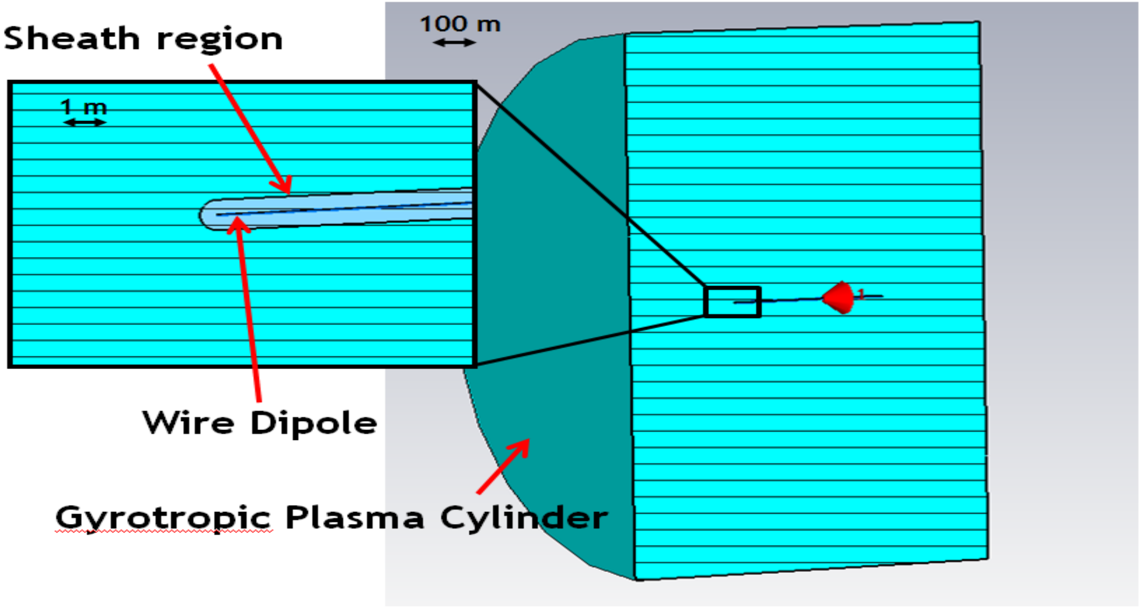
- Satellite in elliptical orbit
- Plasma density depends on altidude
- Investigate effect on the 250 m radial antennas
- Earth magnetic field requires gyrotropic extension of Drude model



www.nasa.gov

NASA IMAGE RPI in Magnetosphere

- Farfield pattern, antenna impedance
- Gyrotropic Drude model



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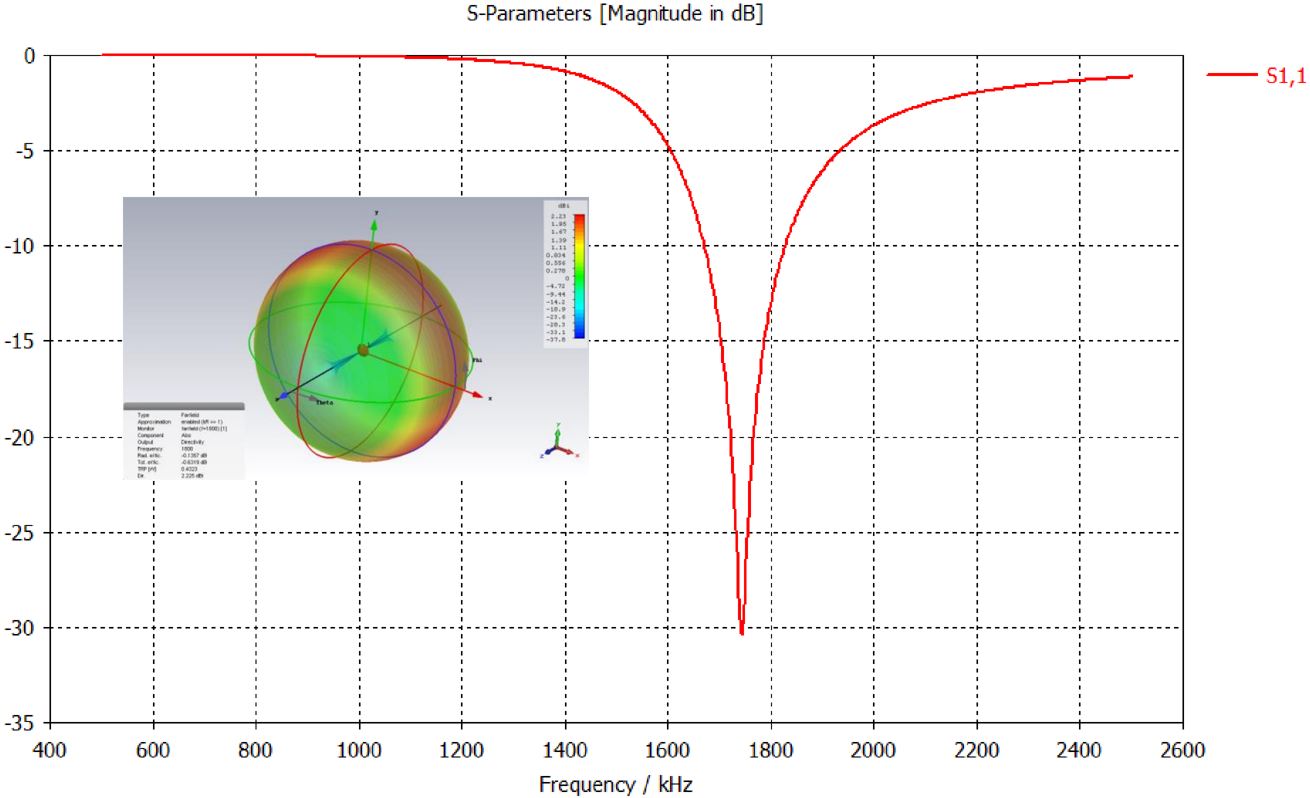
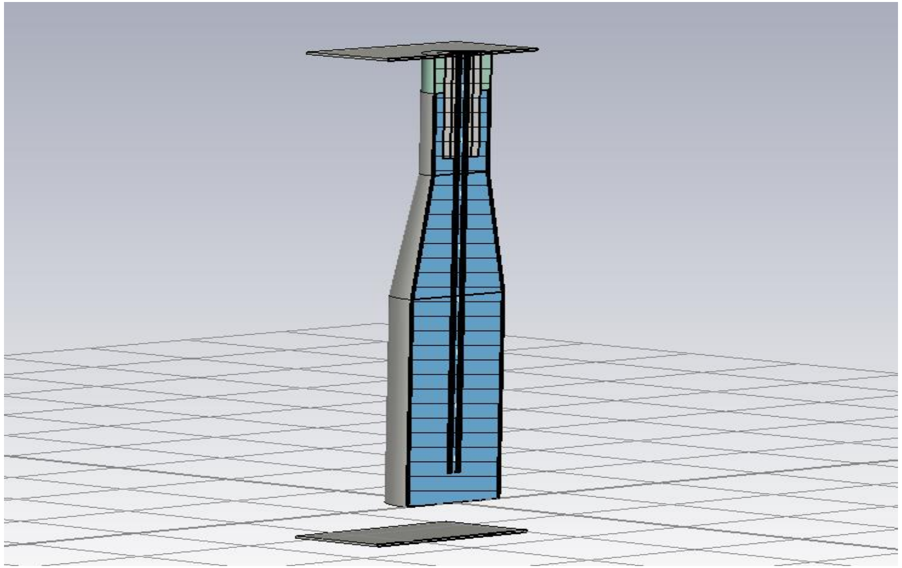
NASA IMAGE RPI in Magnetosphere



Type	Farfield
Approximation	enabled (kR >> 1)
Monitor	farfield (f=1800) [1]
Component	Abs
Output	Directivity
Frequency	1800
Rad. effic.	-0.1357 dB
Tot. effic.	-0.6319 dB
TRP [W]	0.4323
Dir.	2.225 dBi

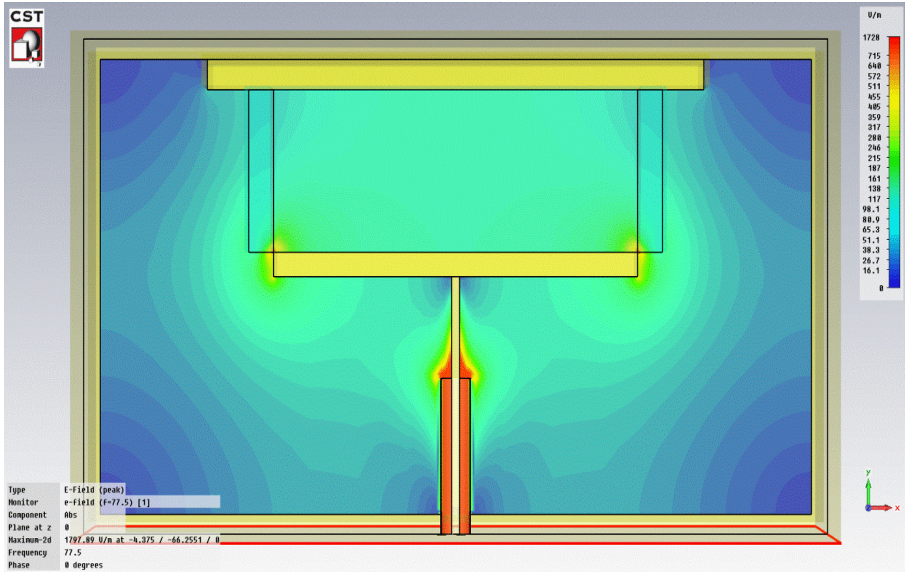
Non-destructive Sterilization

PET bottles



steves@aept.ruhr-uni-bochum.de

Medical tools



Type E-Field (peak)
Monitor e-field (f=77.5) [1]
Component Abs
Plane at z 0
Maximum-2d 1797.89 V/m at -4.375 / -66.2551 / 0
Frequency 77.5
Phase 0 degrees

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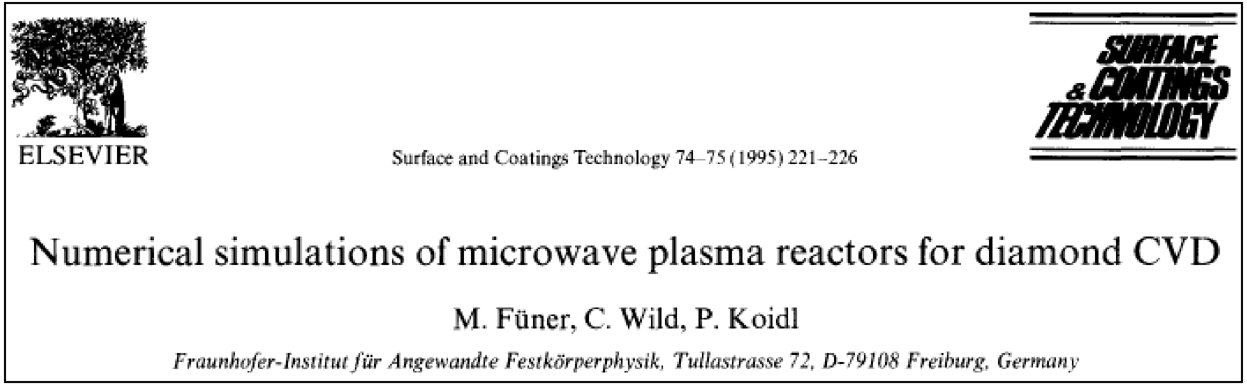
Non-Linear Global Model



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Surface and Coatings Technology 74–75 (1995) 221–226

SURFACE & COATINGS TECHNOLOGY

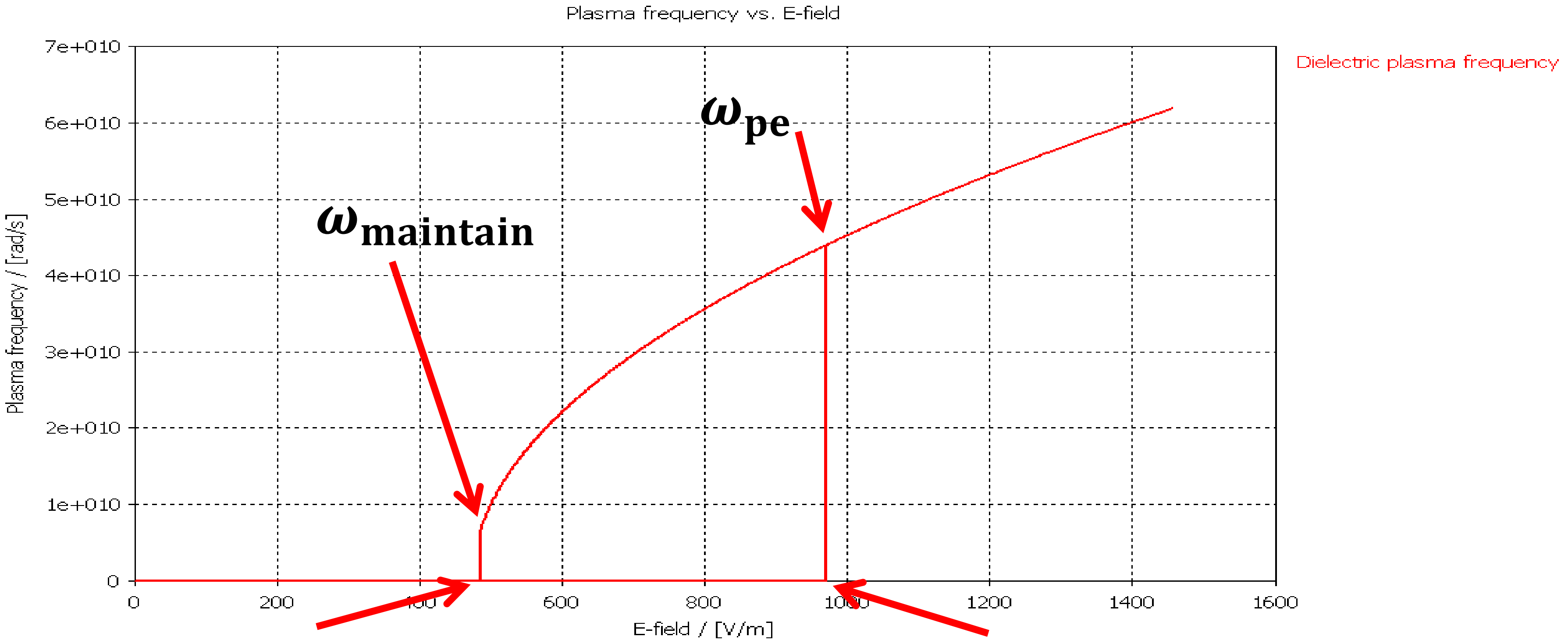
Numerical simulations of microwave plasma reactors for diamond CVD

M. Füner, C. Wild, P. Koidl

Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, D-79108 Freiburg, Germany

- The authors allow the plasma frequency to vary depending upon the local electric field

Nonlinear Material Properties



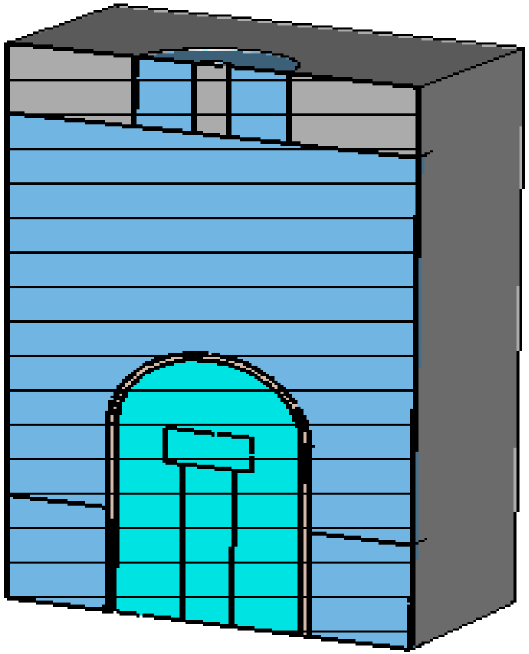
ω_{maintain}

ω_{pe}

“OFF”

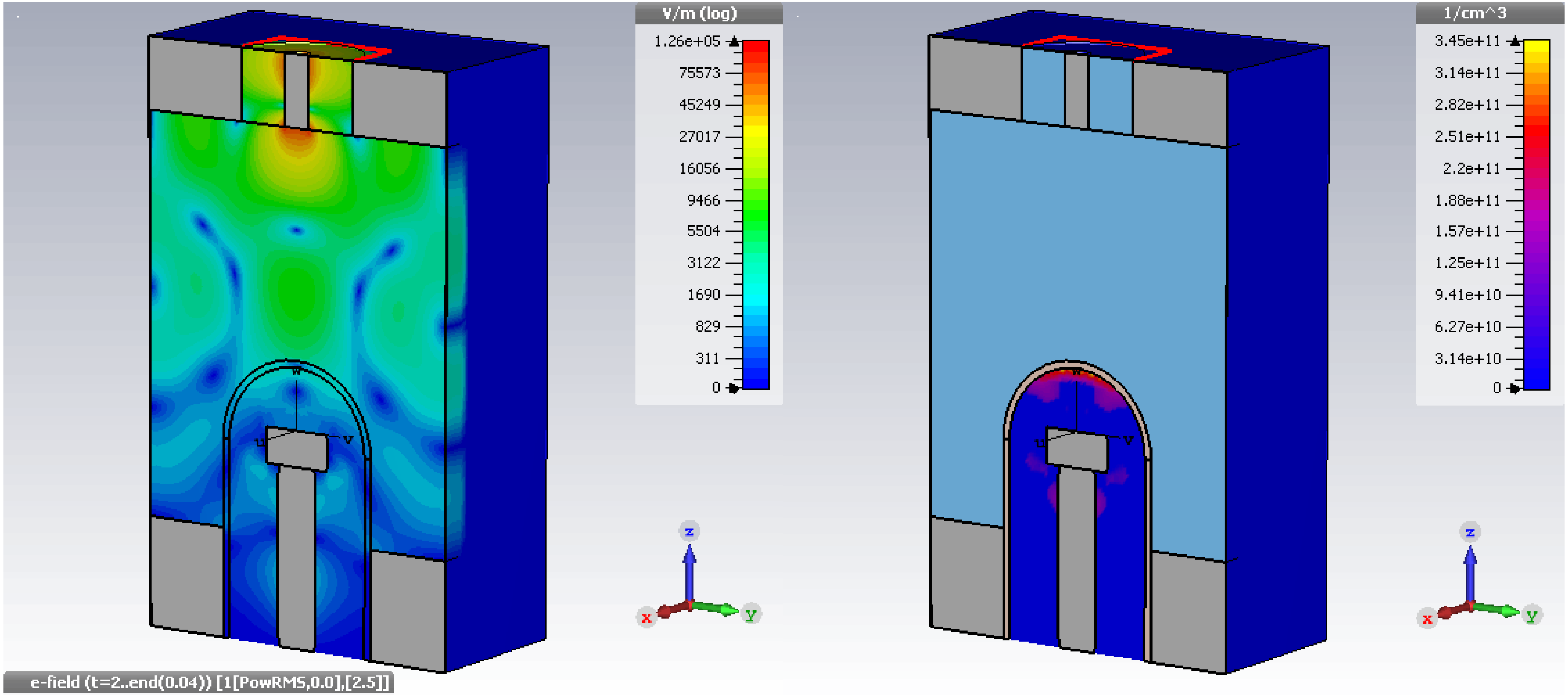
“ON”

Example: CVD Plasma Reactor



F Silva et al., *MW engineering of plasma-assisted CVD reactors for diamond deposition*, J. Phys. Condens. Matter **21** (2009) 364202 and references therein

E-Field and Plasma Density



Thank You!

Questions?