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

Dr.-Ing. Frank H. Scharf
CST of America
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

\[ \omega_{pe} = \sqrt{\frac{n_e e^2}{m_e \epsilon_0}} \]

- 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
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
  \[ \mathbf{F} = m\mathbf{a} \]
Basic Physics behind Simulation

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

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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:

$$\frac{df(\ddot{x}, \ddot{v}, t)}{dt} = f_c$$

Simple enough - or is it? Let’s apply it to a simple case!
The Near-Cathode Region in HIDs

D-Lamp for automotive headlights

http://www.aept.rub.de
Different Spot Attachments

Solving the Boltzmann Equation

\[ \frac{\partial f_i}{\partial t} - \frac{\beta}{n_i} \frac{\partial f_i}{\partial v} + \nabla \cdot (3f_i + \nabla_n f_i + \nabla_v f_i) = n_i f_i - \gamma (1 + \gamma)n_i^2 f_i + \tilde{v}_i \left( 3f_i + \nabla v f_i + \nabla_v f_i \right) \]

\[ = \frac{\partial}{\partial t} \int_\mathbb{R} \int_\mathbb{R} g^3 \left[ \alpha_{ii}(f_i(v - \frac{g'e}{2} + \frac{g'\tilde{v}}{2})f_i(v - \frac{g'e}{2} - \frac{g'\tilde{v}}{2}) - f_i(v)f_i(v - g'\tilde{v})) \right. \]

\[ + \alpha_{ii}(f_i(v - \frac{\tilde{v}}{2} + \frac{g'e}{2})f_i(v - \frac{g'e}{2} - \frac{g'\tilde{v}}{2}) - f_i(v)f_i(v - g'\tilde{v})) \]

\[ \times \, dg'\, d\Omega' \]  \hspace{1cm} (4.50)

\[ \frac{df(\vec{x}, \vec{v}, t)}{dt} = \mathbf{f}_c \]

\[ \frac{\partial f_a}{\partial z} = -n_i f_a + \gamma (1 + \gamma)n_i^2 f_i + \tilde{v}_i \left( 3f_a + \nabla v f_a + \nabla_v f_a \right) \]

\[ + \frac{\partial}{\partial t} \int_\mathbb{R} \int_\mathbb{R} g^3 \left[ \alpha_{aa}(f_a(v - \frac{g'e}{2} + \frac{g'\tilde{v}}{2})f_a(v - \frac{g'e}{2} - \frac{g'\tilde{v}}{2}) - f_a(v)f_a(v - g'\tilde{v})) \right. \]

\[ + \alpha_{ai}(f_a(v - \frac{\tilde{v}}{2} + \frac{g'e}{2})f_a(v - \frac{g'e}{2} - \frac{g'\tilde{v}}{2}) - f_a(v)f_a(v - g'\tilde{v})) \]

\[ \times \, dg'\, d\Omega' \]  \hspace{1cm} (4.51)

Solve for Density and Velocity

Solid: Ions
Dashed: Neutral particles

Mach 1
Particle-In-Cell

- Use a computer to create an ensemble of particles

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

A magnetic field is used to focus the beam:

Without magnetic field:

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

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

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: $\text{Kn} = \frac{\lambda}{L}$
- Fluid approximation is good if $\text{Kn} << 1$

- Surprisingly robust, due to conservation of mass, momentum, energy
Solving the Fluid Dynamic Equations

\[ \frac{d}{dz}(n_i v_i) = k_i n_in_a - k_r n_i^3 \]
\[ \frac{d}{dz}(n_a v_a) = -k_i n_in_a + k_r n_i^3 \]
\[ \frac{d}{dz}(n_a m_i v_i^2) = -(T_h + T_e) \frac{dn_i}{dz} - n_i n_a k_{cr} m_i (v_i - v_a) + k_i n_i n_a m_i v_a - k_r n_i^3 m_i v_i \]
\[ \frac{d}{dz}(n_a m_i v_a^2) = -T_h \frac{dn_a}{dz} + n_i n_a k_{cr} m_i (v_i - v_a) - k_i n_i n_a m_i v_a + k_r n_i^3 m_i v_i \]

Solve for Density and Velocity

Solid: Ions  Dashed: Neutral particles

Supersonic neutrals! Artifact of the fluid model
Global Models
Approach 3: Global model

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

\[
\epsilon_{\text{eff}} = \epsilon_0 \left(1 - \frac{\omega_p^2}{\omega^2 + \nu^2}\right) - i \frac{\epsilon_0 \nu \omega_p^2}{\omega(\omega^2 + \nu^2)}
\]

where \(\omega_p\) is the local plasma frequency, which depends on the electron density \(n_e\):

\[
\omega_p^2 = n_e \frac{e^2}{m_e \epsilon_0}
\]
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

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
NASA IMAGE RPI in Magnetosphere

- Satellite in elliptical orbit
- Plasma density depends on altitude
- 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

jon.schoenberg@ll.mit.edu
NASA IMAGE RPI in Magnetosphere
Non-destructive Sterilization

PET bottles

steves@aept.ruhr-uni-bochum.de

Medical tools

stapelmann@aept.ruhr-uni-bochum.de
Non-Linear Global Model

Numerical simulations of microwave plasma reactors for diamond CVD

M. Funer, 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

Plasma frequency vs. E-field

Dielectric plasma frequency

ω_{pe}

ω_{maintain}

“OFF”

“ON”
Example: CVD Plasma Reactor

E-Field and Plasma Density
Thank You!
Questions?