16.522: Session 18
C Courtesy of Prof. Eduardo Ahedo Universidad Politecnica de Madrid

Types of models

- • **Kinetic:** based on Boltzmann eq.; unaffordable except for particular aspects of the problem
- \bullet **Fluid:** familiar formulation but important difficulties arising from
	- 1. Weak collisionality (Kn large)
	- 2. Wall interaction
	- 3. Curved magnetic topology
	- 4. 2D subsonic/supersonic ion flows
- •**Particle In Cell & MonteCarlo methods (PIC/MCC):** good for weak collisionality; simple to implement, but subject to 'numerical effects'; important difficulties in dealing with disparate scales of electron and ions. MCC model collisions statistically.
- • **Hybrid (PIC/MCC for heavy species & fluid for electrons):** best compromise today; allows 2D (geometrical and magnetic) effects; avoids small electron scales and admits quasineutrality

Simulation of the plasma discharge

- •2D, axisymmetric model
- •Quasineutral plasma except for sheaths around walls.
- •Plasma wall interaction treated in separate sheath models.
- •Boundaries: 1) anode $+$ gas injector, 2) cathode surface, 3) lateral walls
- •3 or 4 species: neutrals, ions $(+, ++)$, and electrons
- • Ion dynamics: unmagnetized, near collisionless, internal regular sonic transitions, singular sonic transitions at sheath edges.
- • Electrons: magnetized, diffusive motion, and weakly <http://ocw.mit.edu/help/faq-fair-use/>. collisional (local thermodynamic equilibrium is not assured)
- •Fluid modelling: complex and uncertain.
- • There is no fully 2D model yet. Two existing options:
	- a) Approximate 1D (axial) fluid model
	- b) Near 2D hybrid model: fluid eqs. for electrons; particle model for ions & neutrals

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2D fluid model

- Basic hypotheses: 1) azimuthal symmetry: $\frac{d}{d\theta} = 0$, $u_{\theta i} = 0$, $u_{\theta n} = 0$ • Basic hypotheses: 1) azimuthal symmetry: $\frac{\partial}{\partial t} = 0$, $u_{\alpha} = 0$, $u_{\alpha} = 0$ ∂
- 2) Quasineutrality: $|n_e = n_{i+} + 2n_{i++}| \implies$ boundary conditions at sheath edges
	- 3) Simplified treatment of pressure tensors

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Continuity equations:
$$
\frac{\partial n_e}{\partial t} + \nabla \cdot n_e \vec{u}_e = S_{ion}
$$
 $S_{ion} \approx n_e n_n R_{ion}(T_e) \leftarrow$ ionization

$$
\frac{\partial n_i}{\partial t} + \nabla \cdot n_i \vec{u}_i = S_{ion}, \qquad \frac{\partial n_n}{\partial t} + \nabla \cdot n_n \vec{u}_n = -S_{ion}
$$
 (here $n_e = n_i$ only)

 $\frac{1}{t} \left(m_e \vec{n}_e \vec{u}_e \right)$ Electron momentum: ∂ •∂ $\widetilde{\vec{u}}_e + \nabla \cdot \vec{m}_e \vec{m}_e \widetilde{\vec{u}_e \vec{u}_e} = -\nabla (n_e T_e) - e n_e (\vec{E} + \vec{u}_e \times \vec{B}) + \vec{M}_e$

$$
\vec{M}_e \approx -n_e n_n R_{en} (T_e) m_e \vec{u}_e \quad \leftarrow \quad \text{e-n momentum transfer}
$$

Ion momentum: $\left| \frac{\partial}{\partial t} \left(m_i n_i \vec{u}_i \right) + \nabla \cdot m_i n_i \vec{u}_i \vec{u}_i \right| = -\nabla (n_i \vec{T}_i)$ $\begin{array}{c} \widehat{\mathcal{O}} \ -(\,m_{\cdot}n_{\cdot}\vec{u}_{\cdot}\,)+\nabla\cdot m_{\cdot}n_{\cdot}\vec{u}_{\cdot}\vec{u}_{\cdot}=-\nabla\vec{v} \end{array}$ •∂ G GG $i + en_i \vec{E} + \vec{M}_i$

 $\vec{M}_i \approx S_{ion} m_i \vec{u}_n - S_{cx} m_i (\vec{u}_i - \vec{u}_n)$ \leftarrow ionization + charge-exchange mom. transf.

2D fluid model

• Electron (total) energy equation :

$$
\frac{\partial}{\partial t} \left(\frac{3}{2} T_e + \frac{1}{2} m_e u_e^2 \right) n_e + \nabla \cdot \left[\left(\frac{5}{2} T_e + \frac{1}{2} m_e u_e^2 \right) n_e \vec{u}_e + \vec{q}_e \right] = -e n_e \vec{u}_e \cdot \vec{E} + Q_e
$$

 $Q_e \approx -n_e n_n R_{ion} (T_e) E_{ion} \alpha_{ion}$ \leftarrow ionization $(E_{ion} = 12.1 \text{eV}, \alpha_{ion} \sim 1.5 - 2.5 \text{ for Xe})$

• Internal energy = total energy – mechanical energy

$$
\frac{\partial}{\partial t} \left(\frac{3}{2} T_e n_e \right) + \nabla \cdot \left[\frac{3}{2} T_e n_e \vec{u}_e + \vec{q}_e \right] = -n_e T_e \nabla \cdot \vec{u}_e + Q'_e
$$

$$
Q'_{e} = Q_{e} - \vec{M}_{e} \cdot \vec{u}_{e} + \frac{1}{2} m_{e} u_{e}^{2} S_{e} \approx n_{e} n_{n} \left[\left(R_{en} + \frac{1}{2} R_{ion} \right) m_{e} u_{e}^{2} - R_{ion} E_{ion} \alpha_{ion} \right]
$$

• Heat flux (diffusive model): (Bittencourt)

$$
\vec{o} = -\frac{5}{2} p_e \nabla T_e - e \vec{q}_e \wedge \vec{B} - m_e v_e \vec{q}_e \rightarrow \vec{q}_e = -\overline{\vec{K}}_e \cdot \nabla T_e
$$

• Energy equations for ions and neutrals.

From 2D to 1D model

 Electron continuity equation: \bullet

$$
\frac{\partial n_e}{\partial t} + \frac{\partial n_e u_{ze}}{\partial z} + \frac{1}{r} \frac{\partial r n_e u_{re}}{\partial r} = n_e v_i
$$

The 1D axial model works with values averaged over each ('doughnut') radial section \bullet

$$
0 = \frac{2}{r_{ext}^2 - r_{int}^2} r_{int}^{r_{ext}} \left[\frac{\partial n_e}{\partial t} + \frac{\partial n_e u_{ze}}{\partial z} + \frac{1}{r} \frac{\partial r_{de} u_{re}}{\partial r} - n_e v_i \right] \longrightarrow \left[\frac{\partial \overline{n}_e}{\partial t} + \frac{\partial \overline{n}_e \overline{u}_{ze}}{\partial z} = \overline{n}_e (\overline{v}_i - \overline{v}_w)
$$

with $\overline{n}_e \equiv \overline{n}_e(z)$,..., and 'source' $\left[\overline{n}_e \overline{v}_w - 2 \frac{(r n_e u_{re})|_{int}^{ext}}{r_{ext}^2 - r_{int}^2} \right]$ evaluating losses at lateral walls.

 $e^{\lambda t}$ *i* w $\frac{n_e}{\partial t} + \frac{cn_e u_{ze}}{\partial z} = \overline{n}$ $V_{\rm r} - V$

An auxiliary <u>radial model</u> (at each *z*) is needed to \bullet

compute \overline{v}_w & determine radial profiles: $\left| \frac{1}{n} \frac{\partial m_e u_{re}}{\partial x} \right| \ge n_e \overline{v}$

$$
\frac{1}{r} \frac{\partial r n_e u_{re}}{\partial r} \approx n_e \overline{v}_w
$$

- This is a variable-separation type of solution; $\overline{v}_w(z)$ is an eigenvalue of the radial model. i
- We proceed similarly with the rest of fluid equations.

1D axial model

- Neglect jet divergence, doubly-charged ions, p_i , p_n ,... i
- Wall interaction terms appear as source terms (instead of BCs) i
- Conservation of species flows: i

$$
\frac{d}{dz}(n_e u_{zi}) = n_e (v_i - v_w)
$$

 v_i : ionization frequency v_w : recombination frequency

 $m_n u_{z_n} + n_e u_{z_i} = \text{const} = \dot{m}_A / A m_i$

 $n_e u_{zi} - n_e u_{ze} = \text{const} = I_d / Ae$

Ion axial momentum equation: i

$$
\frac{d}{dz}(m_{i}n_{e}u_{zi}^{2}) = -en_{e}\frac{d\phi}{dz} + m_{i}n_{e}(v_{i}u_{zn} - v_{w}u_{zi})
$$

Neutral axial momentum equation \bullet

$$
\frac{d}{dz}(m_{i}n_{n}{u_{zn}}^{2}) = m_{i}n_{e}(v_{wn}u_{znw} - v_{i}u_{zn})
$$

 u_{znw} velocity of neutrals from recombination ($\neq u_{zi}$)

1D axial model

Electron Ohm´s law: \bullet

$$
-u_{ze} = \frac{v_e}{m_e \omega_e^2} \left[e \frac{d\phi}{dz} - \frac{1}{n_e} \frac{d}{dz} (n_e T_e) \right] \left[u_{\theta e} = -u_{ze} \frac{\omega_e}{v_e} \right]
$$

$$
{\theta e}=-u{ze}\frac{\omega_e}{v_e}
$$

 $V_e = V_{en} + V_{ei} + V_{wm} + V_{turb}$: effective collision frequency

 (v_{wmn}) due to wall interaction, v_{turb} due to plasma turbulence)

Electron internal energy: \bullet

$$
\frac{d}{dz}\left(\frac{5}{2}n_eT_eu_{ze} + q_{ze}\right) = u_{ze}\frac{d(n_eT_e)}{dz} + v_e n_e m_e u_e^2 - v_i n_e E_{ion}\alpha_{ion} - \beta_e v_w n_e T_e
$$

 $(\beta_e \sim 6 - 100$: factor for energy losses at lateral walls)

- Heat conduction: $0 = -\frac{1}{2} p_e \nabla T_e e \vec{q}_e \wedge B m_e \nu_e \vec{q}_e \rightarrow |q_{ze} = -\frac{\nu_e}{2m} \frac{e}{\omega^2}$ on: $0 = -\frac{5}{2} p_e \nabla T_e - e \vec{q}_e \wedge \vec{B} - m_e v_e \vec{q}_e \rightarrow \begin{vmatrix} q_{ze} = -\frac{5r}{2} \end{vmatrix}$ $e^{Q}T_e - e\vec{q}_e \wedge B - m_eV_e\vec{q}_e \longrightarrow$ $|q_{ze} = -\frac{e}{2} - \frac{e}{2} - \frac{e}{2}$ *e e* $p_e \nabla T_e - e \vec{q}_e \wedge \vec{B} - m_e \vec{v}_e \vec{q}_e \rightarrow \begin{vmatrix} q_{ze} = -\frac{5n_e T_e}{2} \frac{V_e}{r_e} \frac{dT_e}{r_e} \frac{dV_e}{dr_e} \end{vmatrix}$ m_a ω_a^2 dz $v_e \vec{q}_e \rightarrow \begin{vmatrix} q_{ze} = -\frac{3n_e I_e}{2m_e} \frac{V_e}{\omega} \end{vmatrix}$ $=-\frac{3}{2} p \nabla T - e \vec{q} \cdot \Delta \vec{B} - m \nabla \vec{q} \rightarrow |q_{-} = -$
- Normalized set of equations: $|(T_e m_i u_{zi}^2) \frac{dI}{dt} \vec{F}(\vec{Y})|$ *dY* $T_e - m_i u_{zi}^2$ $\frac{dE}{dz} = F(Y)$ \rightarrow \rightarrow \rightarrow \bullet

 $Y = (n_e, n_n, u_{zi}, u_{ze}, u_{zn}, T_e, q_{ze}, \phi)$ vector of 8 plasma variables \rightarrow

Singular (sonic) points of the equations at : $M = \frac{u_{zi}}{\sqrt{T_e/m_i}} = \pm 1$ \bullet

1D axial model

- 2 $\frac{2}{e}$ $\frac{2q_{ze}}{1}$ $\frac{2q_{ze}}{1}$ $\frac{2q_{ze}}{1}$ $\frac{2q_{ze}}{1}$ lnFor instance: $\frac{u u_{zi}}{u} = v_i - u_{zi} \frac{d u}{dx}$ $1 - \frac{-q_{ze}}{5n_a T_a u_{ze}} - \nu_i m_i (2 u_{zi} - u_{zn}) + m_i u_{zi}^2 \frac{d^2 u_{ze}}{d^2 u_{ze}}$ i α_{zi} *zi* α_{zi} $e^{i\theta}$ *i* i^{μ} *zi e ze* $e^{i\theta}ze^{-i\theta}$ *z* θ *z* θ *z* θ *z* θ *i* θ *i* θ *i* θ *zi* θ *zi* θ *zi* θ *i* θ *zi* θ *zi e e e ze* $\frac{du_{zi}}{dz} = v_i - u_{zi} \frac{d \ln A}{dz} - u_{zi} \frac{G}{T_a - m_i u}$ $G = -\frac{\omega_e^2}{V_a} m_e u_{ze} \left(1 - \frac{2q_{ze}}{5n_a T_a u_{ze}}\right) - v_i m_i (2u_{zi} - u_{zn}) + m_i u_{zi}^2 \frac{d \ln A}{dz}$ $=$ V_i $u_{\scriptscriptstyle \rm rel}$ $\frac{\omega_e}{v_a} m_e u_{ze} \left(1 - \frac{2q_{ze}}{5n_a T_e u_{ze}} \right) - v_{ze}$ − $\begin{pmatrix} 2q \end{pmatrix}$ $=-\frac{v_e}{v_e}m_e u_{ze} \left(1-\frac{-q_{ze}}{5n_e T_e u_{ze}}\right)-v_i m_i (2u_{zi} - u_{zn})+$ \bullet
- **A** singular transition exists at anode sheath edge (point B): $M_B = -1$ & $G_B = \infty$
- A regular subsonic/supersonic transition exists inside the channel (point S) with \bullet

$$
M_s = 1
$$
 & $\vec{F}(\vec{Y}_s) = \vec{0}$, i.e. $G_s = 0$

- Point S is equivalent to the critical s ection of a Laval nozzle, where \bullet $0 = G_s \equiv m_i u_{zi}^2 d \ln A/dz$ corresponds to $dA/dz = 0$. In a Hall thruster, $G_s = 0$ corresponds to a certain balance between ionization and electron diffusion.
- 8 boundary conditions are set at points B, S and P: \bullet
	- Discharge voltage (1)
	- Density and velocity of injected gas at anode (2)
	- Electron temperature at cathode (1)
	- Regularity condition at point S (1)
	- Anode sheath conditions (3)

Anode sheath in a Hall thruster

- For Maxwellian-type VDF electron flux to anode $\sim n_{_{eA}}\sqrt{T_{_e}/2\pi m_{_e}}$, •
- In normal conditions this is much larger than the quasineutral flux in the channel, $g_{ze} \equiv n_e u_{ze} (> 0)$ •
- A negative anode sheath AB is formed i n order to •

satisfy
$$
g_{zeB} = g_{zeA}
$$
:
$$
n_{eB}u_{zeB} \approx -n_{eB} \exp\left(-\frac{e\phi_{AB}}{T_{eB}}\right)\sqrt{\frac{T_{eB}}{2\pi m_e}}
$$

This equation determines the sheath potential fall, ϕ_{AB} .

- Bohm condition at sheath edge: $|u_{_{zib}} \approx -\sqrt{T_{_{eB}}/m_{_{\tilde t}}}$ •
- Electron energy flux deposited: a) at the anode A, •

$$
q_{zeA}^{tot} = -\int \frac{1}{2} m_e w^2 w_z f_{eB}(w) d^3 w \approx 2 T_{eB} g_{zeB}
$$

b) at the sheath edge B :

$$
q_{zeB}^{tot} = g_{zeB} (2T_{eB} + e\phi_{AB})
$$

These are 3 boundary conditions for the axial quasineutral model •

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Axial structure

Acceleration region:

•

- Presents most of the potential drop & ion acceleration
- For electrons: Joule heating competes with wall cooling
- Heat conduction smooths T_e profile
-
- Plasma production = plasma recombination
Plasma density decreases (due to ion
acceleration)
 $\begin{bmatrix} \frac{5}{8} & 60 \\ 1 & \frac{1}{12} & 40 \end{bmatrix}$ Plasma density decreases (due to ion acceleration)
- • **Ionization region**:
	- Electron cooling due to ionization
	- Maximum of plasma density inside
- • **Ion backstreaming region**:
	- Electric force very small
	- Ion reverse flow is small
	- Pressure drop (towards anode) dominates electron diffusive flow
	- Length depends on ionization rate (i.e. T_e)

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- Magnetic field is adjusted for each case:
	- solid lines: 110V, 110G
	- dashed lines: 600V, 330G

Axial structure

Influence of anode mass flow

Influence of magnetic field shape

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External B-field profiles

- solid lines: $L_{b1} = 9.5$ mm, $B_{max} \sim 380$ G

- dashed lines: $L_{b1} = 30$ mm, $B_{max} \sim 140$ G

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Thrust

- Plasma momentum flow: $F_p(z) = \sum F_a(z)$, $F_a(z) = (m_a u_{z\alpha}^2 + T_a) n_\alpha A$, , *ien*α=• Plasma momentum flow: $F_p(z) = \sum F_\alpha(z)$, $F_\alpha(z) = (m_\alpha u_{z\alpha}^2 +$
- Axial momentum equation for the plasma:

Thrust

- Integrating the preceding equation between anode and far downstream:
- 2 Electric force: $F_{elec} = \left| A \frac{\epsilon_0}{2} \right|$ Thrust: $F = F_{p\infty} - D_{plume} = F_{mag} + F_{pA} - F_{elec} - D_{wall}$ Magnetic force: $F_{mag} = \int_{A} j_{\theta e} B_r A dz$ *elec d* $F_{elec} = \left| A \frac{z_0}{2} \right| \frac{d\phi}{dz}$ Electric force: $F = \left[4 \frac{\varepsilon_0}{4} \left(\frac{d\phi}{dr} \right)^2 \right]$ ∞ • Thrust: $F = F_{\text{max}} - D_{\text{atym}} = F_{\text{max}} + F_{\text{max}} - F_{\text{atym}}$ $-$ magnetic force: $r_{\text{max}} =$ $=\left[A\frac{\omega_0}{2}\left(\frac{a\varphi}{dz}\right)\right]_A$ ∫ Ion wall impact drag: $D_{wall} = \int_{V_w} v_m (u_{zi} - u_{zaw})$ *E wall* $\int_{A}^{V} w^{H}v_{i} \, dv_{zi}$ *w_{znw}* \int_{e}^{v} ν *D*_{*m*} μ _{*l*} μ _{*l*} μ _{*l*} μ _{*l*} μ _{*l*} μ ^{*n*}_{*addz*} μ _{*n*} μ ^{*n*}_{*addz*} *dA*∞ ⎥⎥ ∫
	- Jet divergence drag: $D_{\text{plume}} = \int_{A} n_{e} T_{e}$ $D_{\text{plane}} = \int n_a T_a - d z$ *dz* $-$ Jet divergence drag: $D_{\text{down}} =$ ∫
- Therefore, thrust is transmitted to the thruster through the magnetic reaction force of elect rons on the thruster magnetic circuit.
	- − Notice the contribution of the external magnetic field to thrust.
	- − Pressure forces at the anode make a marginal contribution
	- − Ion energy accommodation at walls acts as a drag force.

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Particle-in-cell (PIC) methods

- •Individual motion of macroparticles, subject to electromagnetic forces, is followed in a computational grid. (see Birdsall-Langdon)
- •<u>Cell size,</u> l_{cell,} smaller than plasma gradients
- •Timestep, $\Delta \tau$, such that particles advance less than cell size.
- \bullet Number of macroparticles per cell, N_{cell} , depends on good statistics and small numerical oscillations.
- \bullet Mass of macroparticle depends on species density
- •Different species \rightarrow different sets of macroparticles
- • Example for Hall thruster (only ions and neutrals)
	- –axisymmetric, 30mm \times 15 mm \rightarrow 900 (toroidal) cells \rightarrow 1_{cell}~0.5mm
	- – N_{cell} (per species) ~ 30 \rightarrow 27.000 macroparticles/species
		- \rightarrow 10⁹ -10¹¹ atoms/macroparticle
	- macroparticle mass \sim atom mass \times (atom/macroparticle)
	- $\Delta \tau$ ~ 10⁻⁸ s (ions), 10⁻⁷ s (neutrals), 10⁻¹⁰ s (electrons)

Video of particle motion

Courtesy of Professor Ahedo, Universidad Carlos III de Madrid. Used with permission.

Video of plasma dynamics

Courtesy of Professor Ahedo, Universidad Carlos III de Madrid. Used with permission.

Time-averaged 2D behavior

:][ifY`fYa cjYX`XiY`hc`Wcdnf][\hfYghf]Whcbg"`D`YUgY`gYY`:][ifY`%%`]b`9gWcVUfž`8"ž`5"`5bhtEbž`UbX`9"`5\YXc" "G]a i `Uh]cb cZ<][\!GdYWZJW=a di `gY UbX 8ci V`Y!GHJ[Y <U``H\fi ghYfg"" =b DfcW'&- h\ =bhYfbUh]cbU`9`YWf]W Dfcdi `g]cb`7cbZYfYbWžDf]bWhcbžlG5" &\$\$)"

Time-averaged 2D behavior

7ci fhYgmcZDfcZYggcf 5\YXcžl b]j Yfg]XUX 7Uf cg = XY A UXf]X" I gYX k]h\ dYfa]gg]cb"

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