MIPSE Seminar December 8 (Wed), 2021

Dynamics of Low Temperature Magnetized Plasmas: Self-Organization and Anomalous Electron Transport

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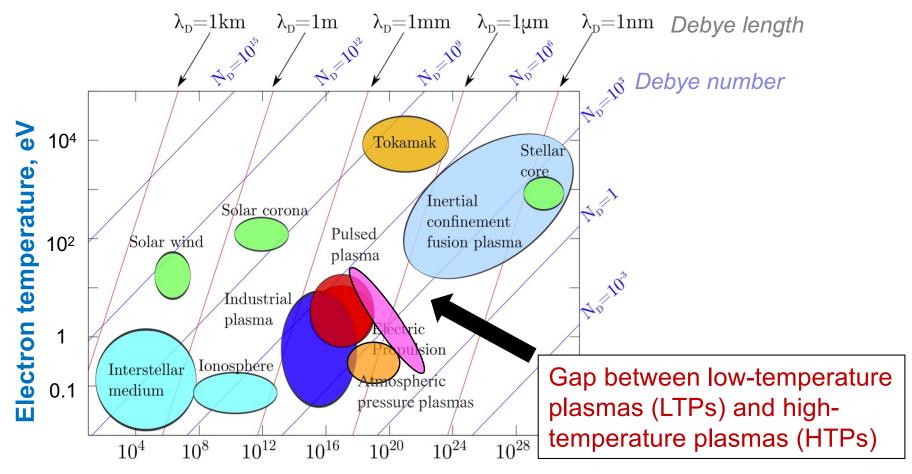


Outline

- 1. Introduction: Low temperature magnetized plasmas
- 2. Computational plasma modeling
- 3. Physics and modeling of low-temperature magnetized plasmas
 - Kinetic theory/modeling of plasma instabilities and turbulence
 - Fluid modeling of low-temperature magnetized plasmas
 - Data-driven online estimation for plasma chemistry

4. Conclusion







Electron (plasma) density, m⁻³

Low temperature magnetized plasmas

Using applied magnetic fields leads to higher electron temperature and density

Multiscale

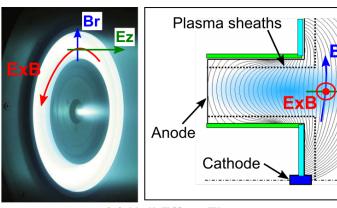
- High-frequency: Instabilities, turbulence
- Low-frequency: Self-organization

Multiphysics

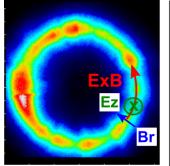
- Collisional (intermolecular, walls)
- Collisionless (non-Maxwellian, kinetic, waves, gyromotion)

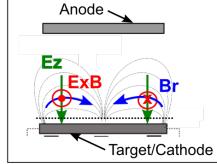
Multispecies

- Electrons, ions (singly, multiply charged)
- Excited state



(a) Hall Effect Thruster



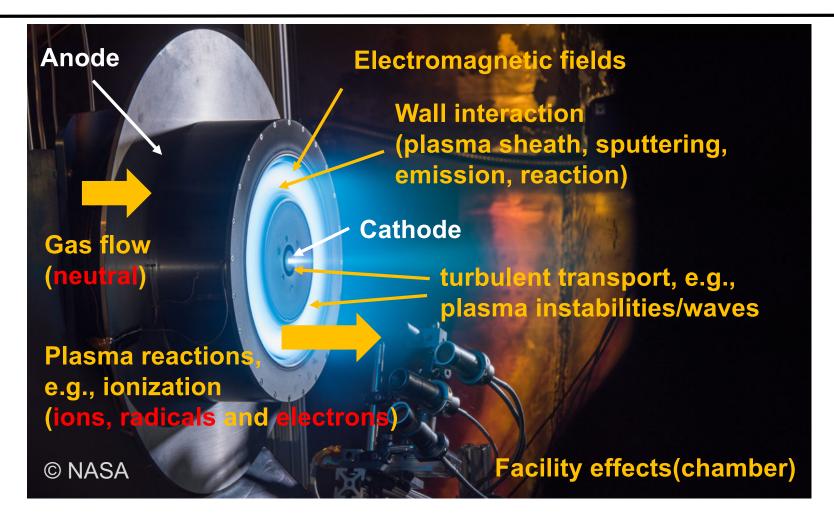


(b) Magnetron Discharge





Nonlinear coupling of dynamic plasma processes





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Why computational modeling?

Verification / Benchmarking

- Theoretical understanding
- Numerical understanding

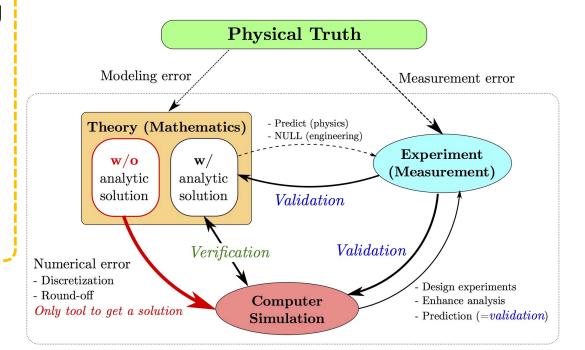
Validation

- vs. Experiments
- Modeling of Diagnostics
- Understanding of physical phenomena



Designing tool

- Predictive modeling
- System analysis
- Product designing



Why simulation? [with Professor Bram Van Leer (UM, Aero)]



Low temperature plasma (LTP) models

OP PUBLISHING

JOURNAL OF PHYSICS D: APPLIED PHYSIC

J. Phys. D: Appl. Phys. 42 (2009) 194013 (20pp)

doi:10.1088/0022-3727/42/19/194013

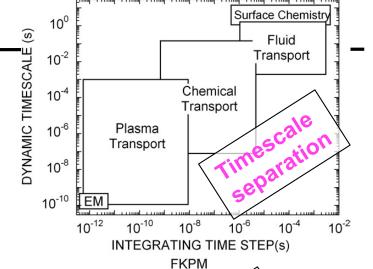
REVIEW ARTICLE

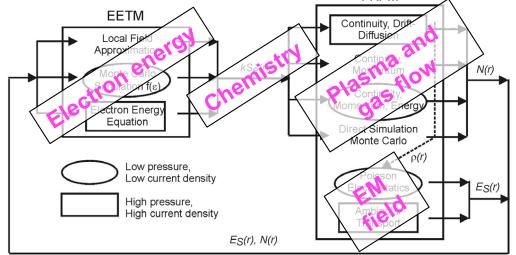
Hybrid modelling of low temperature plasmas for fundamental investigations and equipment design

Mark J Kushner

Electrical Engineering and Computer Science Department, University of Michigan, 1301 Beal Ave., Ann Arbor, MI 48109-2122, USA

- Multiscale nature
- Multiphysics
 - Electrons
 - Heavy species
 - Wall interaction (boundary condition)







Physics-based modeling techniques for plasma flows

(a) Fluid (continuum) models

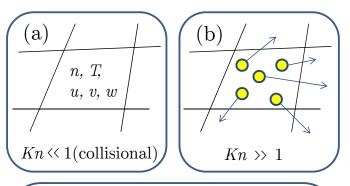
- Drift-diffusion model
- Euler/Navier-Stokes/MHD/Two-fluid
- Numerically inexpensive

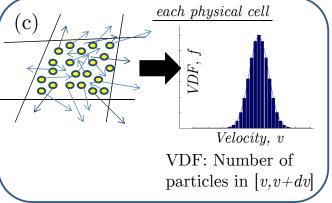
(b) Particle-based kinetic methods

- 1 macroparticle ≈ 10⁵-10⁸ real particles
- Particle-in-cell (PIC), DSMC, MCC

(c) Grid-based direct kinetic (DK) methods

- Solve kinetic equations directly in discretized phase space
- No statistical noise vs. particle method









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Classical vs anomalous electron transport

Chapter 5 in Chen's book

(Using single-fluid resistive MHD,) the flux associated with diffusion is

$$\Gamma = n\boldsymbol{u}_{\perp} = -D_{\perp}\nabla n.$$
 [5.98]

Where

$$D_{\perp} = \frac{2m\nu_{ei}k_BT}{e^2B^2} = 2\frac{\nu_{ei}}{\omega_{ce}}\frac{k_BT}{eB}.$$
 [5.99] Classical

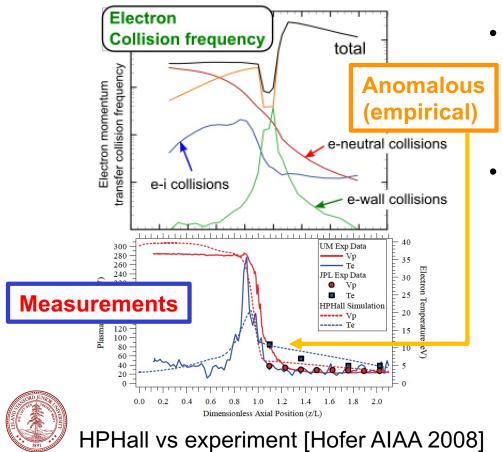
... In almost all previous experiments, D_{\perp} scaled as B^{-1} , rather than B^{-2} , Furthermore, the absolute value of D_{\perp} was far larger than that given by Eq. [5.99]. This anomalously poor magnetic confinement was first noted in 1946 by Bohm, Burhop, and Massey, Bohm gave the semiempirical formula

$$D_{\perp} = \frac{1}{16} \frac{k_B T}{eB} = D_B.$$
 [5.111]

Anomalous (cf. Bohm)



The way we *thought* about cross-field electron transport in low-temperature magnetized plasmas



Drift-diffusion flux (e.g., Ohm's law)

$$\mathbf{\Gamma} \equiv n\mathbf{u} = \underbrace{\pm n\bar{\mu} \cdot \mathbf{E}}_{\text{drift}} - \underbrace{\bar{D} \cdot \nabla n}_{\text{diffusion}}$$

Electron mobility (transport

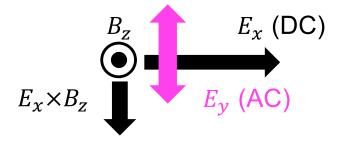
coefficient) Measurement
$$\mu_e = \frac{\Gamma_e}{-n_e \left(E + \frac{1}{e} \nabla p_e\right)}$$

$$= \mu_e^{\text{collisional}} + \mu_e^{\text{turbulent}}$$

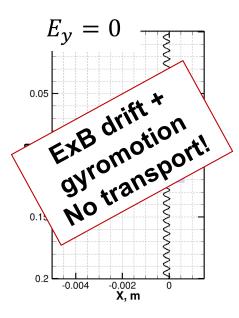
Collisionless cross-field electron transport induced by fluctuations (i.e., plasma waves)

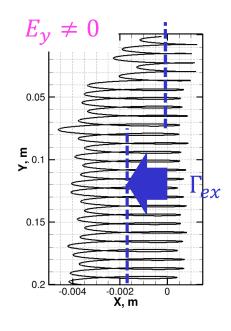
Classical theory: electrons are trapped by the magnetic field

$$\frac{d\vec{x}}{dt} = \vec{v}; \quad \frac{d\vec{v}}{dt} = \frac{q}{m} \left[\vec{E}(\vec{x}) + \vec{v} \times \vec{B} \right]$$



What if there is a plasma wave (i.e., fluctuation in the electric field)?







Turbulence: Electron transport enhanced by plasma wave (1D, 2D, 3D?)

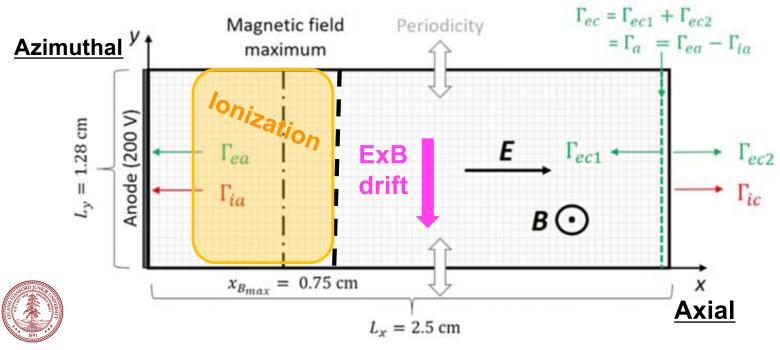
2D z-theta benchmark testcase

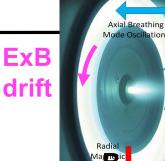
Test case proposed by Boeuf and Garrigues 2018

BC: anode + electron injection

Fixed ionization rate: run time ~30 μs (If neutrals are Emission plane

resolved, 1 ms is needed)





- 500x256 cells
- ~250 ppc
- 200 V
- 0.01 T peak
- $j_i = 400 A/m^2$
- Xe⁺
- 32 CPUs
- 1-2 weeks

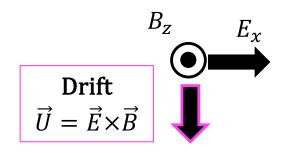
Azimutha

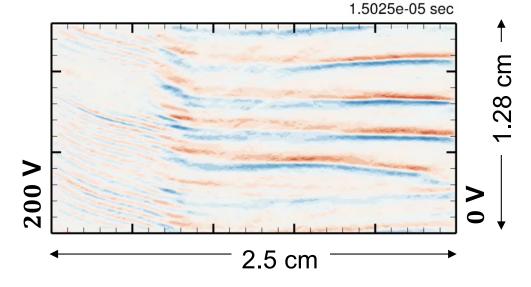
in ExB

Azimuthal plasma wave initiated by electron cyclotron drift instability (ECDI)

Movie

- ExB drift in the y-direction causes the plasma wave formation in the y-direction.
- Upstream: small scale fluctuation (dominant mode: ~1 mm)
- Fluctuating E_{ν} perturbs and detraps the electrons from the magnetic field lines
 - Singly charge ions: Xe⁺
 - Plasma wave (1D in y)



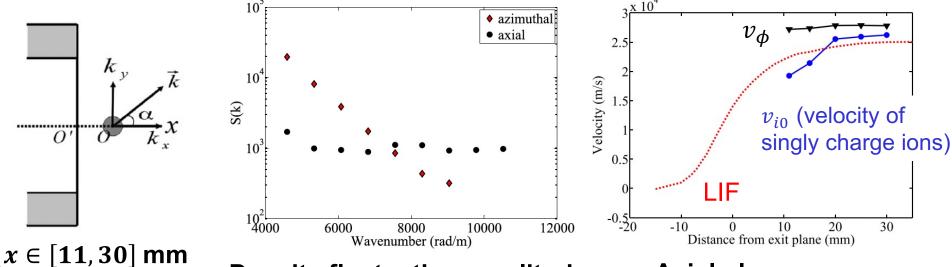




[Charoy T. et al. PSST **28**, 105010 (2019)] [Villafana W. et al. PSST **30**, 075002 (2021)] Azimuthal electric field, E_y

Experimental evidence of axial (cross-field) plasma wave due to ion-ion two-stream instability (IITSI)

- Coherent Thomson scattering (CTS) detected signature of unambiguous axial plasma wave in the plume of a cross-field discharge (with azimuthal wave).
- Phase velocity of axial wave (v_{ϕ}) is faster than Xe⁺ ion velocity (v_{i0})



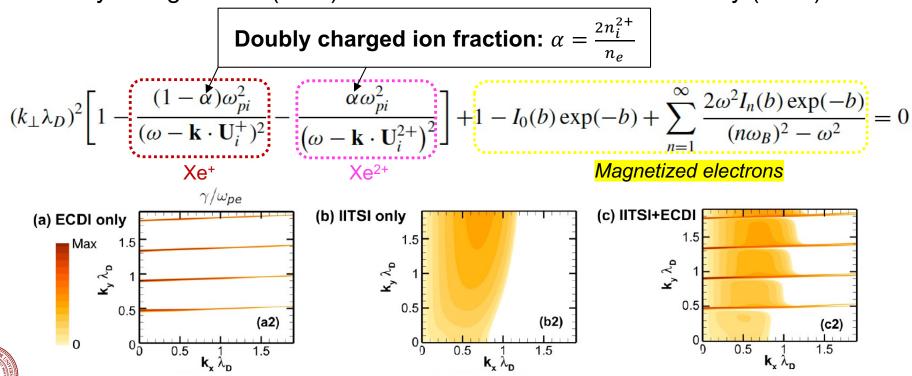
Density fluctuation amplitude

Axial plasma wave

[Tsikata S, Cavalier J, Héron A, et al. Phys. Plasmas 21, 072116 (2014)]

IITSI + ECDI dispersion theory

The CTS measurement suggested that the streams of singly-charged ions (Xe⁺) and doubly-charged ions (Xe²⁺) cause ion-ion two-stream instability (IITSI)



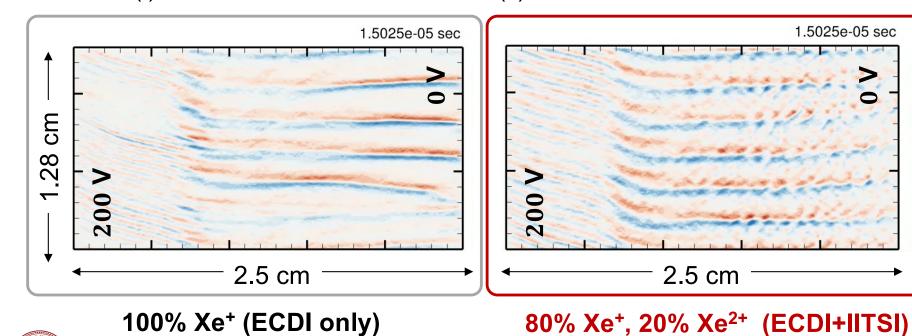


[Hara K and Tsikata S, Phys Rev E 102, 023202 (2020)]

 $x10^4 \text{ V/m}$

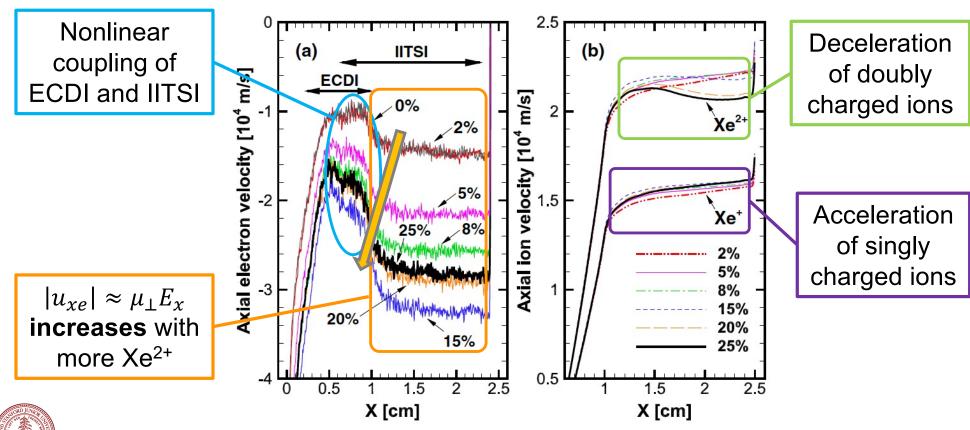
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Multidimensional (2D) plasma wave is observed due to the coupling of (i) **axial** oscillation via IITSI and (ii) **azimuthal** oscillation via ECDI





Cross-field transport: electrons and ions





[Hara K and Tsikata S, Phys Rev E 102, 023202 (2020)]

Time-averaged electron streamline

Fluctuation-based electron transport [Waltz PoF 1982, Liewer Nucl Fusion 1985]

$$\langle \Gamma_{ex} \rangle = \frac{\langle n'_e E'_y \rangle}{B_z}$$

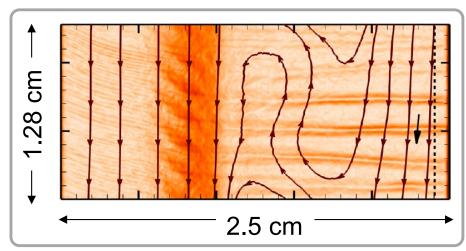
$$\langle \Gamma_{ey} \rangle = -\frac{n_{e0}E_{x0}}{B_z} - \frac{\langle n'_e E'_x \rangle}{B_z}$$

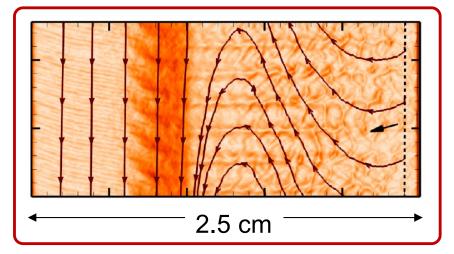
100% Xe+ (ECDI only)

$$|\langle \Gamma_{ex} \rangle| < |\langle \Gamma_{ey} \rangle|$$

80% Xe⁺, 20% Xe²⁺
$$|\langle \Gamma_{ex} \rangle| > |\langle \Gamma_{ey} \rangle|$$

$$|\langle \Gamma_{ex} \rangle| > |\langle \Gamma_{ey} \rangle|$$



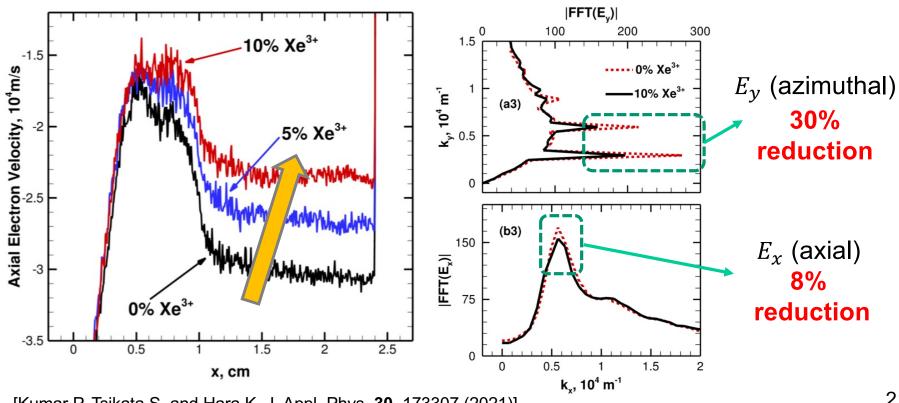




Color: amplitude of electric field. Line: electron streamlines.

Wave damping due to addition of third species (Xe³⁺) leading to *reduced* cross-field electron diffusion

 $|u_{xe}| \approx \mu_{\perp} E_x$ decreases with more Xe³⁺ due to damping of plasma waves





[Kumar P, Tsikata S, and Hara K, J. Appl. Phys. 30, 173307 (2021)]

Azimuthal IVDF: Nonlinear trapping

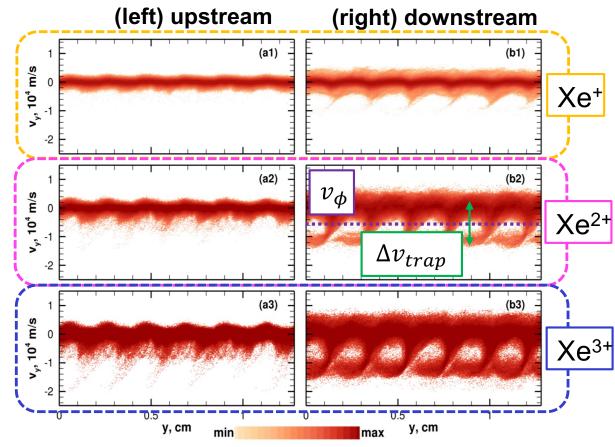
Phase velocity θ -wave

$$v_{\phi} = 6 \times 10^3 \text{ m/s}$$

Trapping velocity

$$\Delta v_{trap} = \left(\frac{2Ze\phi_0}{m_i}\right)^{1/2}$$

 ϕ_0 : potential amplitude





Summary: Part 1 (anomalous electron transport)

- Coupling of ECDI (azimuthal) and IITSI (axial) modes is studied using a 2D parallel PIC code. Analyzed plasma waves and cross-field electron transport.
- The results adding Xe²⁺ and Xe³⁺ suggest that cross-field electron transport/diffusion is affected by the *amplitude* of the multidimensional (2D) plasma wave.
- Recent PIC simulations show the effects of the wavelength of the azimuthal plasma wave on cross-field electron transport. [Kumar, Sewell, Hara, AIAA SciTech 2022]



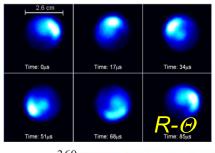
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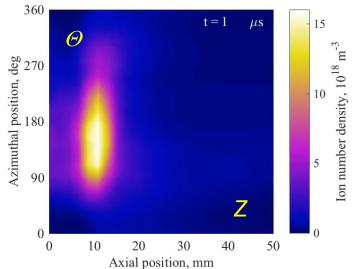


Low-frequency (10-30 kHz) plasma oscillations

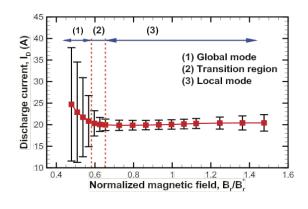
Movie



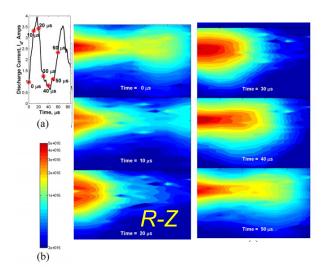
Azimuthally rotating spokes [Ellison 2011]



Gradient drift instability [Kawashima & Hara 2018]



Mode transition: ionization oscillation [Sekerak PhD 2014]



Breathing mode: highspeed probe [Lobbia PhD 2010]

Theory: fluid moment equations



Anisotropic pressure tensor

Fluid equations

$$p_{ij} = mn \iiint (v_i - u_i)(v_j - u_j)\hat{f}(\mathbf{v})d^3\mathbf{v}$$

$$\begin{cases}
\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0 \\
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + \frac{1}{mn}\nabla \cdot \bar{p} - \frac{q}{m}(\mathbf{E} + \mathbf{u} \times \mathbf{B}) = \mathbf{F} \\
\frac{\partial (n\epsilon)}{\partial t} + \nabla \cdot (n\epsilon\mathbf{u} + \bar{p}) \cdot \mathbf{u} + \mathbf{q} = \mathbf{j} \cdot \mathbf{E} + \mathbf{S}
\end{cases}$$

Collision terms



Heat flux

Simulation: plasma fluid modeling strategies

Drift-diffusion (DD) flux models

$$\nabla \cdot \left(\vec{\Gamma}_i - \vec{\Gamma}_e\right) = 0 \Longrightarrow \nabla \cdot \left(n_e \overline{\overline{\mu_e}} \cdot \nabla \phi\right) = f(p_e, \vec{\Gamma}_i)$$

Quasineutral $(n_i \approx n_e)$ DD model:

[HPHall (Fife, Martinez-Sanchez, 1998), HPHall-2/3 (Ahedo 2006, Hofer 2008), Hall2De (Mikellides 2009), Detailed fluid model (Choi and Boyd 2008), other models (Boeuf and Garriques 1998, Barral 2003, Hara 2014)]

Non-neutral $(n_i \neq n_e)$ DD model:

Used in LTP models [Kushner 2009]

neutral
$$(n_i \neq n_e)$$
 DD model:
$$\frac{\partial n_e}{\partial t} + \nabla \cdot \left[-\overline{\mu_e} \cdot \left(n_e \vec{E} + \nabla p_e \right) \right] = \dot{n}_e$$
Scharfetter-Gummel scheme, Dielectric relaxation time
$$\nabla^2 \phi = -\frac{e}{\epsilon_0} (n_i - n_e)$$

Full fluid moment (FFM) model

Need non-oscillatory schemes for the nonlinear inertia term (cf. hyperbolic PDE) Used in other fields, e.g., CFD and HTP [Hakim, Hammett, Srinivasan, Shumlak]



$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{\Gamma} = S$$
, where $U = [n, n\vec{u}, n\varepsilon]$ & $\nabla^2 \phi = -\frac{e}{\epsilon_0}(n_i - n_e)$

Fluid equations for magnetized plasmas

Total energy (TE)
$$\frac{\partial (n\epsilon)}{\partial t} + \nabla \cdot \left(n\epsilon \mathbf{u} + \mathbf{u} \cdot \bar{P} \right) = \mathbf{j} \cdot \mathbf{E} + S,$$
 $S_{heat} = \mathbf{j} \cdot (\mathbf{E} + \mathbf{y} \times \mathbf{B})$

Internal energy (IE)
$$\frac{\partial (ne)}{\partial t} + \nabla \cdot [(ne+p)\mathbf{u}] = S_{\text{trans}} + S$$
, $S_{trans} = -\mathbf{u} \cdot (\mathbf{R} - \nabla p)$,

 $\epsilon = e$ (internal energy) +K (kinetic/drift energy)

- (i) If non-magnetized $(K \rightarrow 0)$, $S_{heat} = S_{trans}$
 - Total energy input $(j \cdot E)$ goes only to the internal energy.
 - Drift-diffusion (DD) approximation can be exactly recovered.
- (ii) If magnetized (e.g., ExB drift; $K \neq 0$), $S_{heat} \neq S_{trans}$
 - $\epsilon = e + K \neq e$: TE and IE equations are NOT identical.
 - DD approximation cannot be used for magnetized plasmas with drift.



Full-Fluid Moment (FFM) Model

Model description

$$\frac{\partial U}{\partial t} + \nabla \cdot \vec{\Gamma} = S$$

• 1D2V/2D2V finite volume model: ions, electrons, and neutrals

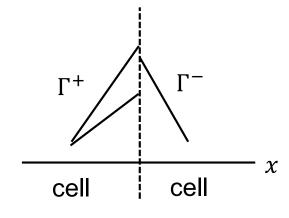
flux source

- 5-moment fluid equation with Poisson equation
- Global Lax-Friedrich flux splitting with MUSCL reconstruction

$$\Gamma = \Gamma^+ + \Gamma^-$$

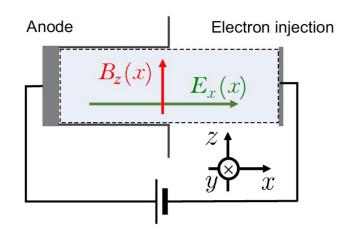
- Time integrator: Strong Stability Preserving Runge-Kutta (RK3-SSP)
- Boundary conditions
 - Kinetic flux treatment
 - Quasineutral electron injection at cathode for 1D
- Message Passing Interface (MPI) for 2D



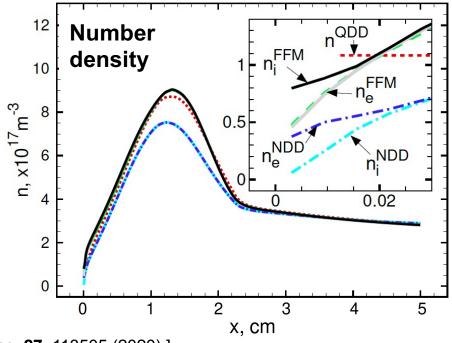


1D cross-field plasma discharge benchmark test

- Xenon mass flow from anode
- lons: collisionless and non-magnetized
- Electrons: collisional and magnetized
- Applied potential drop of 300 V
- Applied magnetic field profile (160 G)
- Anomalous transport for steady state



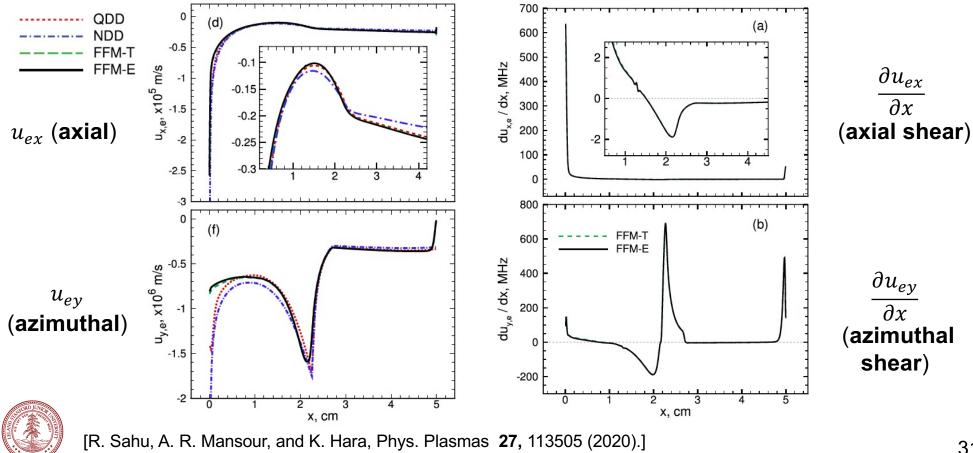
Full-fluid moment (FFM) model vs. Quasineutral drift-diffusion (QDD) and nonneutral drift-diffusion (NDD) models





[R. Sahu, A. R. Mansour, and K. Hara, Phys. Plasmas 27, 113505 (2020).]

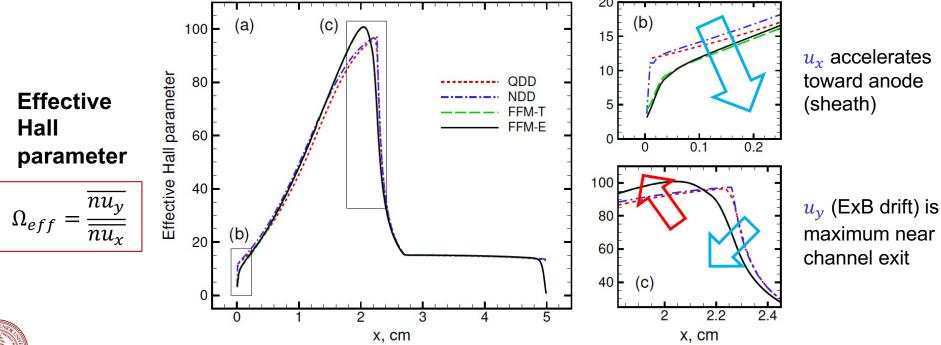
Inertia terms can be captured using the 5-moment FFM



Shear-driven cross-field electron transport

 Effects of the nonlinear inertia term (e.g., shear) on electron transport are observed: shear diamagnetic drift.

$$\vec{u}_{\perp} = \frac{1}{|\vec{B}|^2} \left[-\vec{E} \times \vec{B} + \frac{1}{qn} (\nabla p \times \vec{B}) + \frac{m}{qn} \{ \nabla \cdot (n\vec{u} \otimes \vec{u}) \times \vec{B} \} \right]$$



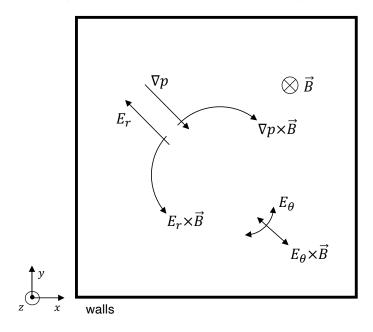


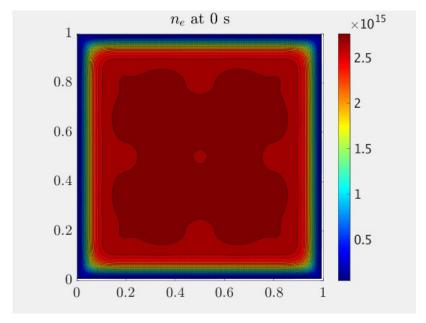
[R. Sahu, A. R. Mansour, and K. Hara, Phys. Plasmas 27, 113505 (2020).]

2D FFM model of Penning discharge

Movie

- Steady-state discharge is maintained with the ionization (source)
- Ambipolar diffusion sets up: electric field and density gradient







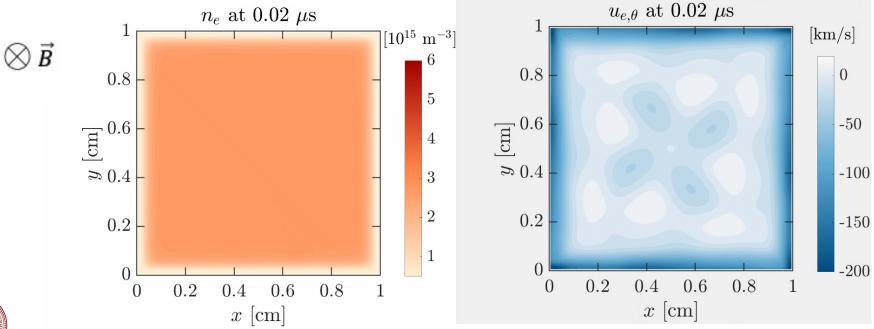
Numerical setup

Unmagnetized case

Rotating spoke in Penning configuration

Movie

- Azimuthally rotating spokes are robustly observed using a 2D full fluid moment (FFM) model.
- Rotation is in the direction of the diamagnetic drift (not ExB drift)





[A. R. Mansour and K. Hara, AIAA 2021, GEC 2021; submitted]

Summary: Part 2 (fluid theory and simulation)

- We showed that drift-diffusion (DD) models can be invalid in magnetized plasmas where the drift is large.
- We developed a 5-moment full-fluid moment (FFM) model
 - 1. 1D cross-field discharge plasma. Benchmarked against quasineutral DD (QDD) and nonneutral (NDD). **Shear-induced electron transport**.
 - 2. 2D self-organizing **azimuthally rotating spokes** in a Penning-type setup. Spoke rotation found to be in the direction of diamagnetic drift.
- Current development: (i) capacitively coupled plasma (CCP) sources, (ii) plasma formation in high-power microwaves (HPMs), and (iii) RF breakdown.
- We are also developing a 10-moment FFM model [Kuldinow, Mansour, and Hara, AIAA SciTech 2022]

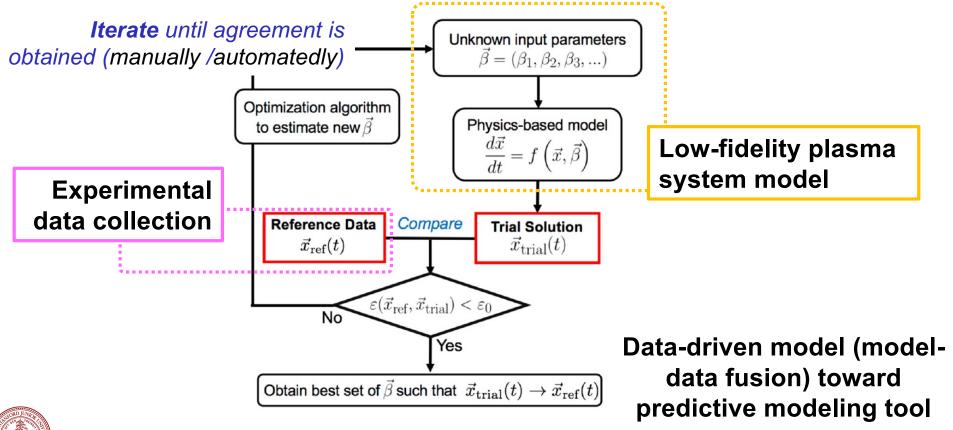


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Data-driven modeling: offline validation

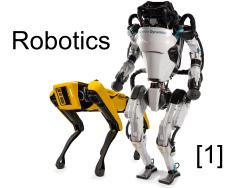




Introduction: online estimation modeling







- Real-time estimation of states, parameters, and associated uncertainties
- Examples: extended/ensemble Kalman filter (linearized model to predict), particle filter (good for highly-nonlinear, unstable systems), recursive least squares (fitting a function), neural network (typically black box; works well when training data are abundant)

[1] Boston Dynamics

Real-time estimation of plasma oscillations

Inverse

problem

Can we estimate the unknown parameter (=Te) from measurement?

Physics-based model. 0D time-dependent predator-prey system [*]:

lons:
$$\frac{dN_i}{dt} + \frac{N_iU_i}{L_{ch}} + \frac{2N_iU_{i,w}}{R_{\Delta}} = N_iN_n\xi_{ion}$$

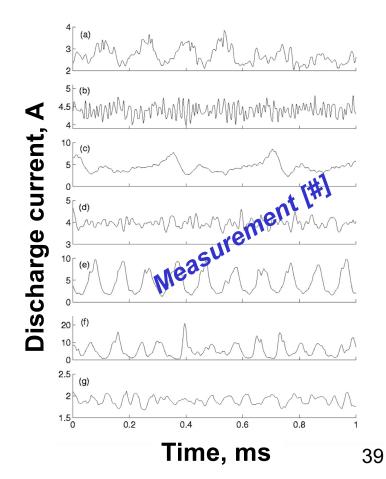
Neutrals:
$$\frac{dN_n}{dt} + \frac{(N_n - N_{int})U_n}{L_{ch}} = -N_i N_n \xi_{ion}$$

Ionization rate coefficient:

$$\xi_{ion} \approx \left[AT_e^2 + B \exp\left(-\frac{C}{T_e}\right)\right] \left(\frac{8eT_e}{\pi m}\right)^{1/2}$$



[*] K Hara, M. Sekerak, I Boyd, A. Gallimore, Phys Plasmas (2014) [#] N Gascon and M Dudeck et al., Phys Plasmas (2003)



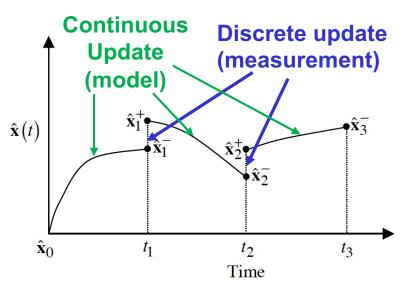
Physics-informed extended Kalman filter (EKF)

$$\frac{dN_i}{dt} = f_1(N_i, N_n, T_e)$$

$$\frac{dN_n}{dt} = f_2(N_i, N_n, T_e)$$

$$\frac{dT_e}{dt} = f_3(N_i, N_n, T_e)$$

Satisfy physical constraints!!



Model forecast (predictor)

$$\dot{\widehat{x}} = f(\widehat{x})$$

- Estimated variables: x̂
- Estimated covariance (error): **P**

Data assimilation (corrector)

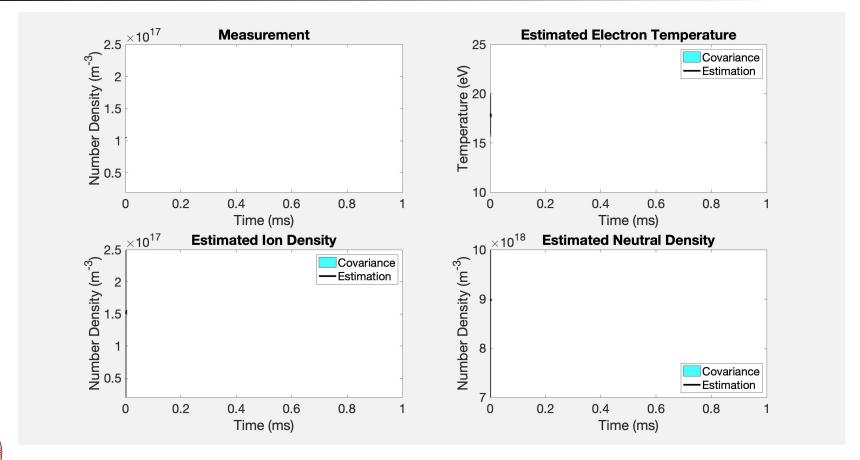
- Measurements: \widetilde{y}
- Measurement error: σ_r
- Update estimated variables:

$$\widehat{x} \leftarrow \widehat{x} + K[\widetilde{y} - h(\widehat{x})]$$

Kalman gain: *K* (a coefficient for how much the estimated quantity is <u>updated/corrected</u> by the measurement)



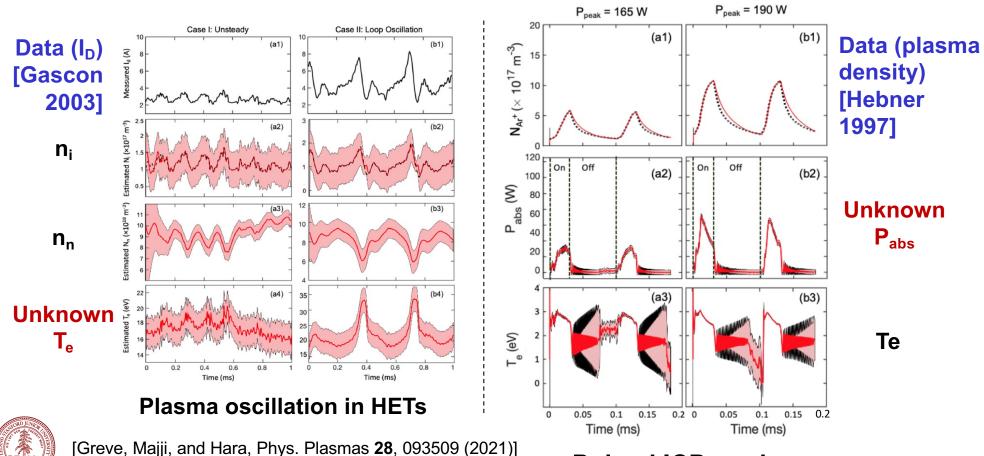
EKF for plasma oscillations in Hall effect thrusters





[Greve, Majji, and Hara, Phys. Plasmas 28, 093509 (2021)]

EKF for plasma chemistry and reaction



[Greve, Majji, and Hara, Phys. Plasmas **28**, 093509 (20 [Greve and Hara, GEC 2021; in preparation]

Pulsed ICP modes

Summary: Part 3 (model-data fusion)

- **Model-data fusion** is an approach to use *low-fidelity* physics-based models and augment/correct the estimates with experimental data.
 - Offline approach: correlation of datasets / data calibration
 - Online (real-time) approach: use incoming measurements and uncertainty propagation to estimate states and parameters
- We are currently applying the EKF model to a few applications
 - Plasma chemistry in semiconductor devices
 - 1D and 2D partial differential equations (PDEs)
 - Circuit and plasma coupling in electric propulsion systems



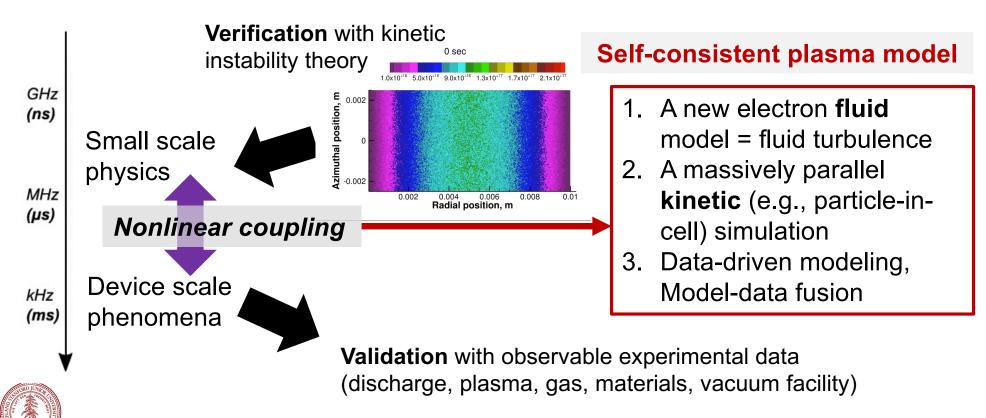
Outline

- 1. Introduction: Low temperature magnetized plasmas
- 2. Computational plasma modeling
- 3. Physics and modeling of low-temperature magnetized plasmas
 - Kinetic theory/modeling of plasma instabilities and turbulence
 - Fluid modeling of low-temperature magnetized plasmas
 - Data-driven online estimation for plasma chemistry

4. Conclusion



Toward a self-consistent model of electron transport in partially magnetized plasmas



Conclusion

We are developing **physics-based** models

- **Kinetic**: particle-in-cell (PIC), Monte Carlo collision (MCC), direct simulation Monte Carlo (DSMC), grid-based direct kinetic (DK)
- Fluid: drift-diffusion (DD), full-fluid moment (FFM)

as well as data-driven models

Online (real-time) state estimation: extended Kalman filter (EKF)
 for a wide range of plasma applications and rarefied gas flows.

These simulations, verified with theory (e.g., linear instability), are used to understand the nonlinear saturation, i.e., turbulence, leading to cross-field plasma transport.

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Thank you for your attention

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