Theoretical & simulation studies of plasma/ wall interactions & boundary plasmas

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Acknowledgement: multidisciplinary LANL team

- **It has been a multi-year LANL effort to set up the collaboration and teaming in the area of PMI and boundary plasmas.**
- **Plasma physics**
  - Plasma Physicists: Gian Luca Delzanno (sheath with surface electron emission and dust) and Xianzhu Tang (sheath, presheath, SOL, stochastic fields, dust, pedestal).
  - Plasma Postdocs: Zehua Guo (theory and kinetic modeling of SOL and sheath); Chris MecDevitt (pedestal transport); Bhuvana Srinivasan (computational two-fluids), Grisha Kagan (pedestal theory), Erinco Camporeale (implicit PIC)
- **Materials science**
  - Materials postdocs: Valery Borovikov (W grain boundary mobility and self-healing)
  - Collaborating material scientists: Art Voter (MD/AMD/materials theory), Danny Perez (AMD/materials theory), Blas Uberuaga (materials theory/radiation damage)
- **Programmatic leverage**
  - Materials side leverages on DOE Energy Frontier Research Center, Nuclear Energy Hub, ASC materials, Fission Advanced Fuel
  - Plasma simulation and staff at XCP-6: Andrei Simakov, William Daughton, Brian Albright.

Overview

- **Three classes of plasma-materials interaction (PMI) issues**
  - distribution of plasma irradiation flux
  - Materials response to plasma and neutron irradiation
  - Wall feedback to the plasma
- **Materials response and wall survivability**
  - Tritium trapping and self-healing of radiation damage by W grain boundary motion
  - Wall recycling & surface morphology change: interatomic potential for surface study
  - Dust transport is a key PMI issue
- **Boundary plasmas: sheath and presheath**
  - Unmagnetized; magnetized with large incident angle; parallel to wall; oblique to wall; reactor-level obliqueness
- **Upstream plasma profile depends on wall recycling (collisionality)**
  - Parallel temperature profile in the long mean-free-path regime (low recycling)
  - Ambipolar potential, parallel flow acceleration, & parallel heat flux
  - Wall potential

Distribution of plasma irradiation flux

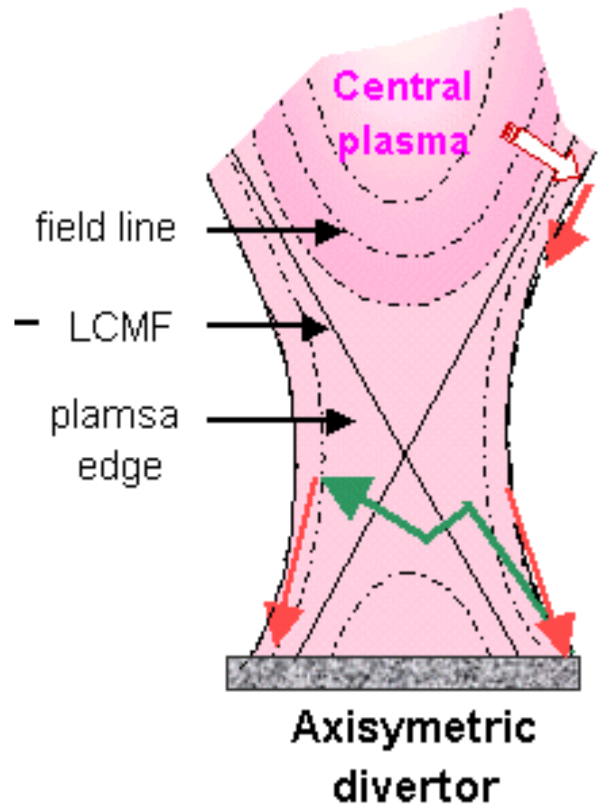
- **A prerequisite for studying wall response: energy and angular distribution function of plasma irradiation flux**
- **Subtlety comes from non-Maxwellian distribution (v.s. shifted Maxwellian)**
  - Gyro-orbit loss with oblique magnetic field -> hole (loss region) in velocity space
  - Parallel streaming loss -> temperature anisotropy
  - Magnetic modulation (e.g. flux expansion) -> extreme non-Maxwellian ions
- **Coupling to surface morphology feature on ion gyroradius scale -> drive surface morphology evolution**
  - In return, surface morphology change modifies local distribution of the plasma irradiation flux, closing the feedback loop.

Materials response to plasma and neutron irradiation

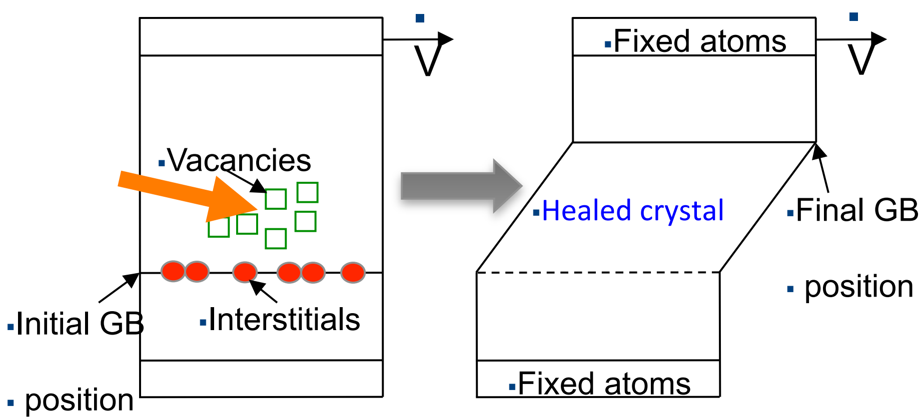
- **There are numerous issues here (eventually integrated to determine engineering performance)**
  - **we will attempt to identify and understand individual controlling physics first, with a focus on those directly affected by and impact plasmas**
- **Surface response:**
  - On plasma ions: what governs steady state recycling?
  - On wall impurity ions: what determines erosion and redeposition rates and how they can be balanced?
  - Stability of the surface morphology
- **Tritium retention**
  - Trapping sites production and removal
  - Tritium transport in materials

Understanding wall feedback

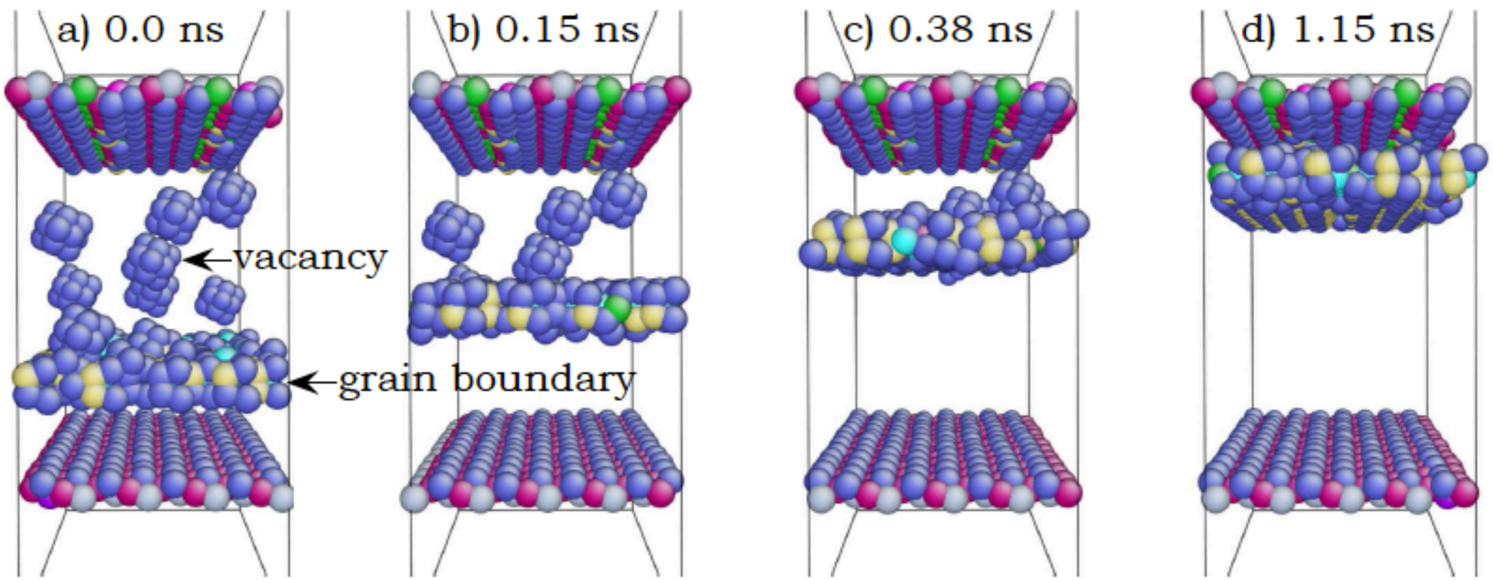
- **Feedback flux of plasma species**
  - Neutral influx via recycling largely determines the collisionality of boundary plasmas
    - Strong collisionality dependence of boundary and upstream plasma profile
    - Control knobs: neutral density control via cryo-pumping; choice of wall materials (solid versus liquid)
- **Feedback flux of impurities (wall material species)**
  - Will it poison the core plasma?
  - Can it be locally redeposited?
- **Dust production and transport**
  - Too many of them survive in dust form -> operational safety issue
  - Even if majority does not survive, source for non-local redeposition
  - A wild card for reactor scenario as for now.



Tritium trapping: self-healing by grain boundary motion



A collision cascade produces vacancies and highly mobile interstitials; the diffusing interstitials find, and are trapped at, a nearby GB. The interstitial-loaded GB is now so easy to shear that internal stresses in the crystal may start it moving, and the coupled motion causes it to sweep past the cascade center, sweeping up the vacancies as it moves through.



Borovikov, et al, PRB, 2012

Interstitial-loading impacts GB coupled motion

- **Interstitial loading can**
  - **lower the sliding friction force and thus reduce the critical stress for the onset of normal migration of grain boundary**
  - **trigger coupled motion in clean GB that does not have coupled motion**
  - **switch the direction of normal migration**

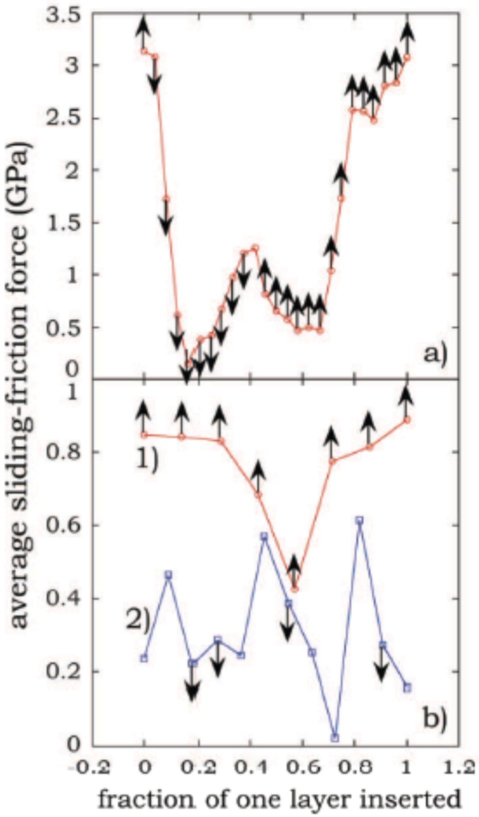


FIG. 2: Average sliding-friction force over a sliding distance of 10 Å, as a function of number of interstitials introduced into: a) Σ5(013)[100] GB, b) 1) $(\bar{3}\bar{1}0)[1\bar{3}\bar{2}]/(51\bar{1})[066]$ and 2) $(\bar{2}04)[231]/(\bar{4}04)[3\bar{2}\bar{3}]$ twist-tilt GBs. The direction of normal GB motion is indicated by the arrows. The points without arrows correspond to pure sliding.

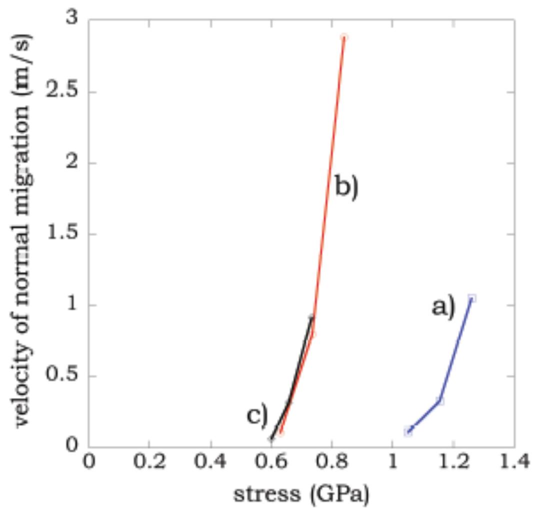


FIG. 3: (a) Velocity vs. stress at T=1000 K for Σ5(012)[100] GB loaded with interstitials, (b) velocity vs. stress at T=2000 K for Σ5(012)[100] GB loaded with interstitials, (c) velocity vs. stress at T=1000 K for twist-tilt GB $(\bar{2}04)[231]/(\bar{4}0\bar{4})[3\bar{2}\bar{3}]$ loaded with interstitials.

Wall recycling and surface morphology evolution (focus of next 5 years): interatomic potential fitting

- **Surface response to plasma irradiation is ideal for molecular dynamics simulation (MD).**
- **Fidelity of molecular dynamics and higher level models is critically dependent on the quality of the interatomic potential.**
  - While using the known W potential in current research on GB and bulk W,
  - We have started a series of new interatomic potential fitting using the LANL expertise in this area.
- **W potential fitting**
  - Current W potential has many local minima
  - We have fitted a new DFT-based W potential and are in the process of testing it.
- **W-He potential fitting**
  - With new Density Functional Theory (DFT) calculation, we have fitted W-He using an existing form of W potential and are in the process of testing it.
  - Next step is to fit W-He with our new W potential.
- **Future fittings include:** W-H and H-He; W-Be, Be-H, Be-He.

Borovikov, et al, 2012

Dust transport is a key PMI issue

- **High heat load -> 100s' kg of dust estimated for ITER**
- **Safety issues: toxicity, reactivity, tritium retention, radiotoxicity**
- **Operational issues:**
  - Dust penetration: core plasma pollution and disruption
  - PMI: dust survivability and non-local redeposition
- **Dust must stay close to wall to survive**
  - Normal: force balance between electrical and ion drag -> levitation or oscillation around equilirium
    - Electric force: local E field, charging versus electron emission (T dependent)
  - Poloidal and toroidal (parallel to wall): unbalanced ion flow drag -> strong acceleration, hence long distance migration
  - Survivability: heating of dust > radiatively cooling -> melting -> nonlocal redeposition.

$$\text{Charging equation}: \frac{dQ_d}{dt} = I_{e,i}\left(Q_d, n_{e,i}(\mathbf{x}_d)\right) - I_{sec}\left(Q_d, n_{e,i}(\mathbf{x}_d)\right) - I_{th}\left(Q_d, n_{e,i}(\mathbf{x}_d), T_d\right)$$

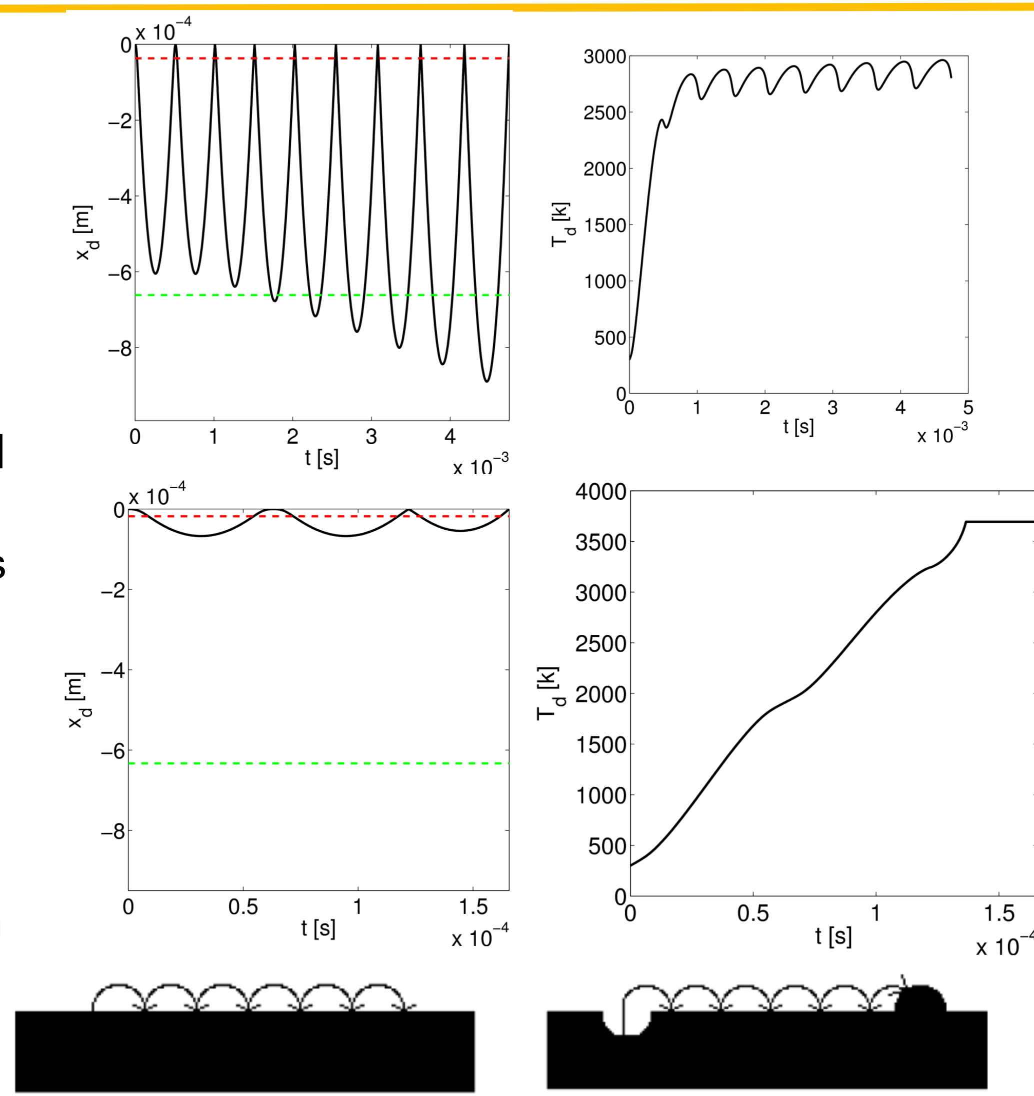
$$\text{Equation of motion}: \frac{d\mathbf{x}_d}{dt} = \mathbf{v}_d;\;\; m_d\frac{d\mathbf{v}_d}{dt} = Q_d\mathbf{E}_{scl}(\mathbf{x}_d) + \mathbf{F}_{drag}\left(\mathbf{V}_{i,scl}(\mathbf{x}_d) - \mathbf{v}_d\right)$$

$$\text{Temperature equation}: m_d C_d\frac{dT_d}{dt} = \pi r_d^2 \Gamma_H,$$

Delzanno, Tang, 2011

Dust survivability strongly reduced in reactor conditions

- **1 micron dust particle can survive in 1 MW/m^2**
  - Radiative cooling prevents melting;
  - accelerated to high speed, travel long distances
- **1 micron dust particle survivability greatly reduced in 10 MW/m^2**
  - Shorter duration, few collisions with wall before melting
  - Thermionic emission induces heat flux collection spike
  - Redeposits non-locally: fixed plasma poloidal flow direction leads to mass migration
- **With 10 MW/m^2, 0.1 micron dust redeposit locally; 10 micron dust can survive**



Delzanno, Tang, 2012

Kinetic model of plasma sheath: unmagnetized and magnetized with low collisionality

- **Bohm's sheath theory requires collisional plasma**
- **Low collisionality poses a problem for ambipolarity in steady state**
  - (pre)sheath electric field leads to trapped electrons.
  - Upstream sourcing fills both the trapped and passing zone in velocity space for electrons
    - Ions are all passing.
  - Ambipolarity demands electron detrapping flux
    - If collision can not do the job, collisionless detrapping by wave-particle interaction must step in
- **Kinetic instabilities to the rescue**
  - Unmagnetized plasma: Weibel instability by T anistropy (Tang, PPCF, 2011)

$$\frac{\partial}{\partial t}\Delta T = -V_x\frac{\partial}{\partial x}\Delta T - 2T_x\frac{\partial V_x}{\partial x} - \frac{2}{n}\frac{\partial}{\partial x}(q^x - q^y). \qquad \Delta T \equiv T_x - T_y$$

$$\gamma = \left(\frac{8}{27\pi}\right)^{1/2}\omega_{pe}\left(\frac{kT_{ex}}{m_e c^2}\right)^{1/2}\frac{T_{ex}}{T_{e\perp}}\left(\frac{T_{e\perp}}{T_{ex}} - 1\right)^{3/2}.$$

  - Magnetized plasma: trapped electron driven whistler instability (Guo & Tang, 2012)
    - Far more virulent than temperature anisotropy driven whistler instability

Kinetic model of plasma sheath: B parallel to wall

- **Gyro-orbit loss is the dominant wall charging mechanism**
  - Large ion gyroradius lends to positive wall charging
- **Well-defined loss region in velocity space**

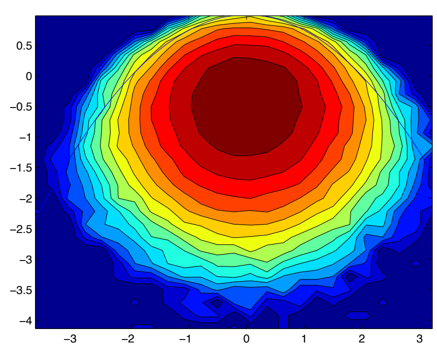
$$\epsilon_0 = \frac{1}{2}m\left[(v_x^0)^2 + (v_y^0)^2 + (v_z^0)^2\right] + q\Phi(L); \;\; p_y^0 = mv_y^0 + qB_zL; \;\; p_z^0 = mv_z^0.$$

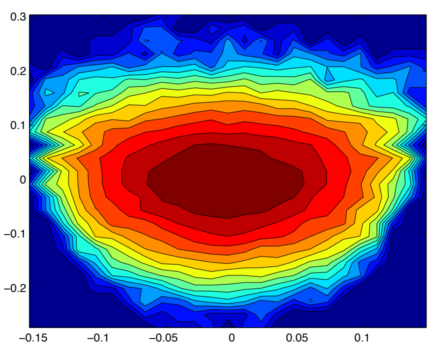
$$\begin{aligned} \frac{1}{2}m(v_x^2 + v_y^2 + v_z^2) + q\Phi(x) &= \epsilon_0 \\ mv_y + qB_zx &= p_y^0 \\ mv_z &= p_z^0 \end{aligned}$$

$$(v_x^0)^2 - \frac{qB_zL}{m}v_y^0 = \frac{q^2B_z^2L^2}{m^2} + \frac{2qV(L)}{m}$$

$$V(L) \equiv \Phi(0) - \Phi(L).$$

Electron



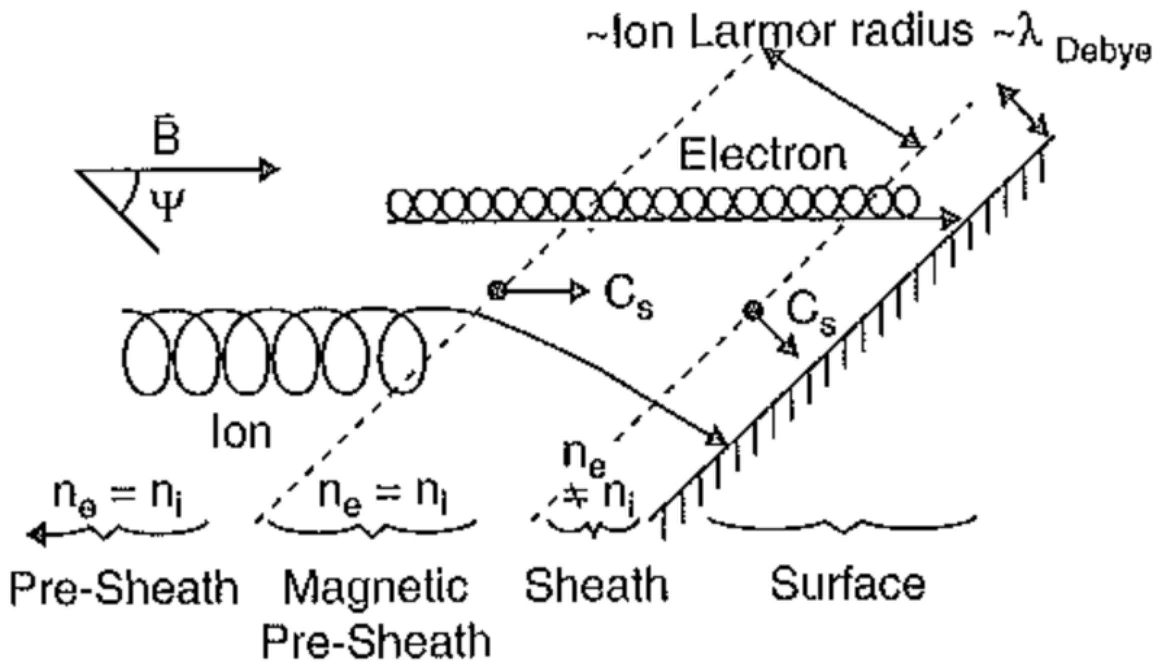


Ion

Krashenennikova & Tang,PoP 2011

Kinetic model of plasma sheath: B oblique to wall

- **Chodura gave the standard magnetized sheath theory (1982)**
  - Three regions: presheath (quasi-neutral); magnetic presheath (quasi-neutral); Debye sheath (non-neutral)
  - Model assumptions: isothermal electrons, ignoring collisional drag, viscosity
  - Bohm condition -> sonic parallel flow and sonic normal flow.



Resolution of Chodura's paradox

- **Chodura predicts a potential drop for the magnetic presheath**

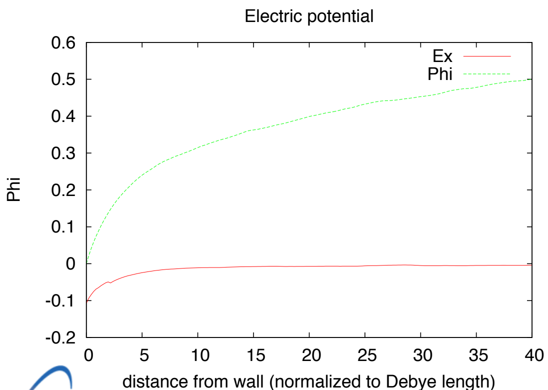
$$\frac{e\Delta\Phi_{CS}}{k_B T_e} = \ln \sin \alpha,$$

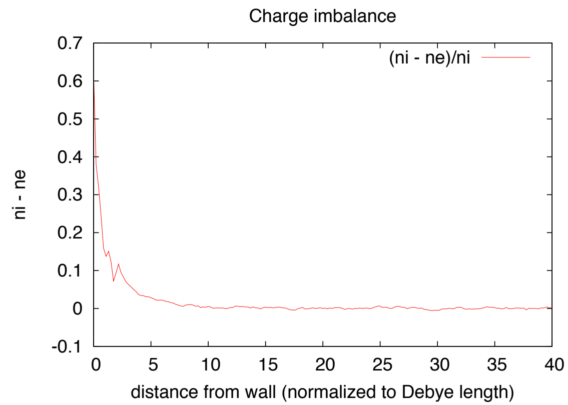
  - Derivation based on continuity, Boltzman electron, and quasineutrality

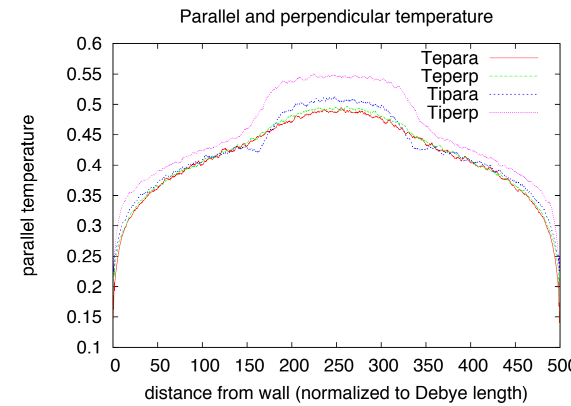
$$n_i^e v_x^e = n_i^f v_x^f, \qquad n_e = n_i = n_s \exp \frac{e(\Phi - \Phi_s)}{k_B T_e}.$$

- **For tokamak experiments, alpha < 4-5 degree, two much drop in potential – what happens to Debye sheath**

- **Resolution: quasi-neutrality is violated, along with Te variation (2 sonic flow condition also ill-defined). Chodura's estimate is way off.**

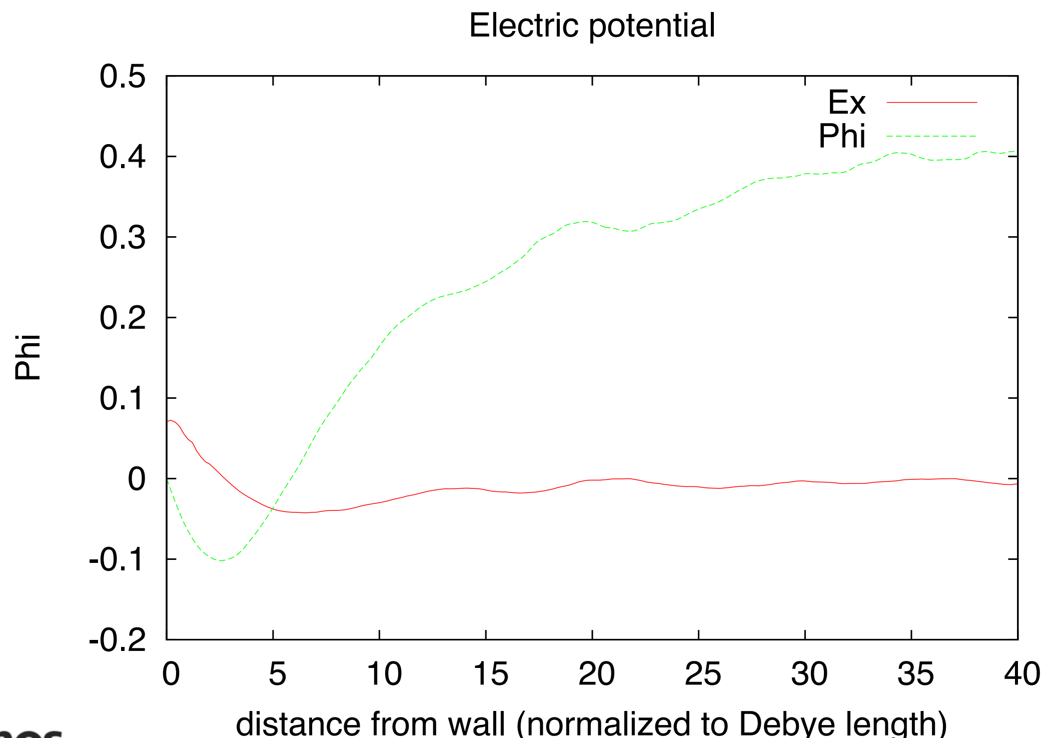






Kinetic model of plasma sheath: reactor level obliqueness

- **What happens if the angle is made reactor-level small: 1 degree or less**
  - Seperation between magnetic presheath and Debye sheath disappears, E in the wall normal direction in magnetic sheath
    - Accelerates ions into the plasma, negative effect on impurity shielding, prevents dust launching.
  - There is no sonic normal flow condition.



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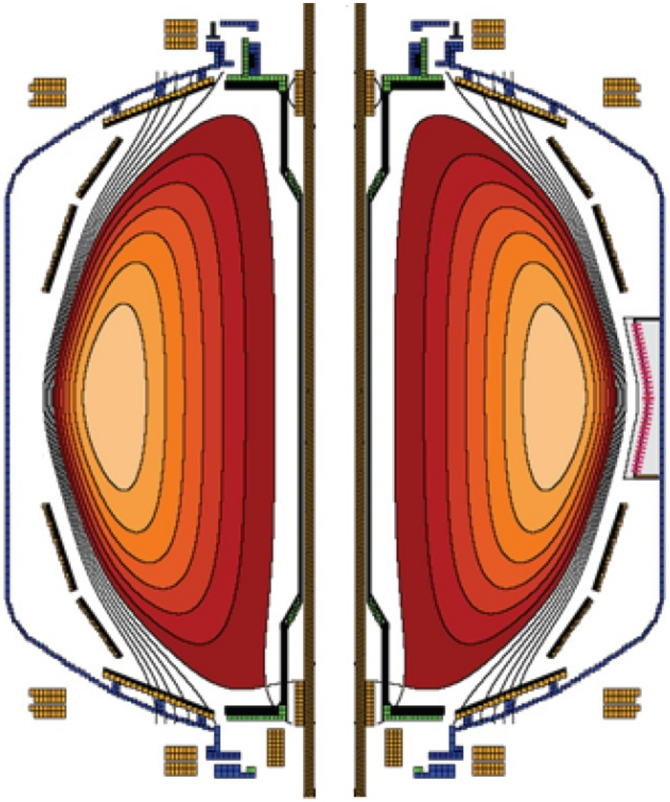
Summary

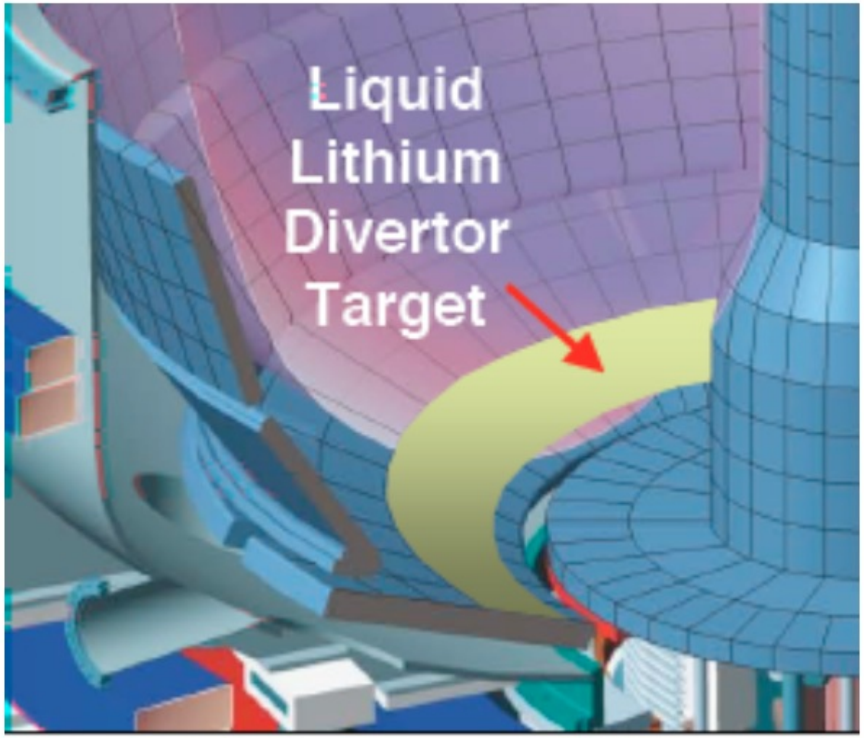
- **PMI requires close collaboration between plasma physicists and materials scientists**
  - There appears to be a well defined geometric interface for information exchange
- **Uncertainties (options) at high and low recycling regimes present bountiful of interesting plasma physics problems**
  - Low recycling -> Long mean-free-path -> plasma kinetics and closures
  - Even in high recycling and hence collisional regime, extreme oblique B field -> gyro-orbit loss -> plasma kinetics
- **Sheath theory has been revisited via kinetic theory & simulation**
  - Unmagnetized: Weibel instability in low collisionality regime.
  - B parallel to wall: sheath structure and scaling law established
  - B oblique to wall: kinetic analysis resolve Chodura paradox
  - Extreme B obliqueness: complicated sheath electric field
- **Dust is a key PMI issue**
- **Materials science aspect taught us a lesson:**
  - Extremely convoluted in processes and scales; may take a while to first isolate individual controlling physics/chemistry, then pursue meaningful integration.

Parallel transport and profile of boundary (SOL) plasmas with a low recycling wall

Motivated by the liquid lithium wall experiments

Low-recycling wall → high-T low-n boundary plasmas





NSTX & LTX: Lithium-divertor/wall → low recycling → high-T and low-n edge plasmas → different (favorable?) plasma confinement modes

Overview

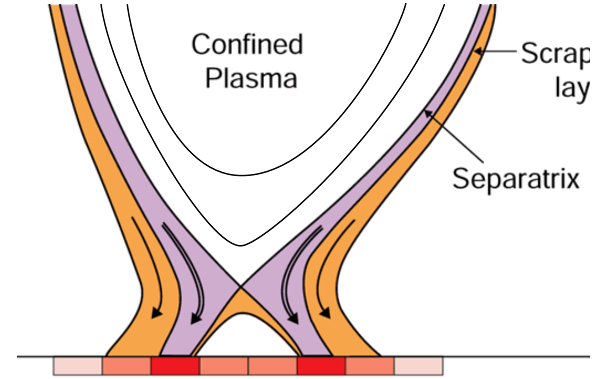
- **Characteristic electron/ion orbits and distribution functions**
  - Uniform magnetic field
  - Modulation of magnetic field strength: flux expansion
  - Trapped versus passing electrons
- **Ambipolarity of parallel transport and collisionless/collisional detrapping of electrons**
  - Trapped electron driven whistler wave & collisionless detrapping via wave-particle interaction
  - Wall potential versus collisionality
- **Relationship between parallel profile variation and B modulation & parallel heat flux**
  - The lowest-order two-temperature fluid model for parallel transport
  - Parallel temperature profile in the long mean-free-path regime (low recycling)
  - Ambipolar potential, parallel flow acceleration, & parallel heat flux
  - Parallel heat flux closure

Orbit: trapped versus passing

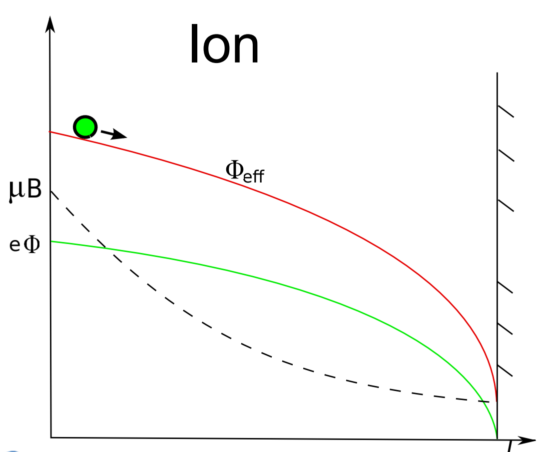
- **Particle parallel motion governed by effective potential**

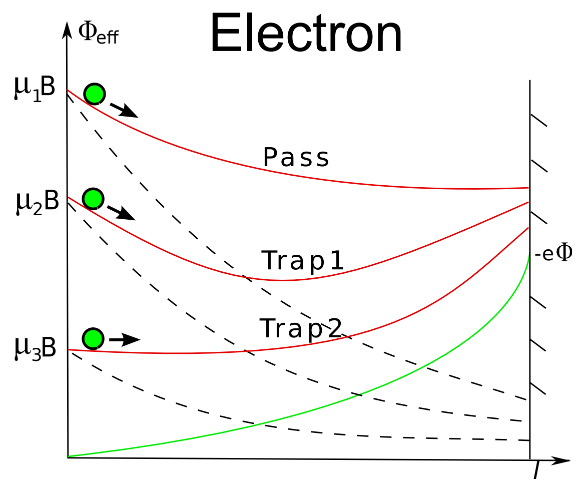
$$\Phi_{eff}(x) = q\Phi(x) + \mu B(x)$$

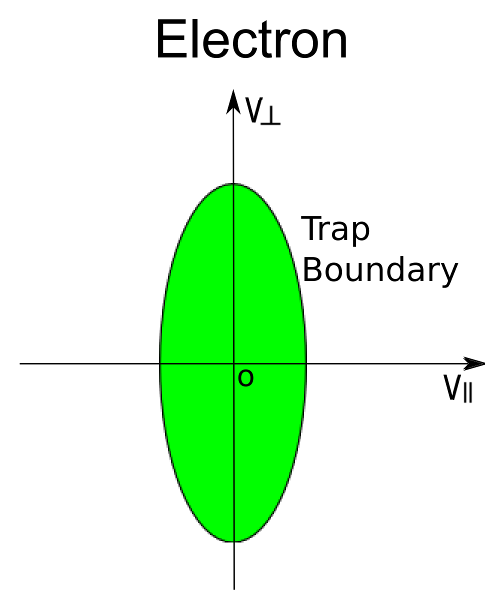
- **Trap-passing boundary:**



$$v_{||}^2 + v_{\perp}^2(1 - B_w/B) = 2e(\Phi - \Phi_w)/m_e \quad \text{or} \quad \epsilon = -e\phi_w + \mu B_w$$

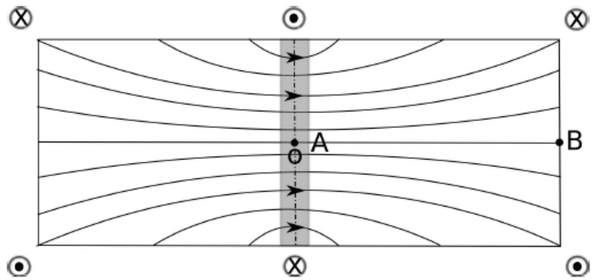


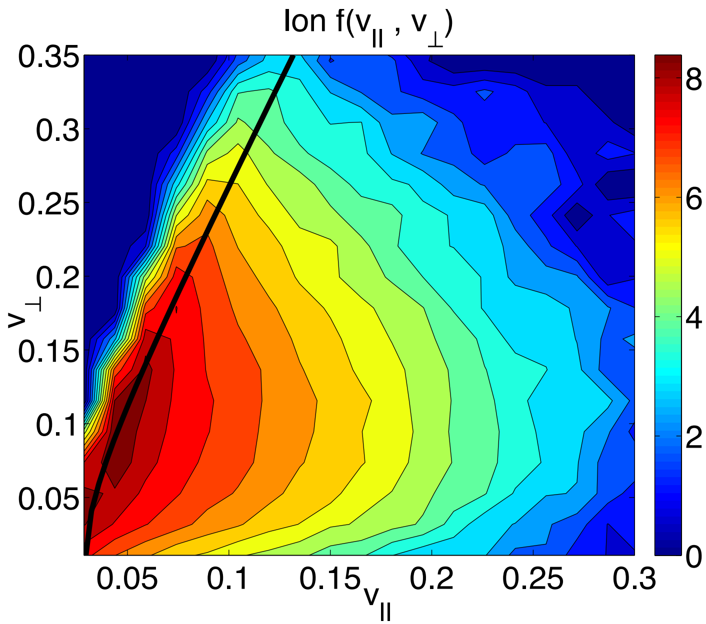


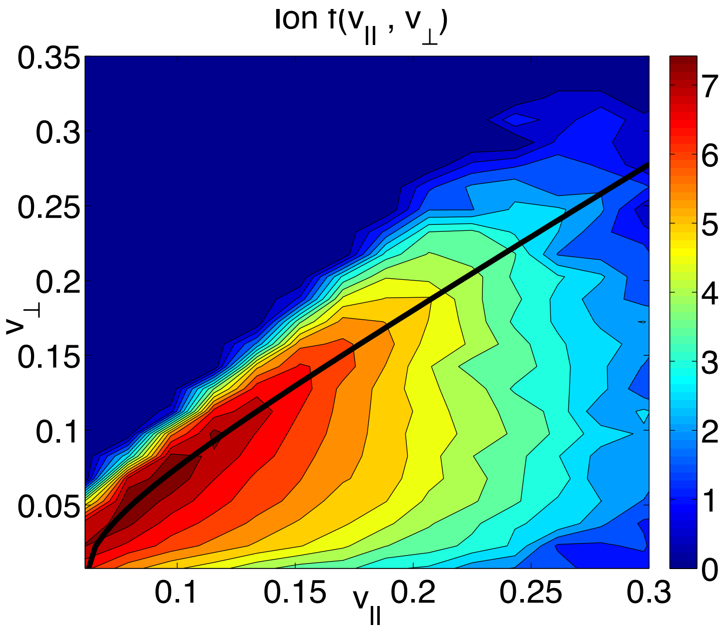


Distribution function: ions are all passing

- **All ions from upstream source, where** $v_{\parallel 0}^2 \geq 0$ **, so**
  $v_\parallel^2 - v_\perp^2 (B_0/B - 1) \geq 2e|\phi|/m_i$ or $\epsilon = \mu B_0$
- **Ion distribution peak on this constraint curve**
- **Ion distribution function compresses in v_perp with decreasing B**





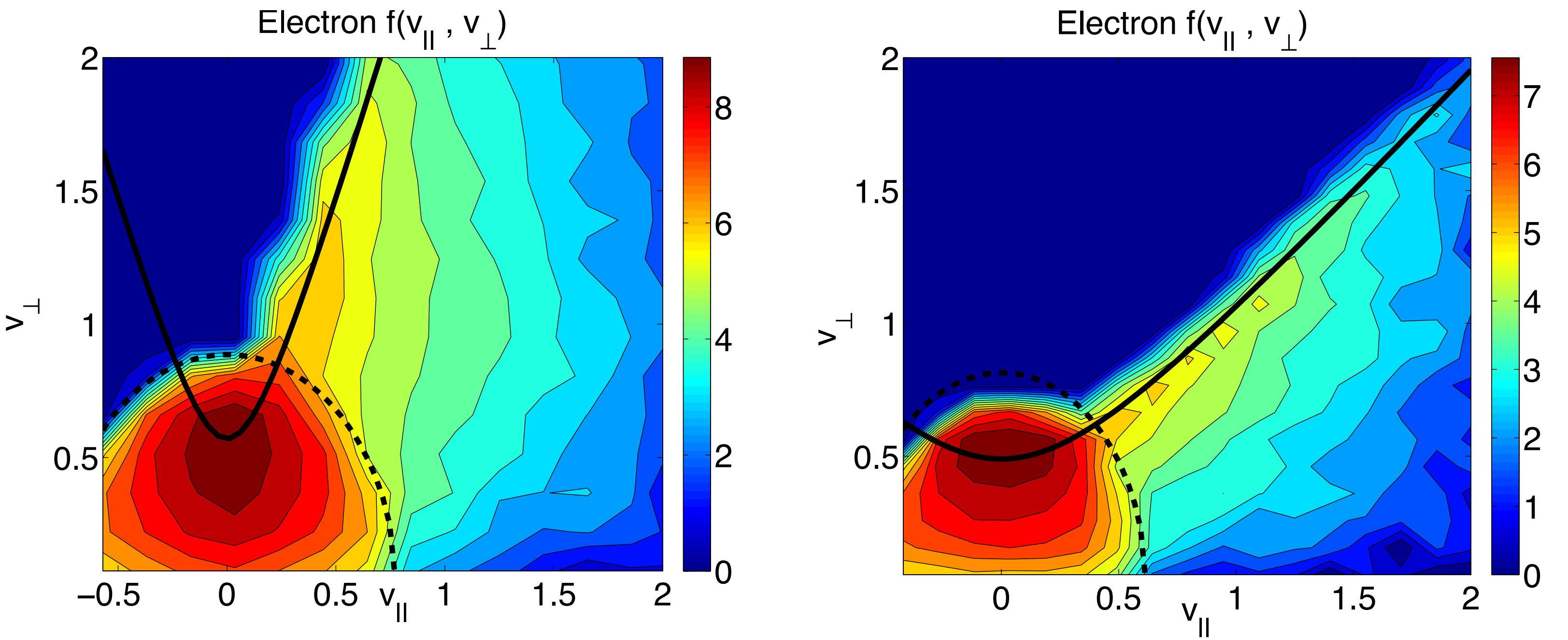


Distribution function: electrostatic trapping of electrons

- **Upstream electron source where** $v_{||0}^2 \geq 0$ **, so**

$$v_\perp^2 (B_0/B - 1) - v_{||}^2 \leq 2e|\phi|/m_e \quad \text{or} \quad \epsilon = \mu B_0$$

- **Passing electrons align with this curve**
- **Electron distribution compresses in v_perp with decreasing B**



Ambipolarity of parallel transport

- **Bohm's sheath/presheath theory requires collisional plasma**
- **Low collisionality poses a problem for ambipolarity in steady state**
  - (Pre)sheath electric field leads to trapped electrons.
  - Upstream sourcing fills both the trapped and passing zones in velocity space for electrons
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  - Ambipolarity demands electron detrapping flux
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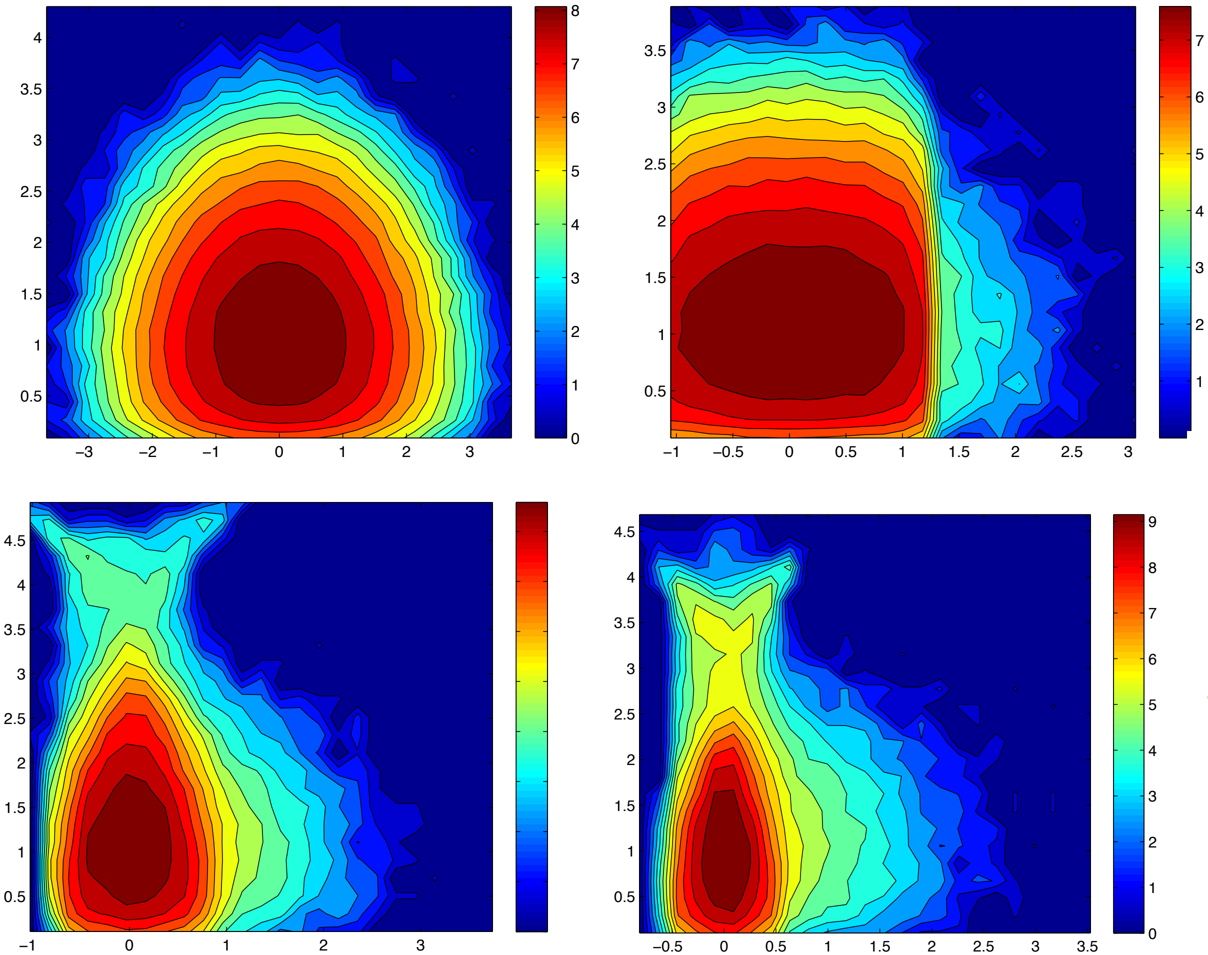
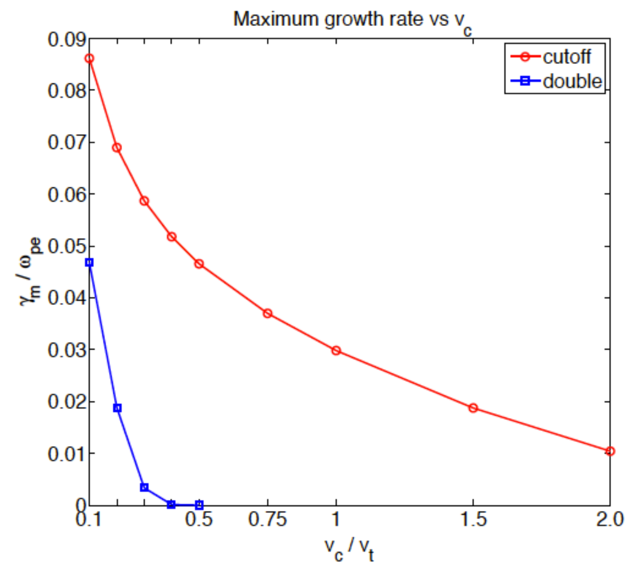
- **Kinetic instabilities to the rescue**
  - Unmagnetized plasma: Weibel instability by T anistropy (Tang, PPCF, 2011)
  - Magnetized plasma: trapped electron driven whistler instability (Guo & Tang, 2012)
    - Far more virulent than temperature anisotropy driven whistler instability

Trapped electron whistler instability & wave-particle inter.

Electron distribution function



Growth rate versus cutoff velocity comparison between T anisotropy and trapped electron **whistler** instabilities.

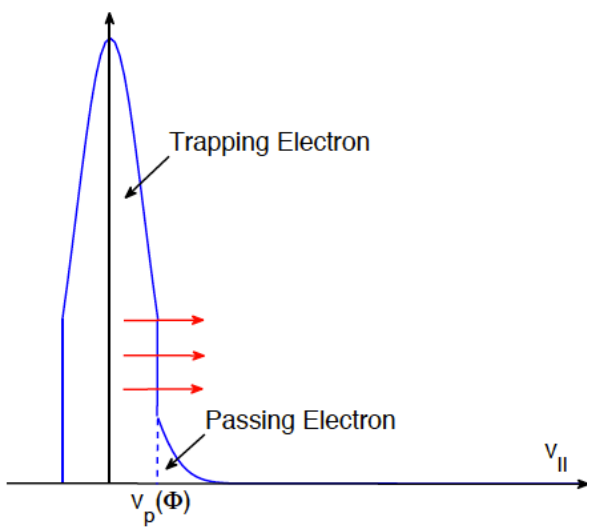


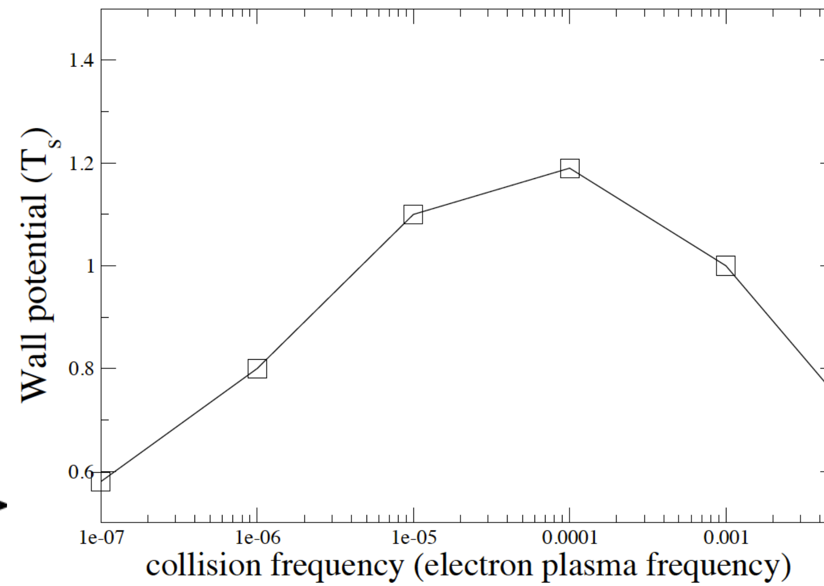
(Guo & Tang, TTF, 2012)

Wall potential

Global kinetic theory provides new insights into the wall potential

- At low collisionality, Φ_{wall} is small so small trapped electron region in velocity space, stronger drive for kinetic instability, more collisionless detrapping via wave-particle interaction.
- Increasing collisonality boosts collisional detrapping, reducing the need for collisionless detrapping, higher Φ_{wall}
- Still greater collisionality accounts for all the required detrapping flux, no need for collisionless detrapping, Φ_{wall} comes down.





Two-T (CGL+) model for plasma parallel profile variation

$$\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + (q/m)(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \partial_{\mathbf{v}} f = S(x, \mathbf{v})$$

$$\partial_t n + \nabla \cdot (n\mathbf{u}) = \Gamma(x)\,,$$

$$nm\mathrm{d}_t\mathbf{u} + \nabla \cdot \mathbb{P} - nq(\mathbf{E} + \mathbf{u} \times \mathbf{B}) + \Gamma(x) m\mathbf{u} = 0$$

$$\mathbb{P} = P_\perp \mathbb{I} + (P_\parallel - P_\perp)\mathbf{b}\mathbf{b}$$

$$\Gamma(x) = \int S(x, \mathbf{v}) d\mathbf{v}$$

$$\mathrm{d}_t P_\parallel + P_\parallel \nabla \cdot \mathbf{u} + 2P_\parallel \mathbf{b} \cdot (\mathbf{b} \cdot \nabla)\mathbf{u} + \nabla \cdot (q_n \mathbf{b}) - 2q_s \nabla \cdot \mathbf{b} = \Gamma_{T_\parallel}$$

$$\mathrm{d}_t P_\perp + 2P_\perp \nabla \cdot \mathbf{u} - P_\perp \mathbf{b} \cdot (\mathbf{b} \cdot \nabla)\mathbf{u} + \nabla \cdot (q_s \mathbf{b}) + q_s \nabla \cdot \mathbf{b} = \Gamma_{T_\perp}$$

$$q_s = m \int f_0 (v_\parallel - u_\parallel)(\mathbf{v} - \mathbf{u})_\perp^2 d\mathbf{v}/2$$

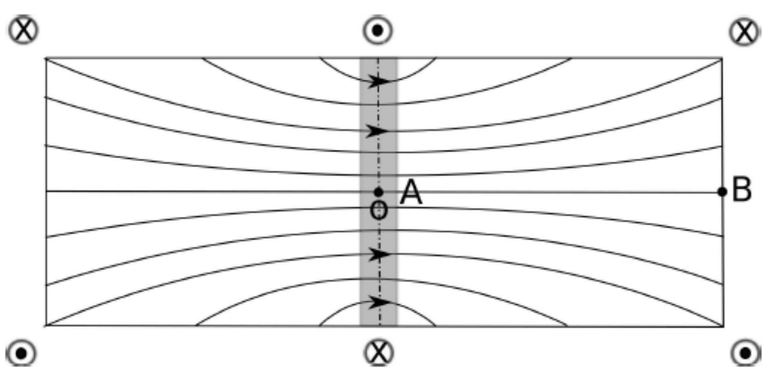
$$q_n = m \int f_0 (v_\parallel - u_\parallel)^3 d\mathbf{v}$$

$$\Gamma_{T_\parallel} = \Gamma(x)(T_{s\parallel} + \tfrac{1}{2} m u^2), \Gamma_{T_\perp} = \Gamma(x) T_{s\perp}$$

Upstream profile depends on collisionality (wall recycling)

- **Conventional expectation of flat electron temperature profile in low recycling regime is based on the collisional closure of electron parallel heat flux**
  - Inconsistent with kinetic analysis and closure calculation (Guo & Tang, PRL, 2012)
- **Trapped electron population makes the upstream plasma a lot colder than usually assumed, implying large T difference between upstream source and plasma (e.g. pedestal and SOL) in low recycling regime**
- **Plasma parallel profile variation is controlled by four parameters:**
  - **Parallel heat flux profile:** q_s/B^2 and q_n/B
  - **Ratio of conductive and convective heat flux at upstream**

$$\alpha_\perp = q_{s0}/n_0 u_0 T_{\perp 0} \qquad \alpha_{||} = q_{n0}/n_0 u_0 T_{||0}$$



(Guo & Tang, 2011)

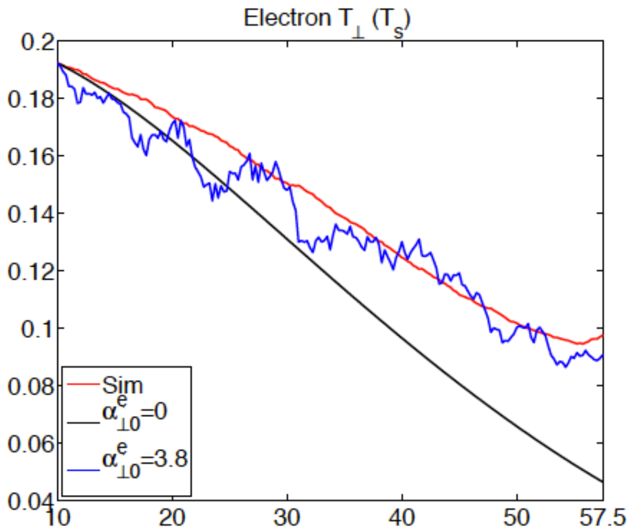
Parallel variation of electron parallel and perpendicular T

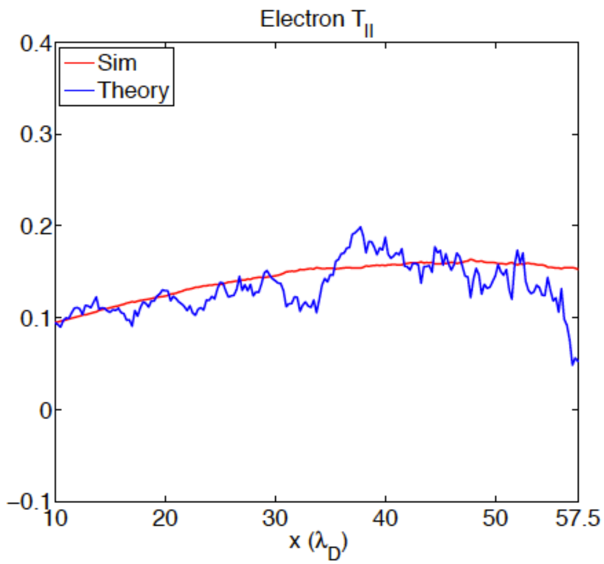
$$T_\perp = T_{\perp 0}\frac{B}{B_0}\left[1+\alpha_\perp(1-\frac{q_s/B^2}{q_{s0}/B_0^2})\right]$$

$\alpha_\perp^i = 0.16, \alpha_\perp^e = 3.8$; the electron $T_\perp$ is significantly modified by q_s.

$$\frac{\partial T_\parallel}{\partial l} = -2T_\parallel\frac{\partial \ln u}{\partial l} - \alpha_\parallel T_{\parallel 0}\frac{\partial}{\partial l}\left(\frac{q_n/B}{q_{n0}/B_0}\right) - 2\alpha_\perp T_{\perp 0}\frac{q_s/B^2}{q_{s0}/B_0^2}\frac{\partial}{\partial l}\left(\frac{B}{B_0}\right);$$

The electron $T_\parallel$ profile is inverted due to the q_s.





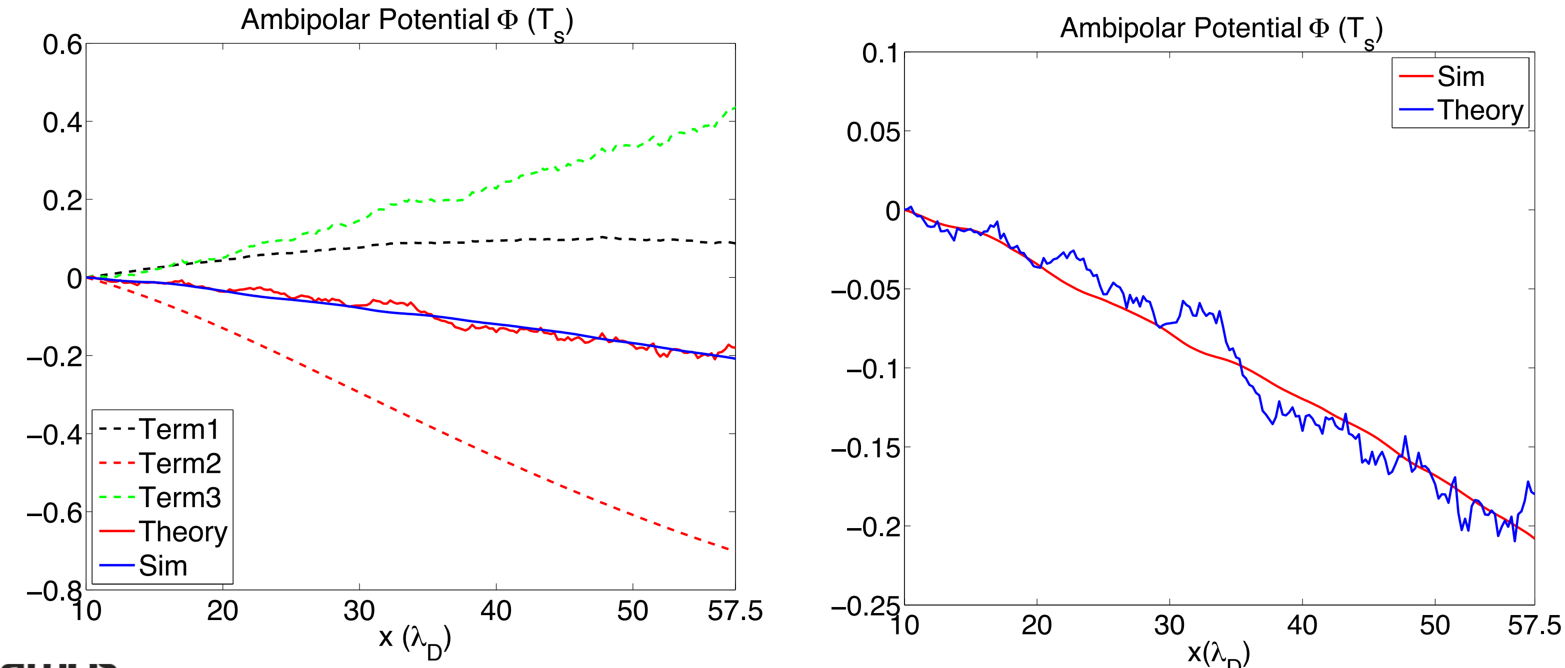
Guo & Tang, PoP, in review,2011

Ambipolar potential & parallel heat flux

- **Electron perpendicular energy drives ambipolar potential**
  - Both mirror force and q_s convert electron perpendicular energy into potential energy
  - Both parallel heat flux components enter to set the coefficients

$$e\Delta\Phi = \frac{3}{2}\Delta T^e_{\parallel} + (1+\alpha^e_{\perp})T_{\perp}{}^e_0\left(\frac{B}{B_0}-1\right) + \frac{1}{2}\alpha^e_{\parallel}T^e_{\parallel 0}\left(\frac{q^e_n/B}{q^e_{n0}/B_0}-1\right)$$

$$\alpha^e_{\perp} = 3.8\,,\alpha^e_{\parallel} = 7.9 \text{ and } \alpha^i_{\perp} = 0.16\,,\alpha^i_{\parallel} = 1.2\,.$$

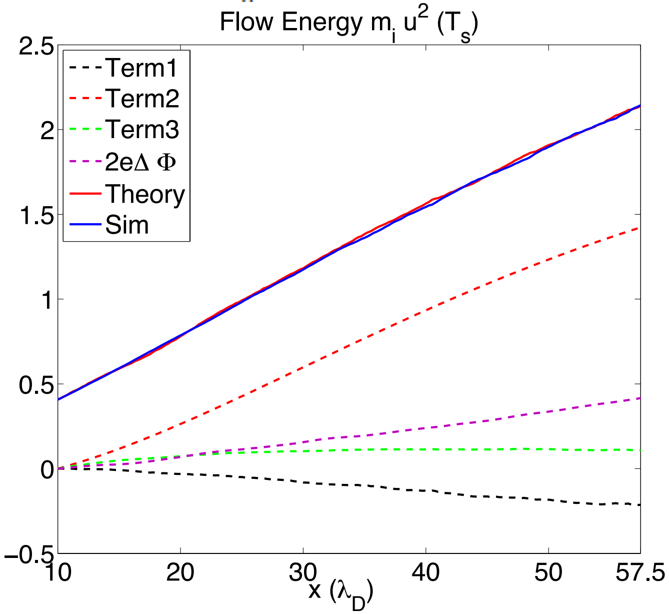


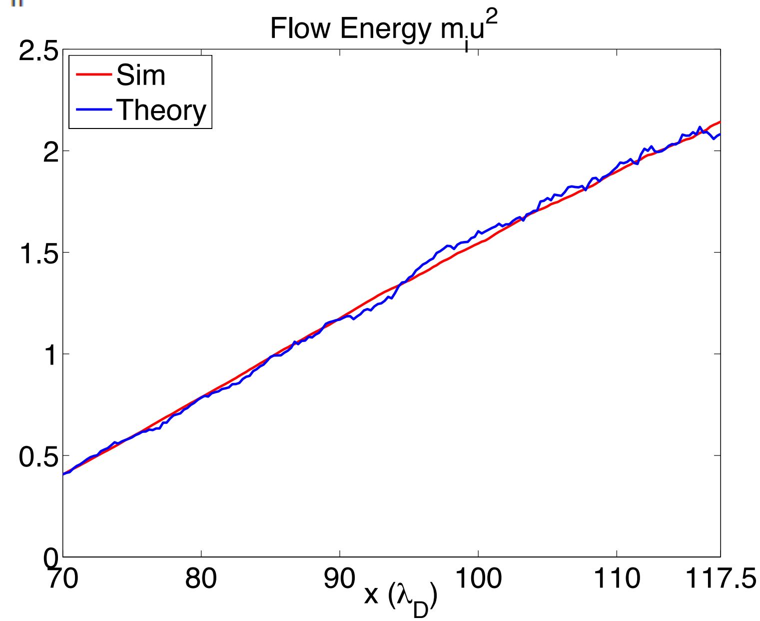
Parallel flow acceleration & parallel heat flux

- **Parallel flow acceleration is strongly modified by the parallel heat fluxes**
  - Both mirror force and q_s convert ion perpendicular energy into parallel flow energy
  - Both parallel heat flux components enter to set the coefficients
  - Definition of sound speed is problematic.

$$m_i \Delta u^2 = \left[-3\Delta T_{\|}^i - 2(1+\alpha_{\perp}^i) T_{\perp 0}^i \left(\frac{B}{B_0} - 1 \right) - \alpha_{\|}^i T_{\| 0}^i \left(\frac{q_n^i / B}{q_{n0}^i / B_0} - 1 \right) \right] - 2e\Delta\Phi$$

$$\alpha_{\perp}^e = 3.8 \, , \alpha_{\|}^e = 7.9 \text{ and } \alpha_{\perp}^i = 0.16 \, , \alpha_{\|}^i = 1.2 \, .$$





Summary

- **In low recycling regime where collisionality is reduced, parallel transport has counter-intuitive behaviors**
  - Due to trapped electrons, much lower temperature than source T.
  - Decompressional cooling also brings down the ion T.
  - Parallel heat flux component can go uphill in parallel temperature
    - A drift kinetic closure showed in a PRL (Guo & Tang, 2012)
  - Parallel temperature can be inverted by flux expansion (colder away from the wall)
- **When collisionality is low, temperature anisotropy and trapped particles drive kinetic instabilities**
  - Ambipolarity in parallel transport requires collisionless detrapping via wave-particle interaction
  - Electromagnetic waves as opposed to electrostatic ones are the primary instabilities (e.g. whistler wave)
- **The CGL equations with parallel heat flux provide a reasonable description of parallel profile variation**
  - Explicit relationship between parallel/perpendicular T, parallel flow, ambipolar potential and B modulation and parallel heat flux.
  - They can be used for direct experimental comparison or inferring unmeasured quantities.