A Review of Recent Progress on Energy Conversion in Plasmas Beyond near-LTE Fluid Models

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November 1, 2023

In Honor of: Bill Dorland

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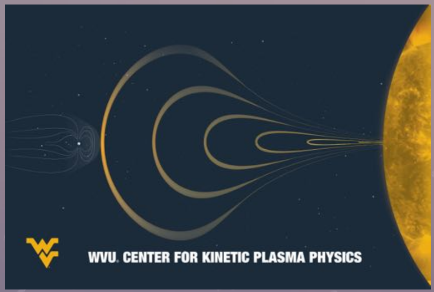
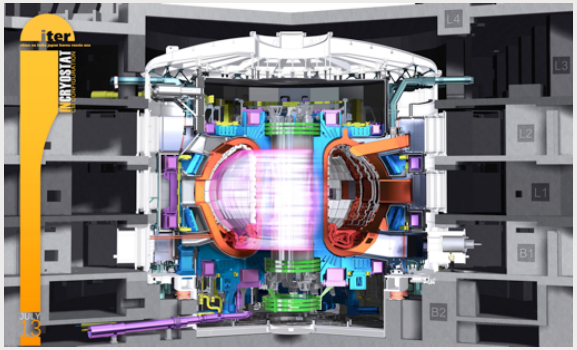


Hasan Barbhuiya

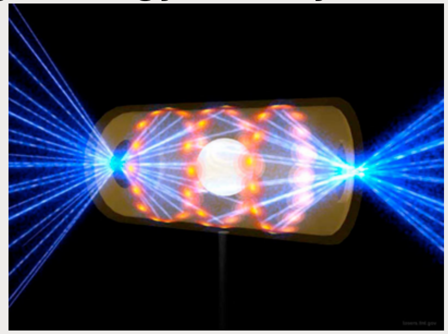

SHERATON

Magnetic Confinement Fusion



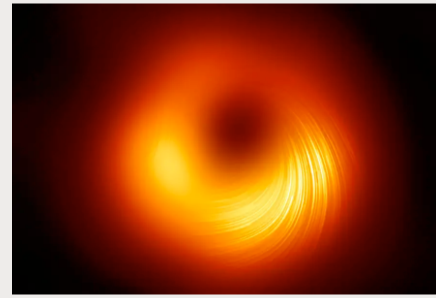
https://www.iter.org/proj/inafewlines

Inertial Confinement Fusion, High Energy Density Plasmas



National Ignition Facility

Compact Objects

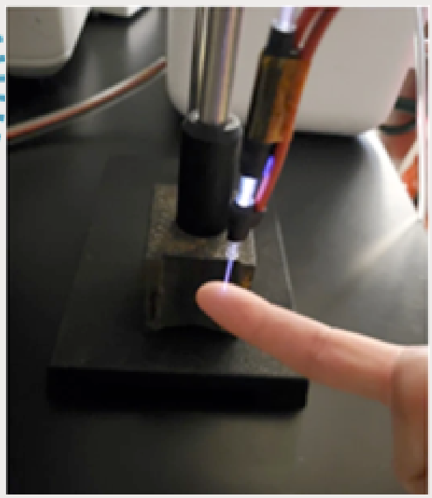


EHT Collaboration/ESO

Astrophysical

nasa.gov

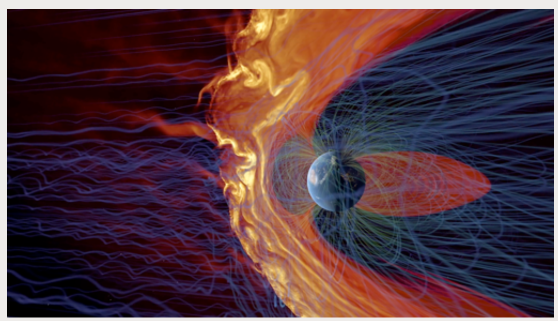
Low Temperature/ Medical/Industrial



Nicol et al., Sci. Reports, 2020

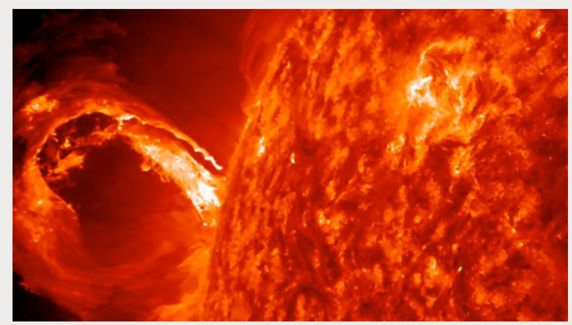
Energy Conversion in Plasmas

Magnetosphere, Interplanetary/stellar



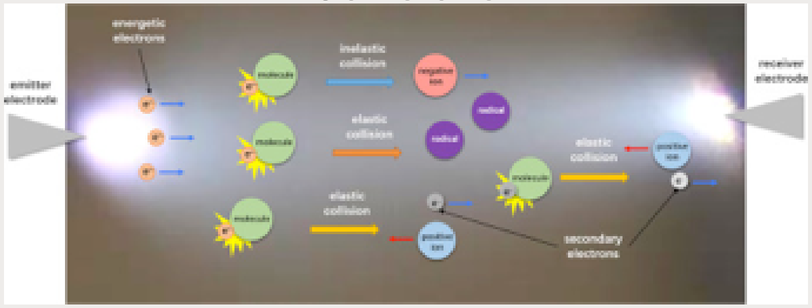
Advanced Visualization Lab, UIUC

Solar/Stellar



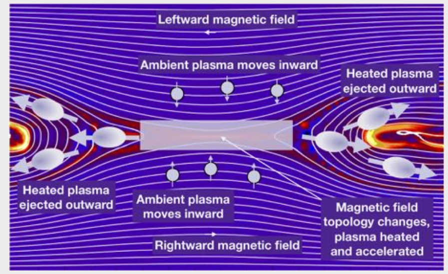
nasa.gov

Collisions



Miao et al., Green Energy and Resources, 2023

Magnetic Reconnection

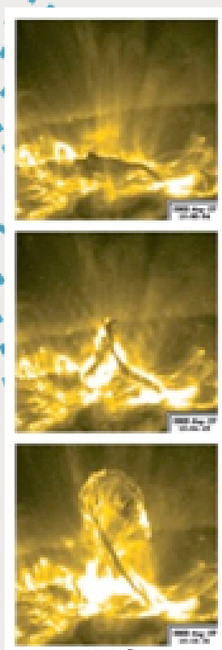


Hesse and Cassak, JGR, 2020

Shocks

NASA and the Hubble Heritage Team (STScI/AURA)

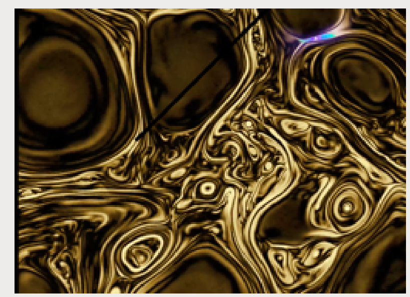
Waves/Instabilities



AAS

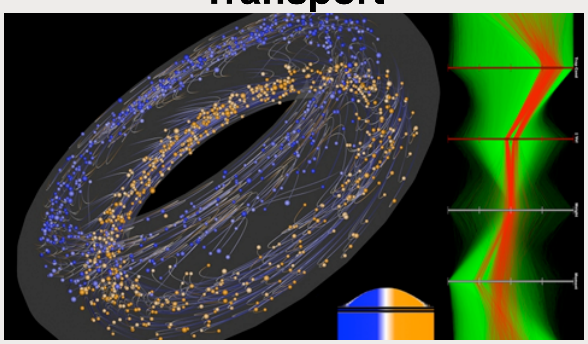
Energy Conversion Mechanisms in Plasmas

Turbulence



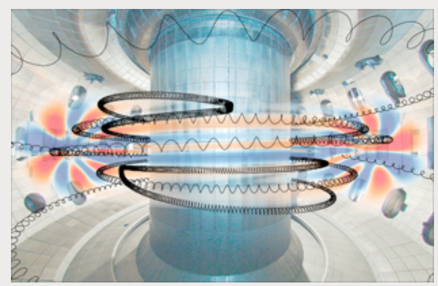
NASA Goddard's Conceptual Image Lab/Lisa Poje

Transport



https://www.alcf.anl.gov/news/plasma-turbulence-simulations-reveal-promising-insight-fusion-energy

Wave-Particle Interactions



Steve Allen (LLNL), adapted by Mike Van Zeeland (General Atomics)

The LTE "Fluid" Approach

- Fluid in local thermodynamic equilibrium (LTE) ⇔ there is a well-defined local temperature
  - In LTE, energy conversion is adiabatic ($p/\rho^\gamma = \text{constant}$)
- Near LTE, departure from LTE is small
  - Viscosity and resistivity cause irreversible conversion into internal energy, conduction transports energy
- Uses of LTE/near-LTE fluid models:
  - Plasma/MHD waves, MHD instabilities, Shocks (Rankine-Hugoniot), Reconnection (Sweet-Parker), turbulence (Kolmogorov), …

www.youtube.com/watch?v=a-_iuXR0FCU

Energy Conversion in near-LTE Fluid Model

- near-LTE fluid energy equations for species σ (n_σ is number density, $\mathbf{u}_\sigma$ is bulk flow velocity, p_σ is pressure, m_σ is constituent mass, q_σ is charge, γ_σ is ratio of specific heats):

Electromagnetic energy density
$\mathcal{E}_{EM} = E^2/8\pi + B^2/8\pi$

$$\frac{\partial \mathcal{E}_{EM}}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{J} \cdot \mathbf{E}$$

Bulk flow energy density
$\mathcal{E}_{\sigma k} = (1/2) m_\sigma n_\sigma u_\sigma^2$

$$\frac{\partial \mathcal{E}_{\sigma k}}{\partial t} + \nabla \cdot (\mathcal{E}_{\sigma k} \mathbf{u}_\sigma) = -\mathbf{u}_\sigma \cdot \nabla p_\sigma + q_\sigma n_\sigma \mathbf{u}_\sigma \cdot \mathbf{E} + \mathbf{R}_{\sigma,\mathrm{coll}}$$

Internal energy density
$\mathcal{E}_{\sigma,\mathrm{int}} = p_\sigma / (\gamma_\sigma - 1)$

$$\underbrace{\frac{\partial \mathcal{E}_{\sigma,\mathrm{int}}}{\partial t} + \nabla \cdot (\mathcal{E}_{\sigma,\mathrm{int}} \mathbf{u}_\sigma)} = \underbrace{-p_\sigma \nabla \cdot \mathbf{u}_\sigma} + \underbrace{\dot{Q}_{\sigma,\mathrm{coll}}}$$

The first law of thermodynamics!

$$\frac{dE_{\sigma,\mathrm{int}}}{dt} + \frac{dW_\sigma}{dt} = \frac{dQ_\sigma}{dt}$$

What Does LTE Mean?

- Phase space density $f_\sigma(\mathbf{r}, \mathbf{v}, t)$ = number density in phase space, *i.e.*, position $\mathbf{r}$, velocity $\mathbf{v}$ space

$$f_\sigma(\mathbf{r}_j, \mathbf{v}_k) \simeq \frac{N_{\sigma,jk}}{\Delta^3 r \Delta^3 v}$$

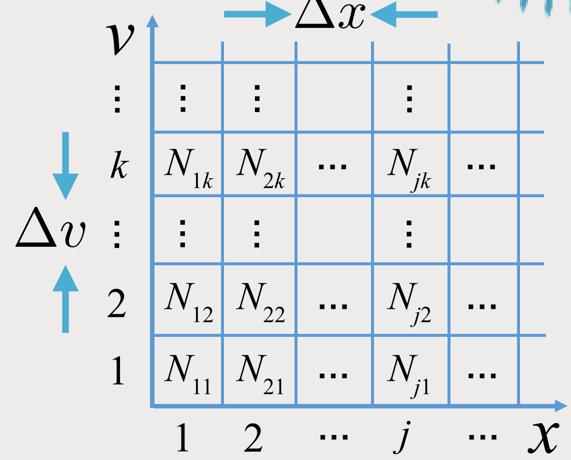
- In LTE, $f_\sigma = f_{\sigma,MB}$, a Maxwell-Boltzmann distribution

$$f_{\sigma,MB} = n_\sigma \left(\frac{m_\sigma}{2\pi k_B T_\sigma}\right)^{3/2} e^{-m_\sigma(\mathbf{v}-\mathbf{u}_\sigma)^2/2k_B T_\sigma}$$

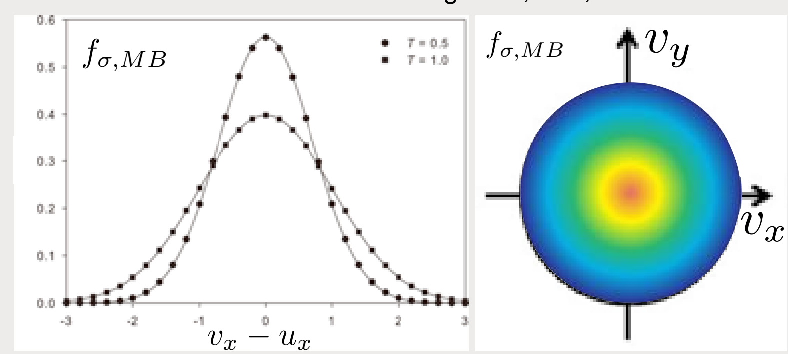
- Temperature T_σ is related to internal energy per particle $E_{\sigma,\text{int}} = (3/2)k_B T_\sigma$

$$E_{\sigma,\text{int}} = \frac{1}{n_\sigma}\int d^3v \left(\frac{1}{2}m_\sigma(\mathbf{v}-\mathbf{u}_\sigma)^2\right) f_{\sigma,MB}$$

1D Phase Space



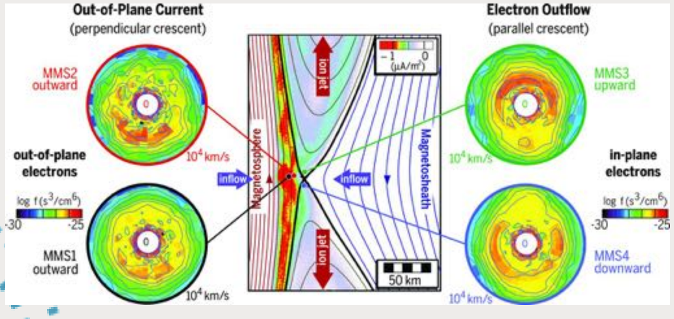
Liang et al., PoP, 2019



Mohazzabi and Shankar, JAMP, 2018

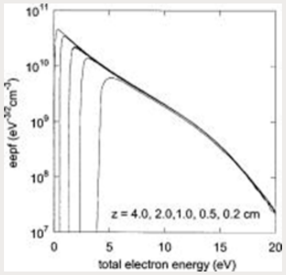
What Does non-LTE Mean?

Earth's Magnetopause (MMS)



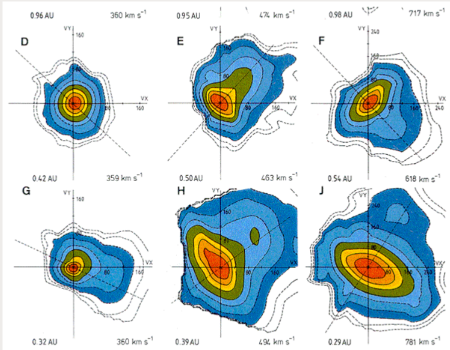
Burch et al., Science, 2016

Low Temperature Experiment



Godyak, PoP, 2005

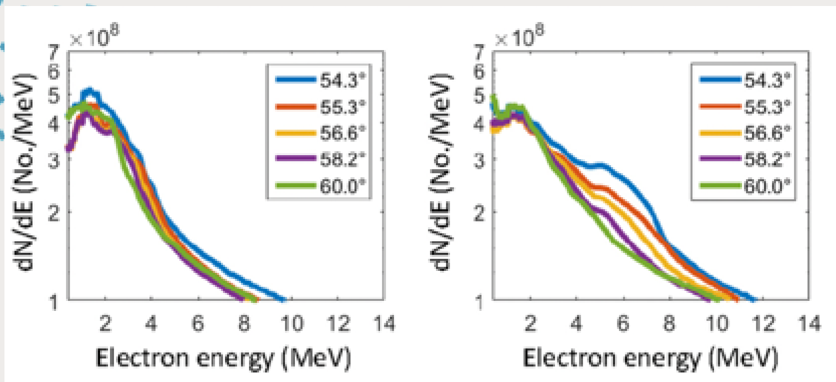
Solar Wind (Helios)



Marsch, Ann. Geophys., 2018

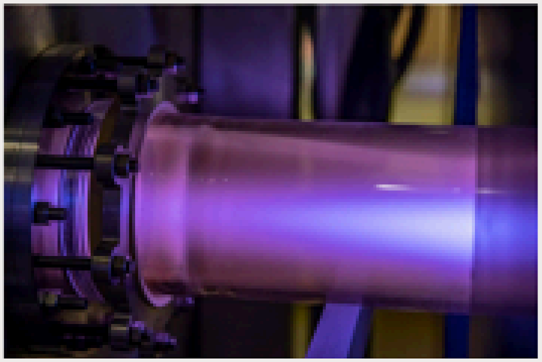
$$f_\sigma \neq f_{\sigma,MB}$$

HEDP Experiment (OMEGA)

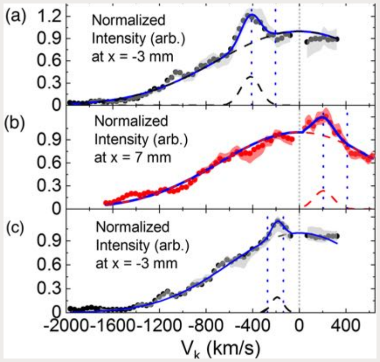


Raymond et al., PRE, 2018

Space/Fusion Experiment (PHASMA, WVU)



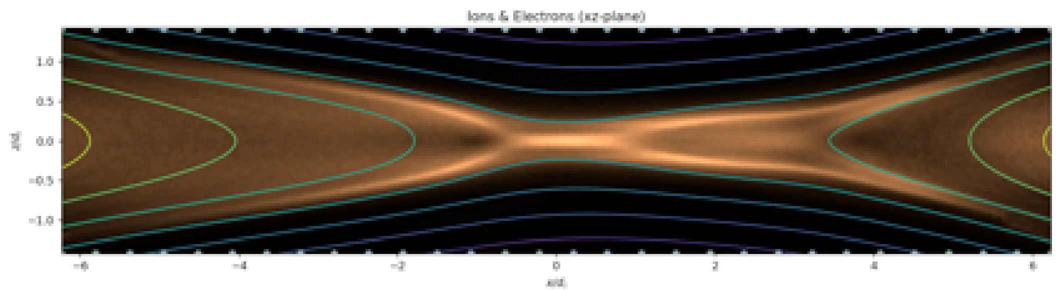
Courtesy of Earl Scime, Jake Stump, WVU



Shi et al., PRL, 2022

Why are Plasmas not in LTE?

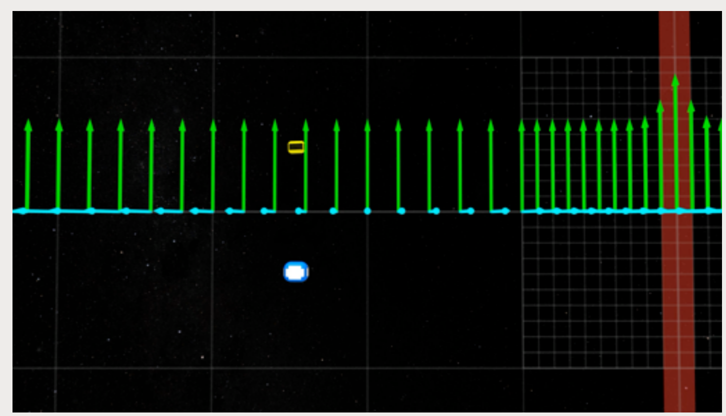
Collisionless Magnetic Reconnection



NASA's Scientific Visualization Studio and Yi-Hsin Liu

- Collisions
  - weak or absent (high temperature, low density)
  - act differently on different species (low temperature)
- Anisotropies, particle trapping, finite-Larmor radius effects, non-thermal heating, …
  - (Howes, PoP, 2017; Matthaeus, ApJ, 2020; Alvarez Laguna et al., PoP, 2022)

Collisionless Shock

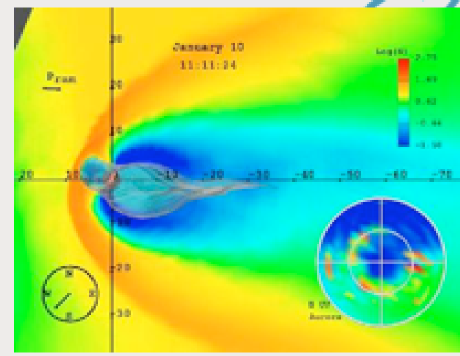


NASA's Scientific Visualization Studio

Overview

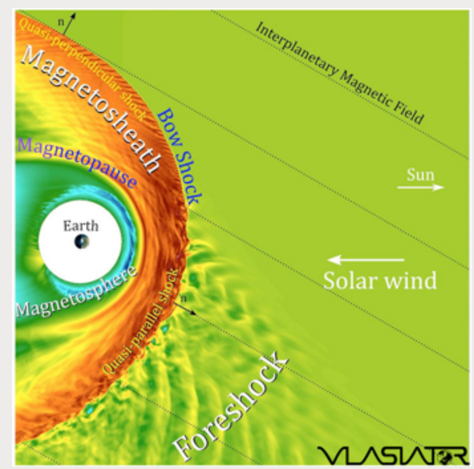
- Non-LTE plasmas - description using kinetic theory
- Review of three approaches to understanding evolution of non-LTE systems
  - Pressure-strain interaction:
    bulk flow energy ↔ internal energy
    (e.g., Yang et al., *Phys. Plasmas*, **24**, 072306, 2017)
  - Field-particle interaction:
    electromagnetic field energy ↔ particle energy
    (Klein and Howes, *Astrophys. J. Lett.*, **826**, L30, 2016)
  - Entropic approach: *all* non-LTE evolution
    (Cassak et al., *Phys. Rev. Lett.*, **130**, 085201, 2023)
- Open questions

Bow shock in:
fluid simulation



https://www.bu.edu/tech/support/research/whats-happening/highlights/spaceweather/

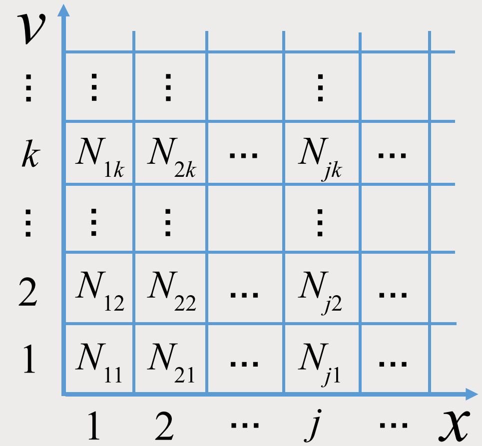
… and kinetic simulation



Goodrich et al., Front. Astron. Space Sci, 2023

Kinetic Theory - How does f_σ Evolve?

- A statistical theory of plasmas
  - Use velocities $\mathbf{v}$ and forces $\mathbf{F}_\sigma$ with Newton's 2nd law to find where the particles $N_{\sigma,jk}$ move in a small time dt, and therefore how f_σ changes in time



Liang et al., PoP, 2019

- The Boltzmann equation (1872)

$$\frac{\partial f_\sigma}{\partial t} + \mathbf{v} \cdot \nabla f_\sigma + \frac{\mathbf{F}_\sigma}{m_\sigma} \cdot \nabla_v f_\sigma = C[f]$$

  - $C[f]$ is an operator describing collisions
    - Here, we leave $C[f]$ unspecified

Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen.

Von Ludwig Boltzmann in Graz.

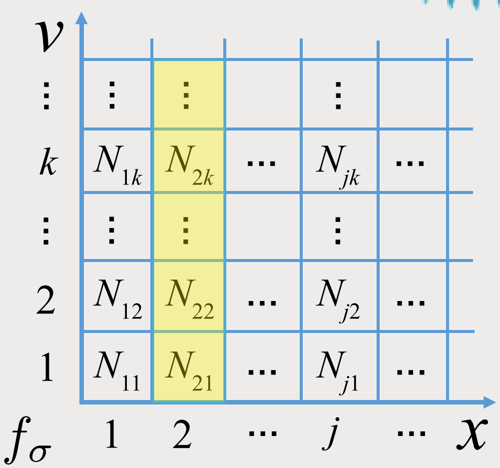
(Mit 1 Holzschnitten.)

(Vorgelegt in der Sitzung am 10. October 1872.)

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} + \eta \frac{\partial f}{\partial y} + \zeta \frac{\partial f}{\partial z} + X \frac{\partial f}{\partial \xi} + Y \frac{\partial f}{\partial \eta} + Z \frac{\partial f}{\partial \zeta} + \int d\omega_1 \int b\,db \int d\varphi\, V(f'f'_1 - f''f'_1) = 0 \quad 44)$$

Fluid Description From Kinetic Theory

- Velocity moments of f_σ give the bulk properties



Liang et al., PoP, 2019

0th moment: Number density

$$n_\sigma(\mathbf{r}, t) = \int d^3v f_\sigma(\mathbf{r}, \mathbf{v}, t)$$

1st moment: Bulk flow velocity

$$\mathbf{u}_\sigma(\mathbf{r}, t) = \frac{1}{n_\sigma(\mathbf{r}, t)} \int d^3v \mathbf{v} f_\sigma(\mathbf{r}, \mathbf{v}, t)$$

2nd moment: Pressure tensor, $P_{\sigma,jk} = n_\sigma k_B T_{\sigma,jk}$

$$P_{\sigma,jk} = \int d^3v m_\sigma (v_j - u_{\sigma j})(v_k - u_{\sigma k}) f_\sigma$$

3rd moment: Tensor heat flux

$$Q_{\sigma,jkl} = \int d^3v m_\sigma (v_j - u_{\sigma j})(v_k - u_{\sigma k})(v_l - u_{\sigma l}) f_\sigma$$

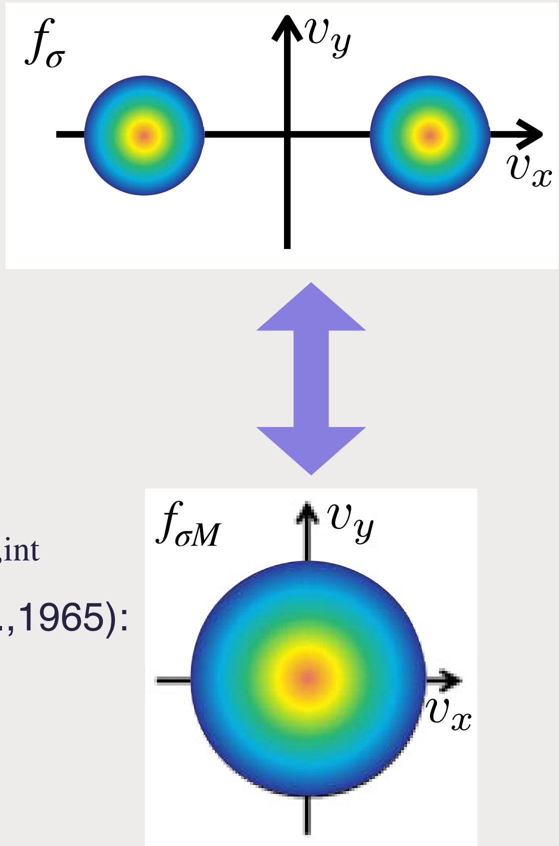
… …

Note, it can take an infinite number of fluid moments to describe the shape of f_σ!

Temperature in Kinetic Theory?!?

- Temperature T_σ is not well-defined for a system not in LTE, but internal energy per particle $E_{\sigma,\text{int}}$ is!

$$E_{\sigma,\text{int}} = \frac{1}{n_\sigma} \int d^3v \left(\frac{1}{2} m_\sigma (\mathbf{v} - \mathbf{u}_\sigma)^2 \right) f_\sigma$$



- Can then define the "effective temperature" $\mathcal{T}_\sigma$ according to

$$E_{\sigma,\text{int}} = \frac{3}{2} k_B \mathcal{T}_\sigma$$

- It is temperature if f_σ were changed to be in LTE with the same $E_{\sigma,\text{int}}$
- "Maxwellianized" distribution $f_{\sigma M}$ (Grad, J. Soc. Indust. Appl. Math.,1965):

$$f_{\sigma M} = n_\sigma \left(\frac{m_\sigma}{2\pi k_B \mathcal{T}_\sigma} \right)^{3/2} e^{-m_\sigma (\mathbf{v} - \mathbf{u}_\sigma)^2 / 2k_B \mathcal{T}_\sigma}$$

Energy Conversion via Fluid Moments

- 2nd moments of Boltzmann equation for species σ gives kinetic theory generalizations of the fluid energy equations (e.g., Braginskii, Rev. Plasma Phys., 1965)

$$\frac{\partial \mathcal{E}_{k\sigma}}{\partial t} + \nabla \cdot (\mathcal{E}_{k\sigma}\mathbf{u}_\sigma + \mathbf{P}_\sigma \cdot \mathbf{u}_\sigma) = (\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma + \boxed{\mathbf{J}_\sigma \cdot \mathbf{E}} + \mathbf{R}_{\text{coll}}$$

Bulk kinetic energy density equation

$$\frac{\partial \mathcal{E}_{\sigma,\text{int}}}{\partial t} + \nabla \cdot (\mathbf{u}_\sigma \mathcal{E}_{\sigma,\text{int}}) = -(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma - \nabla \cdot \mathbf{q}_\sigma + n_\sigma \dot{Q}_{\sigma,\text{coll,inter}}$$

Internal energy density equation

where $\mathbf{J}_\sigma = q_\sigma n_\sigma \mathbf{u}_\sigma$

- Also have Poynting's theorem:

$$\frac{\partial \mathcal{E}_{EM}}{\partial t} + \nabla \cdot \mathbf{S} = \boxed{-\mathbf{J} \cdot \mathbf{E}}$$

  - $\nabla \cdot$ terms ⇔ energy transport
  - coll terms ⇔ energy conversion/transport via collisions
  - $\mathbf{J}_\sigma \cdot \mathbf{E}$ ⇔ rate of energy density conversion between species σ and the electromagnetic field

Energy Conversion via Fluid Moments

- 2nd moments of Boltzmann equation for species σ gives kinetic theory generalizations of the fluid energy equations (e.g., Braginskii, Rev. Plasma Phys., 1965)

$$\frac{\partial \mathcal{E}_{k\sigma}}{\partial t} + \nabla \cdot (\mathcal{E}_{k\sigma}\mathbf{u}_\sigma + \mathbf{P}_\sigma \cdot \mathbf{u}_\sigma) = (\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma + \mathbf{J}_\sigma \cdot \mathbf{E} + \mathbf{R}_{\text{coll}}$$

Bulk kinetic energy density equation

$$\frac{\partial \mathcal{E}_{\sigma,\text{int}}}{\partial t} + \nabla \cdot (\mathbf{u}_\sigma \mathcal{E}_{\sigma,\text{int}}) = -(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma - \nabla \cdot \mathbf{q}_\sigma + n_\sigma \dot{Q}_{\sigma,\text{coll,inter}}$$

Internal energy density equation

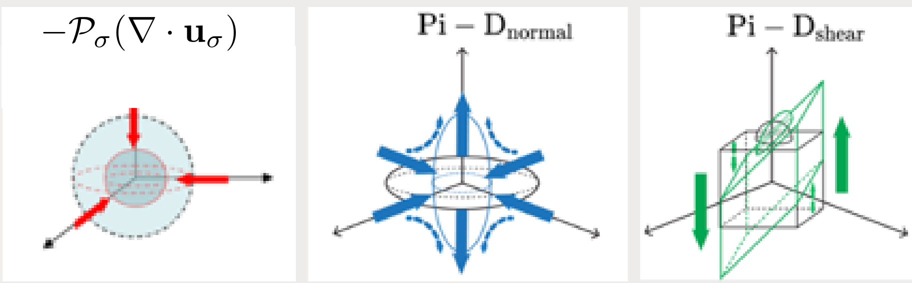
- $-(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma$ = "pressure-strain interaction" = energy density conversion rate between bulk kinetic energy and internal energy (Del Sarto et al., PRE, 2016; Yang et al., PRE/PoP, 2017)
  - It is collisionless; collisions bring in viscosity, resistivity, conductivity, etc.
- Commonly decomposed into compressible and incompressible parts (pressure dilatation, "Pi-D")

$$-(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma = -\mathcal{P}_\sigma(\nabla \cdot \mathbf{u}_\sigma) - \Pi_{\sigma,jk}\mathcal{D}_{\sigma,jk}$$

  - In magnetized plasma (fusion), Pi-D is "gyro-viscosity" (e.g., Hazeltine et al., PoP, 2013)
  - In a closed collisionless system, the pressure-strain interaction describes the net internal energy change (Yang et al., PoP, 2017)

Physics of Pressure-Strain Interaction

- Fluid interpretation (Del Sarto and Pegoraro, MNRAS, 2018; Cassak and Barbhuiya, PoP, 2022)



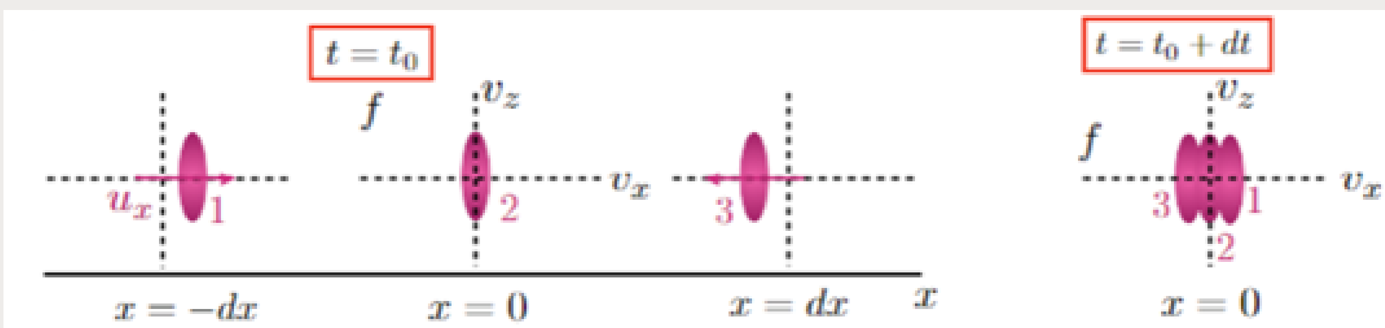
$$\mathrm{Pi-D}_\sigma = \mathrm{Pi-D}_{\sigma,\mathrm{normal}} + \mathrm{Pi-D}_{\sigma,\mathrm{shear}}$$

$$\mathrm{Pi-D}_{\sigma,\mathrm{normal}} = -\left(\Pi_{\sigma,xx}\frac{\partial u_{\sigma,x}}{\partial x} + \Pi_{\sigma,yy}\frac{\partial u_{\sigma,y}}{\partial y} + \Pi_{\sigma,zz}\frac{\partial u_{\sigma,z}}{\partial z}\right)$$

$$\mathrm{Pi-D}_{\sigma,\mathrm{shear}} = -\Bigg[P_{\sigma,xy}\left(\frac{\partial u_{\sigma,x}}{\partial y} + \frac{\partial u_{\sigma,y}}{\partial x}\right)$$

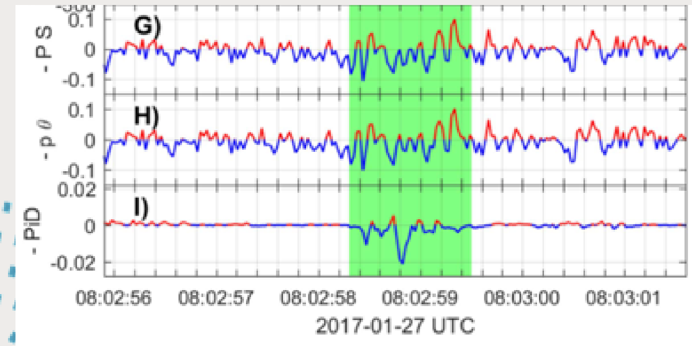
$$+P_{\sigma,xz}\left(\frac{\partial u_{\sigma,x}}{\partial z} + \frac{\partial u_{\sigma,z}}{\partial x}\right) + P_{\sigma,yz}\left(\frac{\partial u_{\sigma,y}}{\partial z} + \frac{\partial u_{\sigma,z}}{\partial y}\right)\Bigg]$$

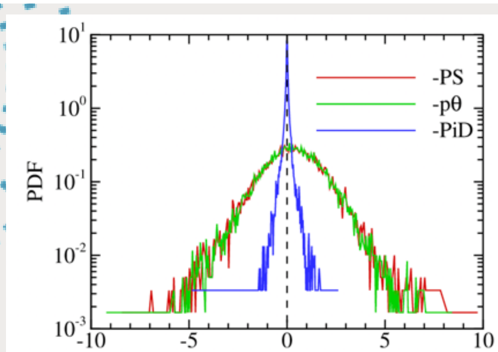
- Kinetic interpretation (Cassak and Barbhuiya, PoP, 2022): example of $-\mathcal{P}_\sigma(\nabla \cdot \mathbf{u}_\sigma)$, $\mathrm{Pi-D}_{\sigma,\mathrm{normal}}$



Pressure-Strain in Observations/Simulations

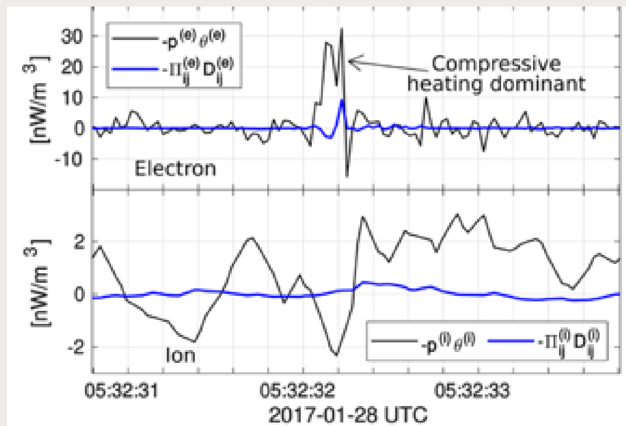
Magnetosheath Turbulence





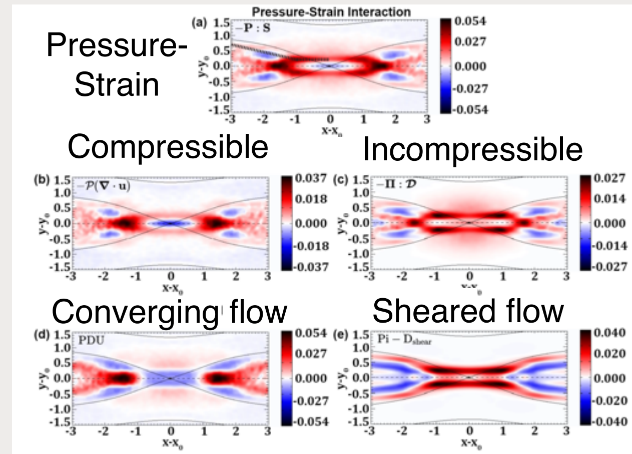
Chasapis et al., ApJ, 2018

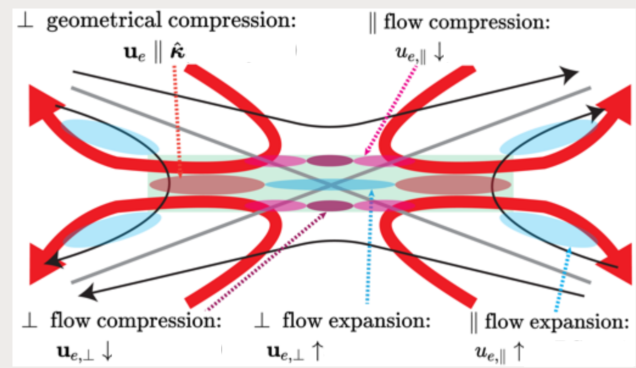
Magnetosheath Reconnection



Bandyopadhyay et al., PoP, 2021

Reconnection PIC Simulations





Barbhuiya and Cassak, PoP, 2022

Pressure-strain interaction can be > 0 or < 0 (unlike viscosity); we can identify fluid physics causing the energy conversion

non-LTE Energy Conversion and the First Law of Thermodynamics

Change in internal energy per particle $E_{\sigma,\mathrm{int}} = \frac{3}{2} k_B \mathcal{T}_\sigma$

Pressure dilatation Compressive heating/ expansive cooling

"Pi-D" Incompressible Deformation

Heat flux density divergence, transport due to non-Maxwellianity

Interspecies collisional heating rate

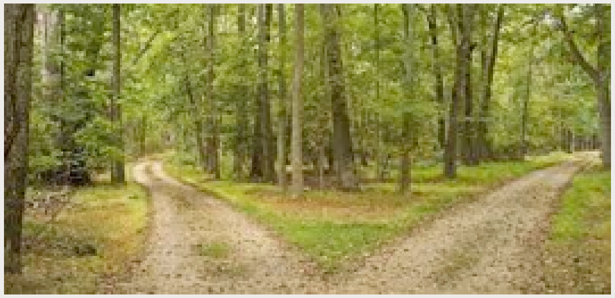
$$n_\sigma \frac{dE_{\sigma,\mathrm{int}}}{dt} = -\mathcal{P}_\sigma(\nabla \cdot \mathbf{u}_\sigma) - \Pi_{\sigma,jk}\mathcal{D}_{\sigma,jk} - \nabla \cdot \mathbf{q}_\sigma + n_\sigma \dot{Q}_{\sigma,\mathrm{coll,inter}}$$

$$\Rightarrow \frac{dE_{\sigma,\mathrm{int}}}{dt} + \frac{dW_\sigma}{dt} = \frac{dQ_\sigma}{dt} + \dot{Q}_{\sigma,\mathrm{coll,inter}}$$

- This is the **non-LTE generalization of the first law of thermodynamics**!

Advantages/Disadvantages

- Advantages
  - Fluid moments are easier to interpret
  - Readily calculable with kinetic simulations: particle-in-cell, Vlasov/Boltzmann, and hybrid
  - Now measurable with state-of-the-art spacecraft: NASA's Magnetospheric MultiScale (MMS) mission (Burch et al., SSR, 2016)



- Disadvantages
  - "Closure problem": fluid moment equations do not close without assumptions
  - Interpretation of the physical cause for the energy conversion is ambiguous
    - Multiple mechanisms can produce $\mathbf{J}_\sigma \cdot \mathbf{E}$ or $-(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma$
      - It is often important to distinguish between energy conversion mechanisms — we have to understand energy conversion as a function of f_σ!

Energy Conversion in Kinetic Theory

- Field-particle interaction approach (Klein and Howes, ApJL, 2016)
  - Particle energy per unit phase space volume w_σ is

$$w_\sigma = \frac{1}{2} m_\sigma v^2 f_\sigma$$

  - w_σ evolves according to

$$\frac{\partial w_\sigma}{\partial t} + \underbrace{\nabla \cdot \left(\frac{1}{2} m_\sigma v^2 \mathbf{v} f_\sigma \right)}_{\text{Energy flux}} + \underbrace{\frac{q_\sigma v^2}{2} \left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c} \right) \cdot \nabla_v f_\sigma}_{\text{Field-particle interaction}} = \underbrace{\frac{1}{2} m_\sigma v^2 C[f]}_{\text{Collisions}}$$

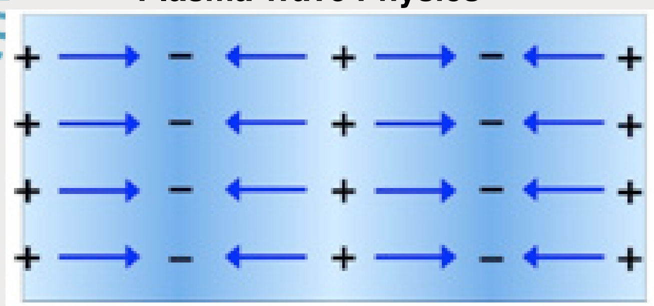
  - Velocity space integral of field-particle interaction term is $\mathbf{J}_\sigma \cdot \mathbf{E}$
    - The field-particle interaction term describes energy conversion rate between fields and particles of species σ per *phase space* volume

Field-Particle Interaction

- Can identify not just the location of energy conversion but where in velocity space it occurs!
  - Crucial to identify the kinetic *mechanism* of the energy conversion

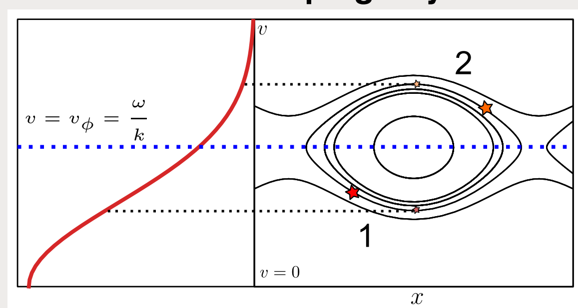
- Example - Landau damping
  - Energy conversion causing the damping is by particles near the phase speed of the wave resonantly gaining energy from the effectively DC electric field

Plasma Wave Physics



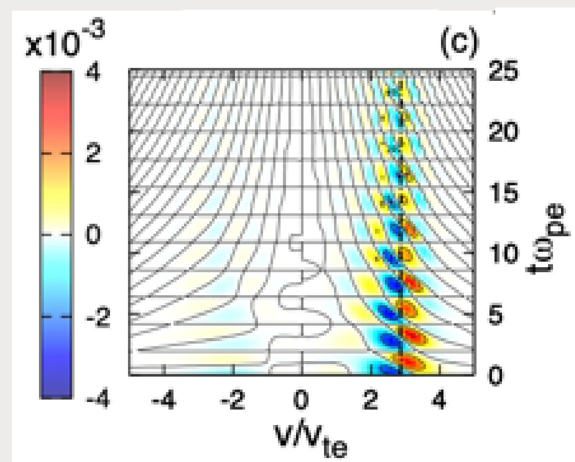
https://www.jeol.com/words/emterms/20121023.060058.php#gsc.tab=0

Landau Damping Physics



Perera et al., Poster BP11.00084

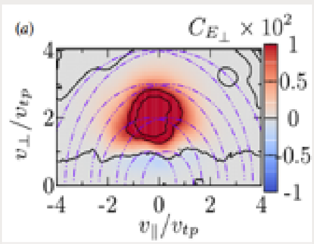
Field-Particle Interaction



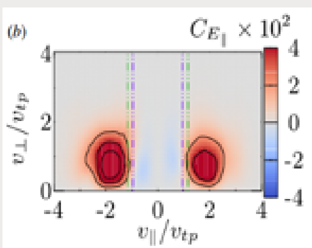
Klein and Howes, ApJL, 2016

Field-Particle in Observations/Simulations

Ion cyclotron damping

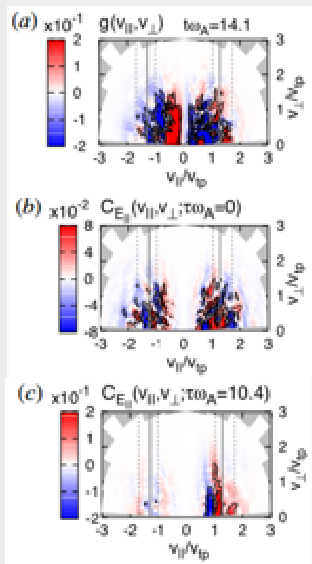


Ion Landau damping



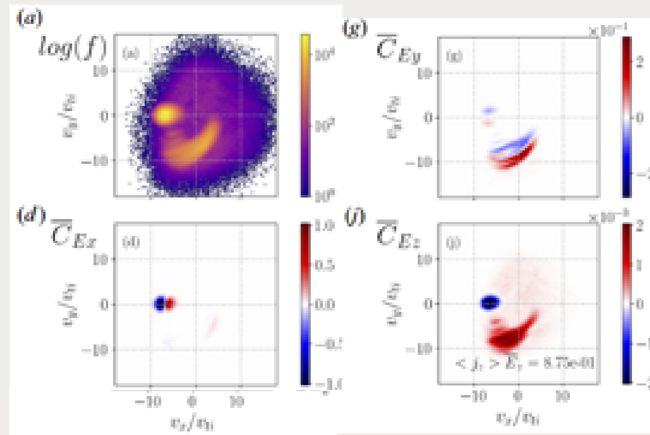
Klein et al., JPP, 2020

Ions in turbulence



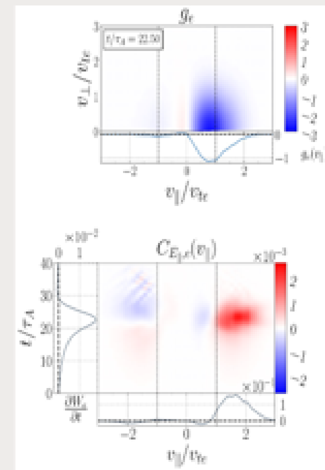
Klein et al., JPP, 2017

Ions in shock



Brown et al., JPP, 2023;
Juno et al., ApJ, 2023

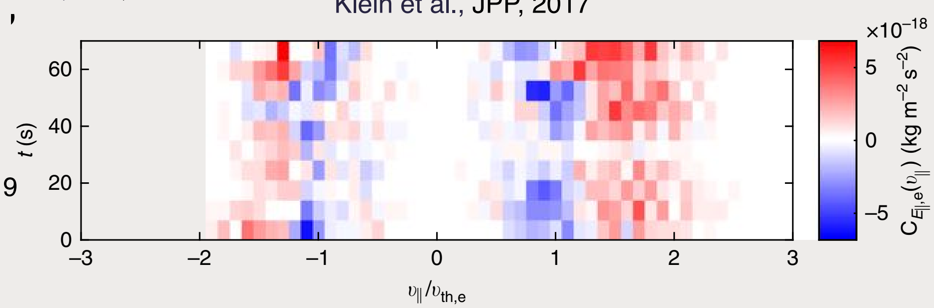
Electrons in reconnection



McCubbin et al., PoP, 2022

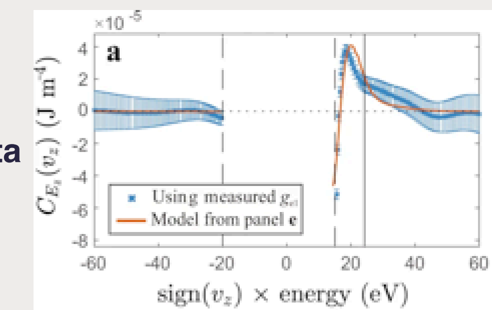
Kinetic Alfvén wave in MMS data

Chen et al., Nat. Comm., 2019



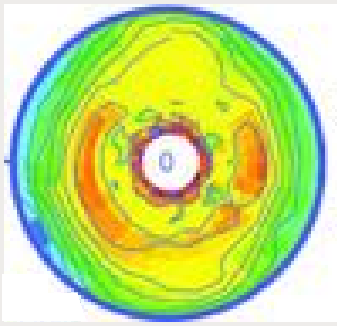
Alfvén wave in LAPD lab data

Schroeder et al., Nat. Comm., 2021



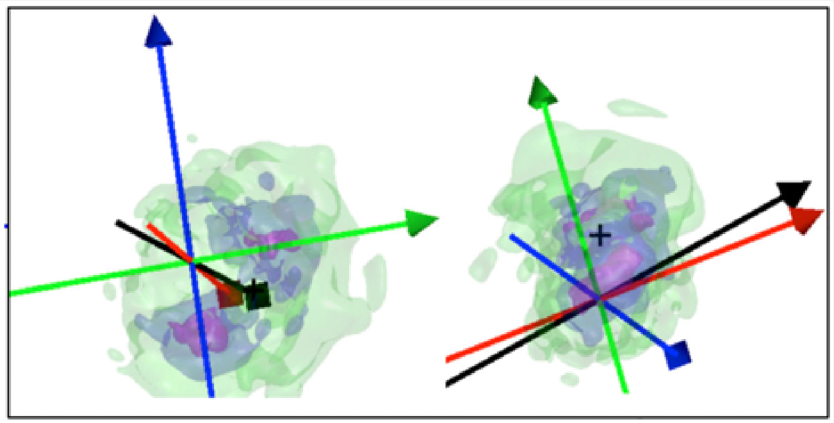
Going Beyond Energy?

- Energy evolution is described by the second moment of f_σ
- The fundamental quantity in kinetic theory is f_σ
  - When not in LTE, there can be infinitely many moments of f_σ!
  - Any moment can change as f_σ evolves!
    - Is there a reason we care about the 2nd moment … but not the 47th?!?



Burch et al., Science, 2016

We argue a complete description of the dynamics requires all moments of f_σ



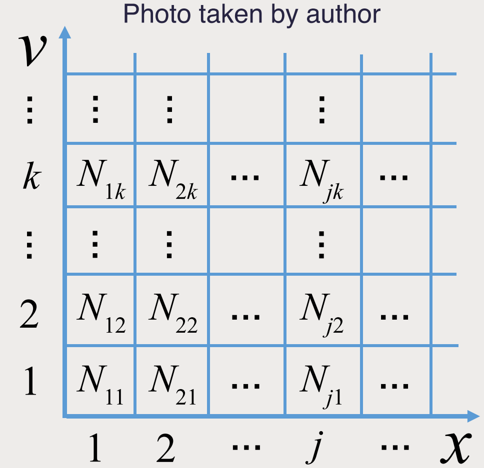
Goldman et al., JGR, 2020

An Entropic Approach

- Potential approaches
  - Direct study of f_σ using Vlasov/Boltzmann equation - hard!
  - Study of fluid equations of all moments - closure problem!
  - Perturbative approach, such as Chapman-Enskog, Onsager relations, Grad 13-moment model/Extended Irreversible Thermodynamics (EIT), gyrokinetics - only formally valid for weakly non-LTE systems
  - Entropic approach
    - Entropy S_σ in kinetic theory is related to the number W_σ of microstates equivalent to a given macrostate, $S_\sigma = k_B \ln W_\sigma$
    - Boltzmann derived kinetic entropy density s_σ for a system with fixed number of particles N_σ (e.g., Bellan's plasma textbook):

$$S_\sigma = \int s_\sigma d^3r, \qquad s_\sigma = -k_B \int f_\sigma \ln\left(\frac{f_\sigma \Delta^3 r_\sigma \Delta^3 v_\sigma}{N_\sigma}\right) d^3v$$

Photo taken by author



Liang et al., PoP, 2019

“Relative Entropy” and Higher Order Moments

- Entropy contains information about all the “internal” moments of f_σ (moments of powers of $v_j - u_j$)

$$s_\sigma = -k_B \int f_\sigma \ln\left(\frac{f_\sigma \Delta^3 r_\sigma \Delta^3 v_\sigma}{N_\sigma}\right) d^3v$$

- Consider the “relative entropy” $s_{\sigma,\mathrm{rel}}$ (Grad, J. Soc. Indust. Appl. Math., 1965)

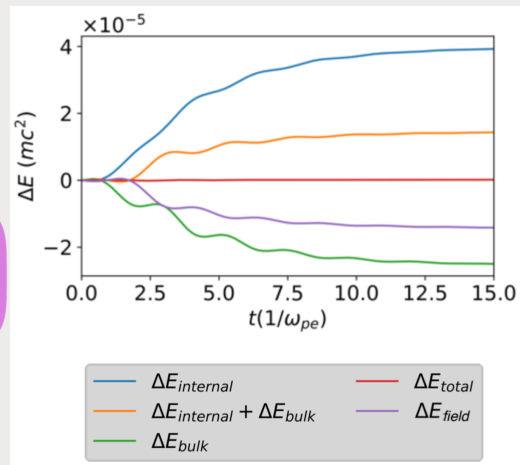
$$s_{\sigma,\mathrm{rel}} = -k_B \int f_\sigma \ln\left(\frac{f_\sigma}{f_{\sigma M}}\right) d^3v$$

- Related to “Kullback-Leibler divergence” (Kullback and Leibler, Ann. Math. Statist., 1951) in information theory
  - Measures statistical separation between distribution f_σ and a reference distribution $f_{\sigma M}$
  - $s_{\sigma,\mathrm{rel}} = 0$ if f_σ is Maxwellian and $s_{\sigma,\mathrm{rel}} < 0$ if not (Grad, J. Soc. Indust. Appl. Math., 1965)
  - It is a measure of non-Maxwellianity of f_σ
    - There are other non-Maxwellianity measures (Kaufmann and Paterson, JGR, 2009; Greco et al., PRE, 2012; Servidio et al., PRL, 2017; Liang et al., JPP, 2020)

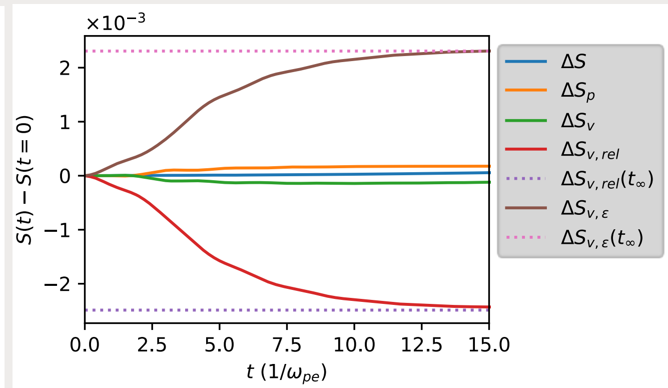
Example - Landau Damping

- Entropy conversion in a 1D traveling plasma wave with charge neutralizing ions
  - Conservation of energy gives final temperature (known since 1960s)
  - Conservation of entropy gives the final position space, velocity space, and relative entropies (Perera et al., in prep)
  - Validated as a function of density perturbation in 1D-1V PIC simulations
    - See also Celebre et al., PoP, 2023

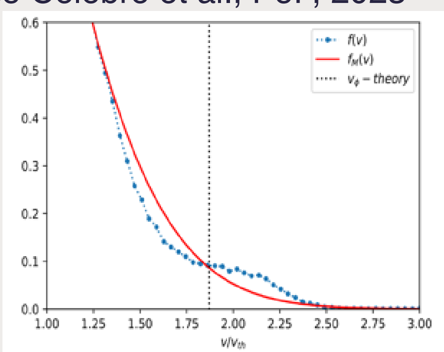
Conservation of energy

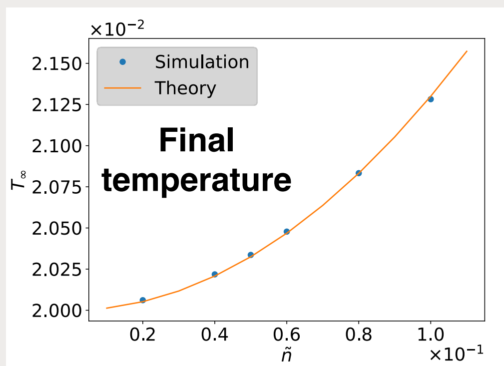


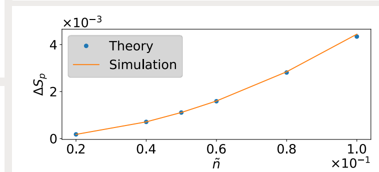
Conservation of entropy



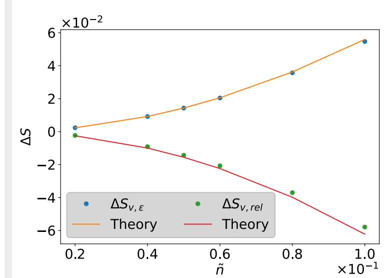
Phase Space Density







Final position space entropy



Final velocity space entropy

Final relative entropy

Perera et al., in prep

Time Evolution of Relative Entropy

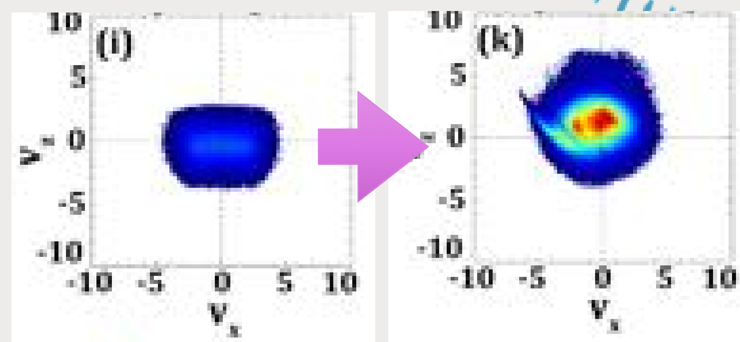
- Time derivative of $s_{\sigma,\mathrm{rel}}$ quantifies the rate at which the shape of f_σ changes (Cassak et al., PRL, 2023)

$\dfrac{d(s_{\sigma,\mathrm{rel}}/n_\sigma)}{dt} > 0$	Evolving towards LTE (thermalizing)
$\dfrac{d(s_{\sigma,\mathrm{rel}}/n_\sigma)}{dt} < 0$	Evolving away from LTE (more non-thermal)

- We defined "Higher ORder Non-Equilibrium Terms" (HORNET) $P_{\sigma,\mathrm{HORNET}}$ with dimensions of power density (Barbhuiya et al., PRE, submitted)

$$P_{\sigma,\mathrm{HORNET}} = -n_\sigma \mathcal{T}_\sigma \frac{d}{dt}\left(\frac{s_{\sigma,\mathrm{rel}}}{n_\sigma}\right)$$

  - If initial f_σ is in LTE and final f_σ is not in LTE, $P_{\sigma,\mathrm{HORNET}}$ quantifies how non-adiabatic the process is
  - Can make direct comparison with power densities, such as $\mathbf{J}_\sigma \cdot \mathbf{E}$ and pressure-strain interaction

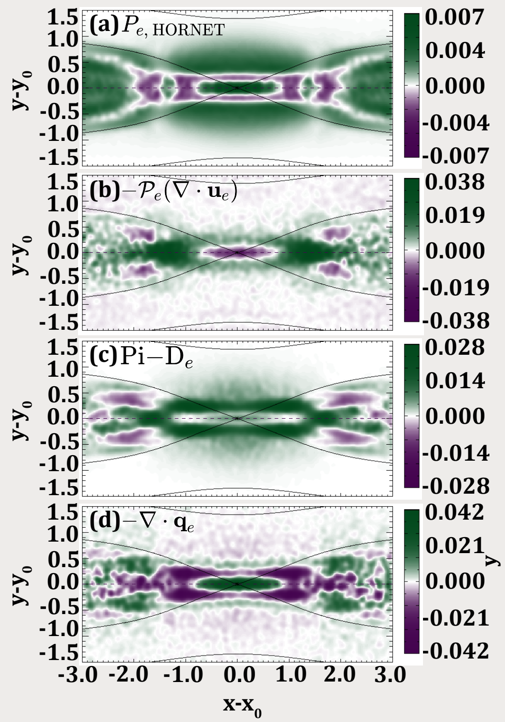


Cassak et al., PRL, 2023

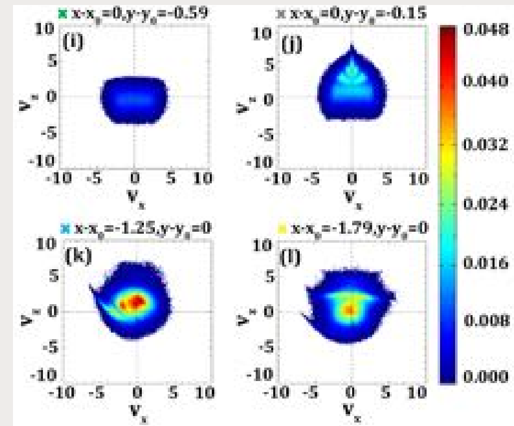
AP photo by Quinlyn Baine / Washington State Department

Examples - Reconnection & Turbulence

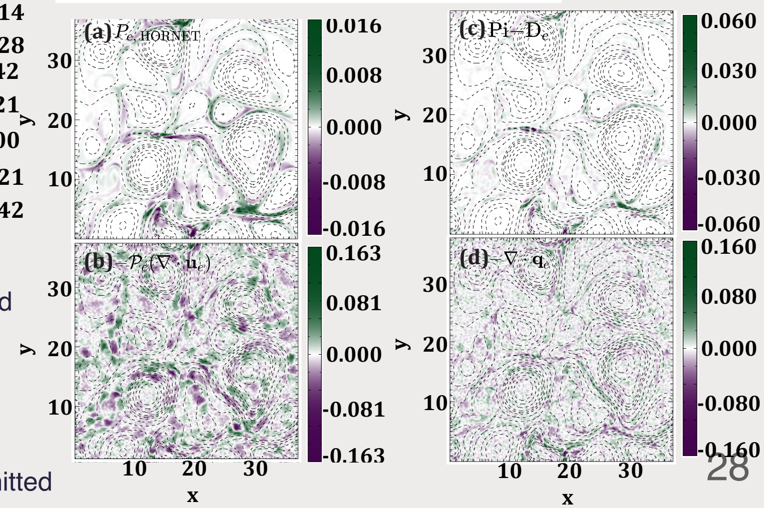
- 2D collisionless particle-in-cell simulations of magnetic reconnection and decaying plasma turbulence (Barbhuiya et al., submitted)
- Results:
  - In reconnection, HORNET has the sign expected from knowledge of evolution of f_σ
    - HORNET can be locally important, but the net is small when integrated over the electron diffusion region
  - In turbulence simulation, system average can be up to 67% of power densities!
    - Non-LTE effects can be dynamically significant!



Barbhuiya et al., PRE, submitted



Cassak et al., PRL, 2023



Barbhuiya et al., PRE, submitted

Kinetic Entropy Evolution

- Evolution equations for s_σ (e.g., Eyink, PRX, 2018) and s_σ/n_σ (Eu, JCP, 1995; Cassak et al., PRL, 2023):

$$\frac{\partial s_\sigma}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{J}}_\sigma = \dot{s}_{\sigma,\mathrm{coll}} \qquad \frac{d}{dt}\left(\frac{s_\sigma}{n_\sigma}\right) + \frac{\nabla \cdot \mathcal{J}_{\sigma,\mathrm{th}}}{n_\sigma} = \frac{\dot{s}_{\sigma,\mathrm{coll}}}{n_\sigma}$$

- A trick: decompose s_σ into 2 terms, $s_{\sigma P}$ and $s_{\sigma V}$ (Mouhot & Villani, Acta Math, 2011; Liang et al., PoP, 2019):

$$s_{\sigma P} = -k_B n_\sigma \ln\left(\frac{n_\sigma \Delta^3 r_\sigma}{N_\sigma}\right) \qquad s_{\sigma V} = -k_B \int f_\sigma \ln\left(\frac{f_\sigma \Delta^3 v_\sigma}{n_\sigma}\right) d^3v$$

- and decompose $s_{\sigma V}/n_\sigma$ into two terms:

$$\frac{s_{\sigma V,\mathcal{E}}}{n_\sigma} = -k_B \int \frac{f_\sigma}{n_\sigma} \ln\left(\frac{f_{\sigma M} \Delta^3 v_\sigma}{n_\sigma}\right) d^3v \qquad \frac{s_{\sigma,\mathrm{rel}}}{n_\sigma} = -\frac{k_B}{n_\sigma} \int f_\sigma \ln\left(\frac{f_\sigma}{f_{\sigma M}}\right) d^3v$$

- After suitable decomposition of $\boldsymbol{\mathcal{J}}_\sigma$ and $\dot{s}_{\sigma,\mathrm{coll}}$, top right equation becomes

$$\frac{dE_{\sigma,\mathrm{int}}}{dt} + \frac{dE_{\sigma,\mathrm{rel}}}{dt} + \frac{dW_\sigma}{dt} = \frac{dQ_\sigma}{dt} + \frac{dQ_{\sigma,\mathrm{rel}}}{dt} + \dot{Q}_{\sigma,\mathrm{coll,inter}} + \dot{Q}_{\sigma,\mathrm{coll,rel}}$$

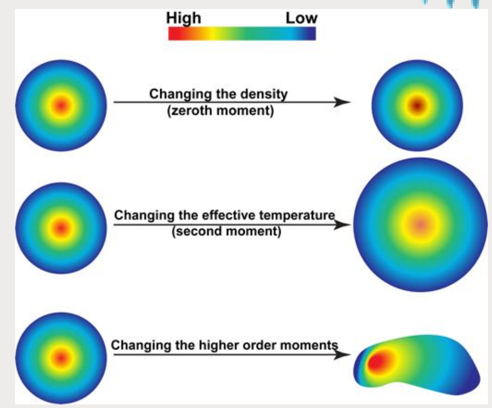
- The entropy equation *contains the non-LTE generalization of the first law of thermodynamics* (and more!)

Interpretations In Context of First Law

- Interpretation 1: In the gyrokinetic limit (Schekochihin et al., ApJS, 2009), $s_{\sigma,\mathrm{rel}}$ is proportional to the "free energy" (Cassak et al., PRL, 2023, Celebre et al., PoP, 2023)
- Interpretation 2: Subtract out the non-LTE generalization of the first law of thermodynamics:

$$\frac{dE_{\sigma,\mathrm{rel}}}{dt} = \frac{dQ_{\sigma,\mathrm{rel}}}{dt} + \dot{Q}_{\sigma,\mathrm{coll,rel}} \qquad \frac{dE_{\sigma,\mathrm{rel}}}{dt} = \mathcal{T}_\sigma \frac{d(s_{\sigma V,\mathrm{rel}}/n_\sigma)}{dt}$$

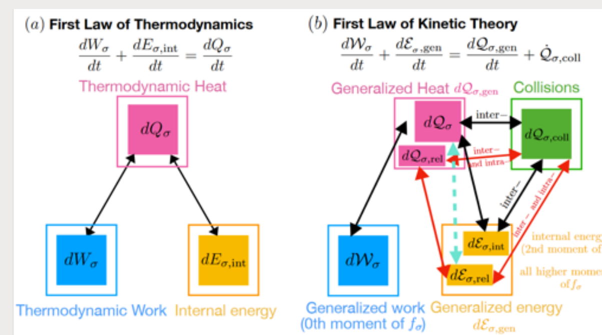
  - First law of thermodynamics describes energy conversion; this equation supplements the first law for non-LTE systems, describing the time evolution the shape of f_σ



- Interpretation 3: Combine the "relative" terms with their non-LTE thermodynamic counterparts, $dE_{\sigma,\mathrm{gen}} = dE_{\sigma,\mathrm{int}} + dE_{\sigma,\mathrm{rel}}$ and $dQ_{\sigma,\mathrm{gen}} = dQ_\sigma + dQ_{\sigma,\mathrm{rel}}$:

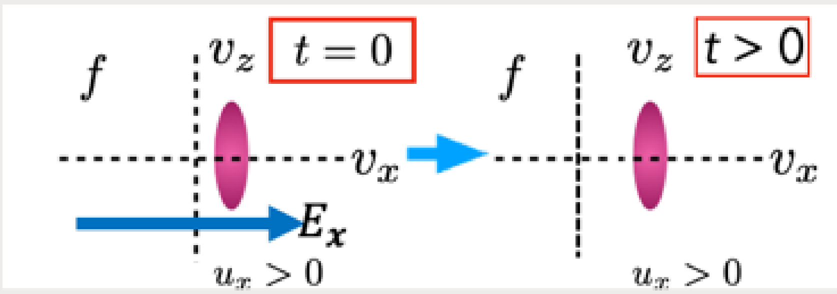
$$\frac{dW_\sigma}{dt} + \frac{dE_{\sigma,\mathrm{gen}}}{dt} = \frac{dQ_{\sigma,\mathrm{gen}}}{dt} + \dot{Q}_{\sigma,\mathrm{coll}}$$

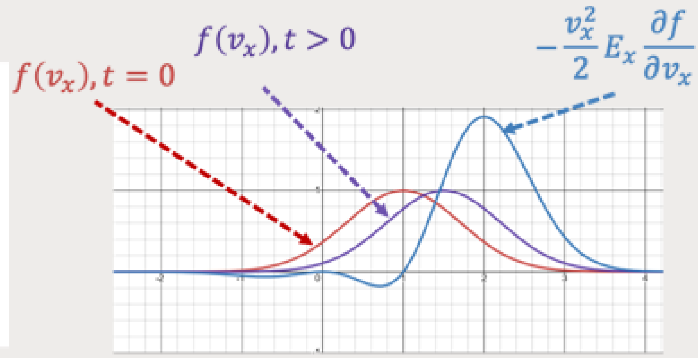
  - Interpret the first law of thermodynamics in LTE as linking the evolution of all the internal moments necessary to describe the system ($n_\sigma \leftrightarrow dW_\sigma$, $T_\sigma \leftrightarrow dE_{\sigma,\mathrm{int}}$); then this expression generalizes the first law of thermodynamics for non-LTE systems that can in principle have an infinite number of internal moments
    - We call it "the first law of kinetic theory" (Cassak et al., PRL, 2023)
    - First principles, only assumption is that N_σ is conserved, valid arbitrarily far from LTE, avoids the "closure problem"



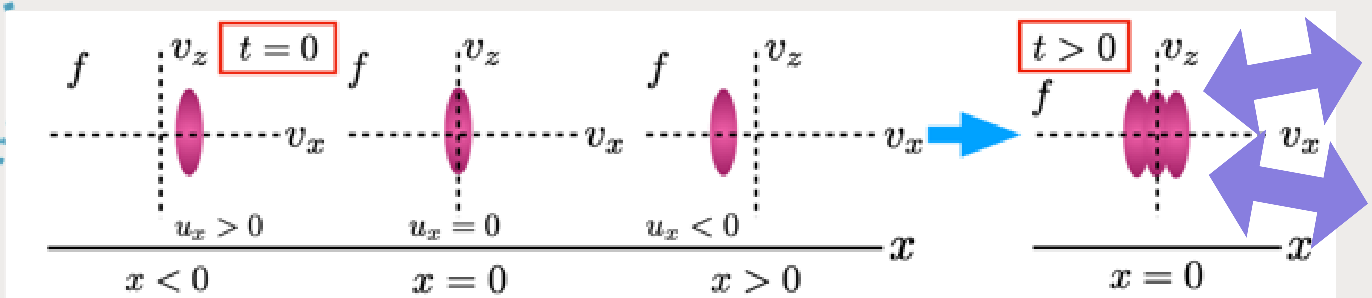
Cassak et al., PRL, 2023

Putting It All Together: PS, FPI, & HORNET





Asymmetry in f_σ parallel to $\mathbf{E} \Rightarrow$ net positive energy conversion from EM to bulk kinetic



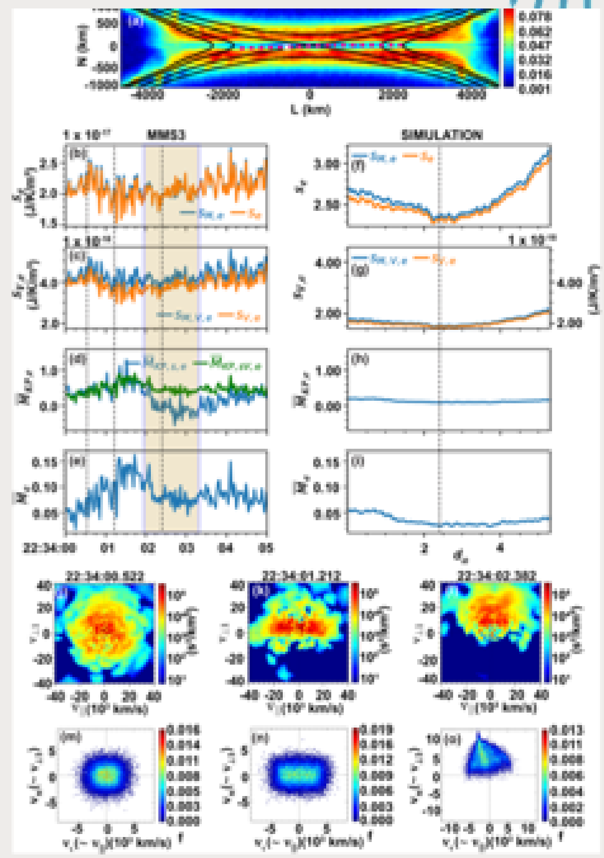
$-(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma > 0 \Rightarrow$ flow convergence broadens f_σ, internal energy increases

$P_{\sigma,\text{HORNET}} < 0 \Rightarrow f_\sigma$ evolving towards Maxwellianity

We're developing the ability to understand energy conversion and phase space density evolution at the phase space density-level

Open Questions

- Can the absolute and relative energy conversion metrics and HORNET be predicted/understood for different ambient plasma parameters and for different physical phenomena? (e.g., Conley et al., JPP, 2023)
- How do the microphysical non-LTE effects described here fit in to meso-scale and macro-scale dynamics? Can non-LTE effects be captured as fluid closures, such as through machine learning?
- What are the role of body forces in changing internal energy?
- How does one relax the assumption about the number of particles being conserved? Seems necessary for applications to low temperature plasmas!
- Are the metrics accessible to observational or experimental scrutiny?
  - MMS has been used to measure field-particle correlation (Chen et al., Nat. Comm., 2019) and pressure-strain interaction (numerous studies)
    - Pressure-strain at ion/MHD scales will be measured by NASA's HelioSwarm
  - MMS has sufficient spatio-temporal resolution to directly measure kinetic entropy reasonably well (Argall et al., PoP, 2022; Lindberg et al., Entropy, 2022; Agapitov et al., arXiv, 2023)
    - These observations did not include relative entropy

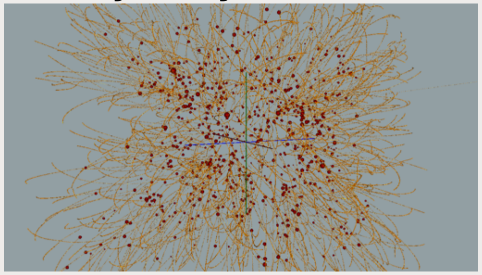


Argall et al., PoP, 2022

Open Questions

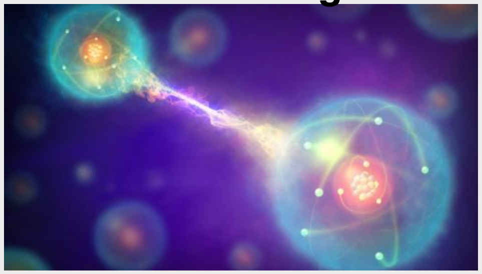
- How can non-LTE approaches describe power-law distributions from particle acceleration? It was recently addressed using entropic approach by Zhdankin (PRX, 2022; J Phys A 2023)
- How do collisions modify non-LTE energy conversion and produce irreversible dissipation (e.g., Pezzi et al., PoP, 2019; Matthaeus et al., ApJ, 2020; Pezzi et al., MNRAS, 2021; Celebre et al., PoP, 2023)?
- How does entropic approach work for systems for which LTE distributions are not the best reference distributions (e.g., Lynden-Bell, MNRAS, 1967; Eu, JCP, 1995; Livadiotis, Europhys. Lett., 2018)?
- Can the entropic approach be applied outside of plasma physics that employ kinetic theory?
  - Jeans equation for stellar dynamics in galaxies, many body simulations of astrophysical systems, molecular dynamics simulations of micro- and nano-fluids for chemical and biological systems
  - There is an analogous result for quantum statistical mechanics with applications to entanglement (Floerchinger and Haas, PRE, 2020)

Many body simulation



https://philippos.info/nbody/

Quantum Entanglement



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Thank you!