Quantifying Dynamics of Plasmas Out of Local Thermodynamic Equilibrium

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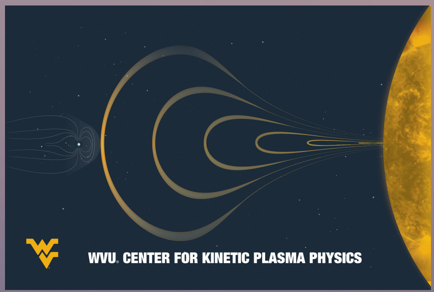
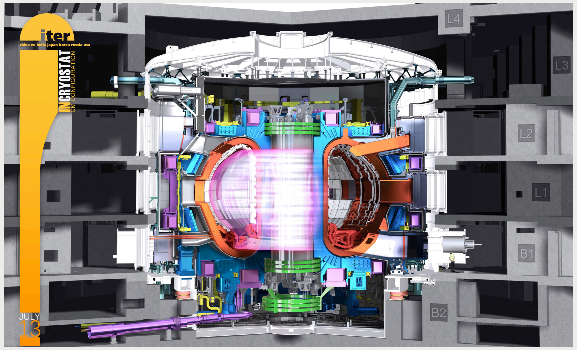


Overview

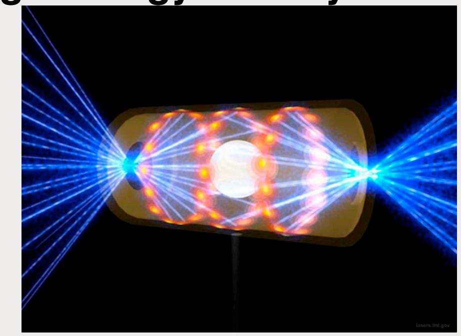
- Plasmas are often out of local thermodynamic equilibrium (LTE)
- We quantify the evolution of *all* non-LTE physics
- We introduce a non-LTE measure with dimensions of power density
- Applications to reconnection, turbulence, and Landau damping
  - Other potential applications - collisionless shocks, wave-particle interactions, low temperature plasmas, laser plasma interaction, …, and beyond plasma physics

Magnetic Confinement Fusion



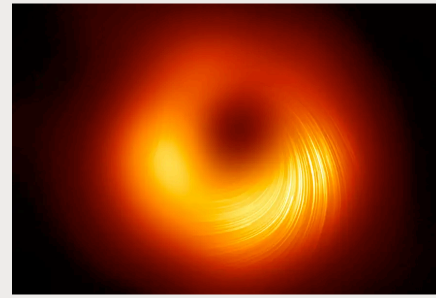
https://www.iter.org/proj/inafewlines

Inertial Confinement Fusion, High Energy Density Plasmas



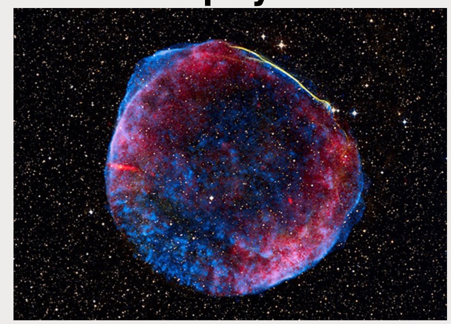
National Ignition Facility

Compact Objects



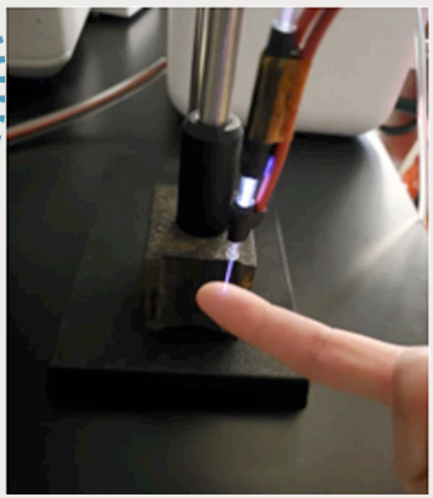
EHT Collaboration/ESO

Astrophysical



nasa.gov

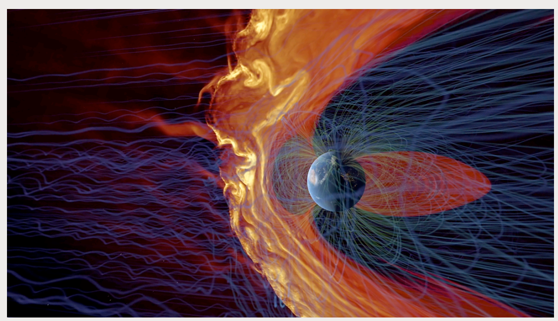
Low Temperature/ Medical/Industrial



Nicol et al., Sci. Reports, 2020

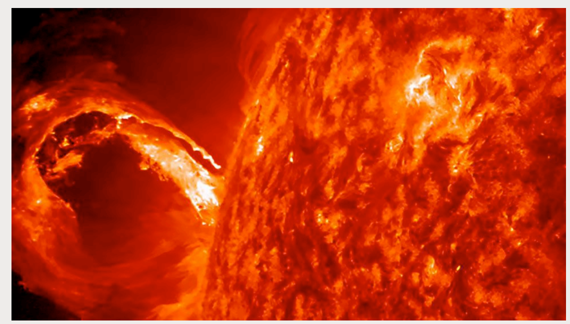
Energy Conversion in Plasmas

Magnetosphere, Interplanetary/stellar



Advanced Visualization Lab, UIUC

Solar/Stellar



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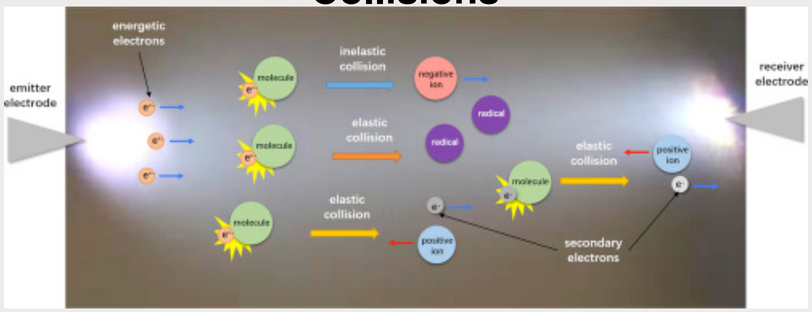
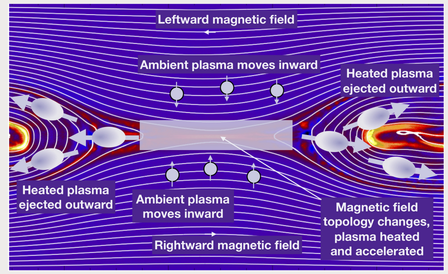
Energy Conversion Mechanisms in Plasmas

Collisions



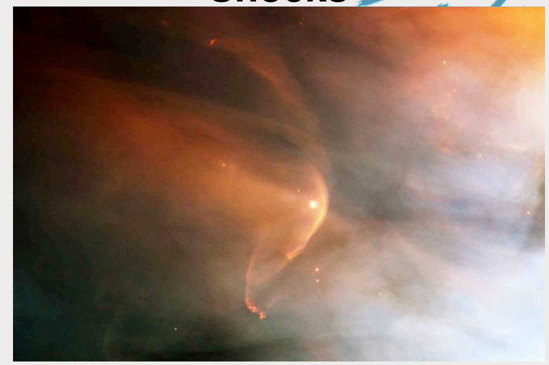
Miao et al., Green Energy and Resources, 2023

Magnetic Reconnection



Hesse and Cassak, JGR, 2020

Shocks

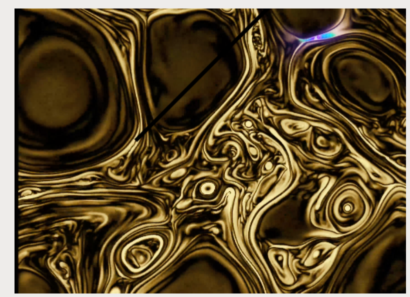


NASA and the Hubble Heritage Team (STScI/AURA)

Waves/Instabilities

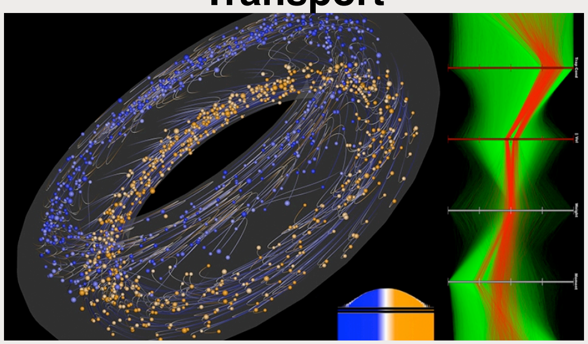
AAS

Turbulence



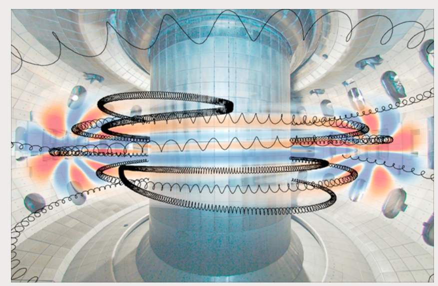
NASA Goddard's Conceptual Image Lab/Lisa Poje

Transport



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

Wave-Particle Interactions

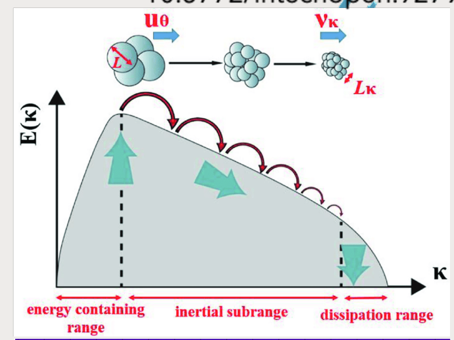


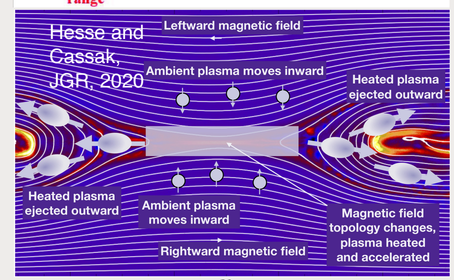
Steve Allen (LLNL), adapted by Mike Van Zeeland (General Atomics)

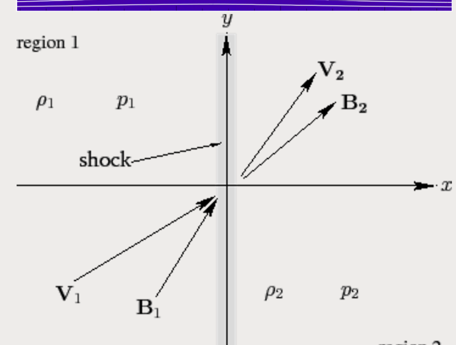
The LTE “Fluid” Approach

- Can describe energy conversion in a plasma using fluid approach
- Fluid in local thermodynamic equilibrium (LTE) ⇔ there is a well-defined local temperature
  - In LTE, energy conversion is adiabatic ($p/\rho^{\gamma} = \mathrm{constant}$)
- 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), …

Aly et al. (2020). 10.5772/intechopen.92794.







https://henry2004y.github.io/Ganymede/shocks/

Energy Conversion – Fluid Approach

- The near-LTE fluid energy density evolution equations for species σ are (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):
  - Bulk flow energy density
    $\mathcal{E}_{\sigma k} = (1/2) m_\sigma n_\sigma u_\sigma^2$
    $$\frac{\partial \mathcal{E}_{\sigma k}}{\partial t} + \nabla \cdot (\mathcal{E}_{\sigma k} \mathbf{u}_\sigma) = -\mathbf{u}_\sigma \cdot \nabla p_\sigma + q_\sigma n_\sigma \mathbf{u}_\sigma \cdot \mathbf{E} + \mathbf{R}_{\sigma,\mathrm{coll}}$$
  - Electromagnetic energy density
    $\mathcal{E}_{EM} = E^2/8\pi + B^2/8\pi$
    $$\frac{\partial \mathcal{E}_{EM}}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{J} \cdot \mathbf{E}$$
  - Internal (thermal) energy density
    $\mathcal{E}_{\sigma,\mathrm{int}} = p_\sigma/(\gamma_\sigma - 1) = 3p_\sigma/2$
    $$\underbrace{\frac{\partial \mathcal{E}_{\sigma,\mathrm{int}}}{\partial t} + \nabla \cdot (\mathcal{E}_{\sigma,\mathrm{int}} \mathbf{u}_\sigma)} = \underbrace{-p_\sigma \nabla \cdot \mathbf{u}_\sigma} + \underbrace{\dot{Q}_{\sigma,\mathrm{coll}}}$$
    - The internal energy density equation is equivalent to the first law of thermodynamics!
    $$\boxed{\frac{dE_{\sigma,\mathrm{int}}}{dt} + \frac{dW_\sigma}{dt} = \frac{dQ_\sigma}{dt}}$$

Validity of the Fluid Model

- The fluid model for species σ assumes the system is in, or very near to, local thermodynamic equilibrium (LTE)
  - This means there is a well-defined temperature T_σ
- The phase space density $f_\sigma(\mathbf{r}, \mathbf{v}, t)$ is the number density of particles in phase space, *i.e.*, position $\mathbf{r}$, velocity $\mathbf{v}$ space:

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

where $N_{\sigma,jk}$ is the number of particles in the jk'th cell of phase space

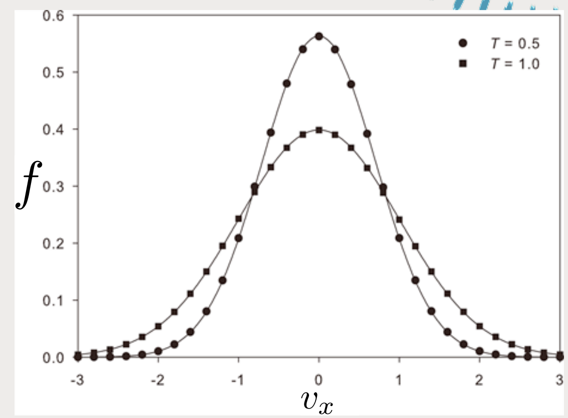
- In LTE, f_σ has a Maxwell-Boltzmann distribution $f_{\sigma,MB}$ (it is "Maxwellian")

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

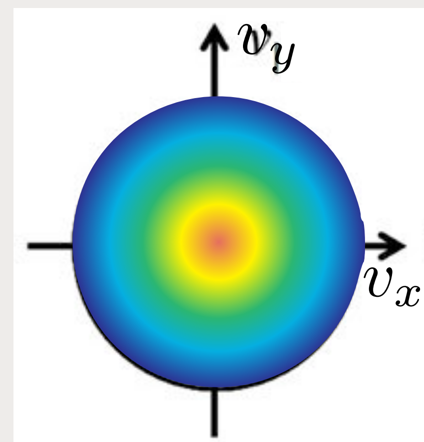
  - The density n_σ is the area under the curve
  - The temperature T_σ is related to the standard deviation (breadth) of f_σ

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

  - The temperature is a measure of the internal (thermal) energy per particle $E_{\sigma,\mathrm{int}}$

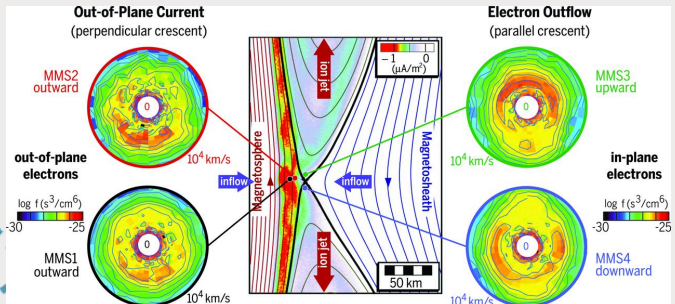


Mohazzabi and Shankar, JAMP, 2018



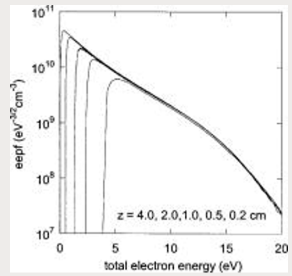
When the Fluid Model is Invalid (non-LTE)

Earth's Magnetopause (MMS)



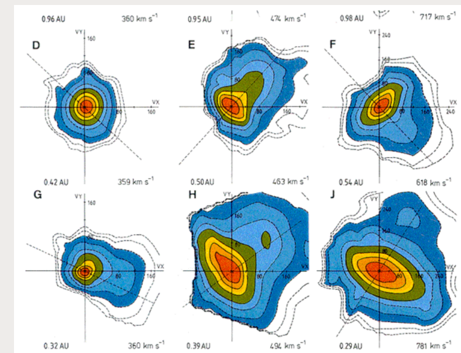
Burch et al., Science, 2016

Low Temperature Experiment



Godyak, PoP, 2005

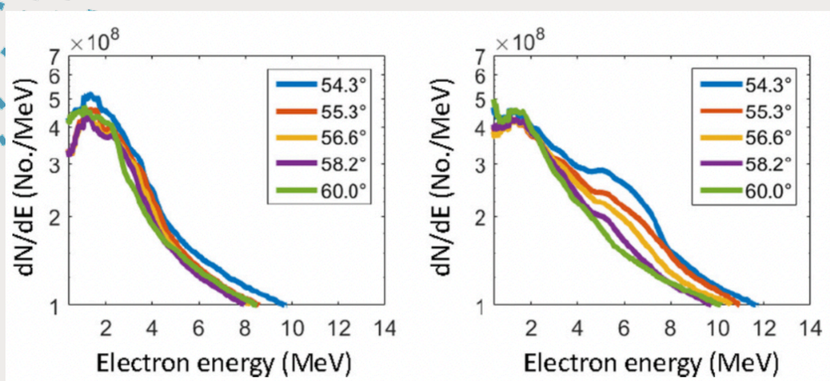
Solar Wind (Helios)



Marsch, Ann. Geophys., 2018

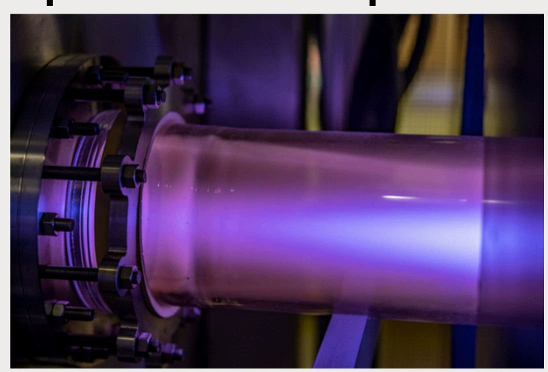
$$f_\sigma \neq f_{\sigma,MB}$$

HEDP Experiment (OMEGA)

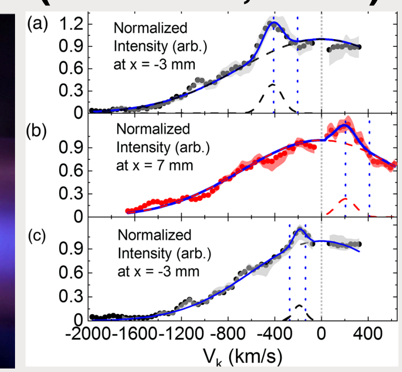


Raymond et al., PRE, 2018

Space/Fusion Experiment (PHASMA, WVU)



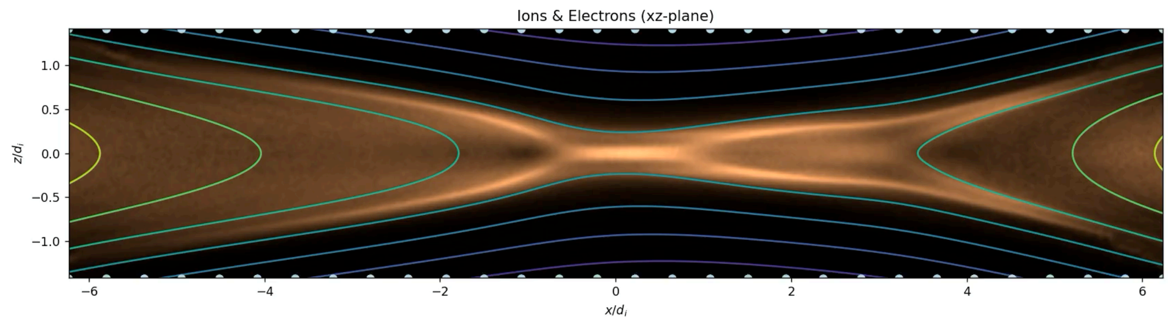
Courtesy of Earl Scime, Jake Stump, WVU



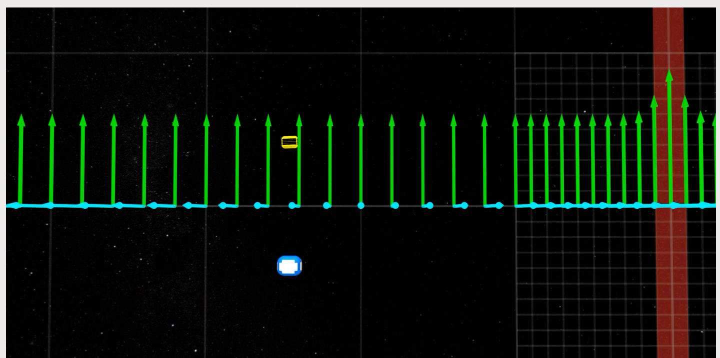
Shi et al., PRL, 2022

Why are Plasmas not in LTE?

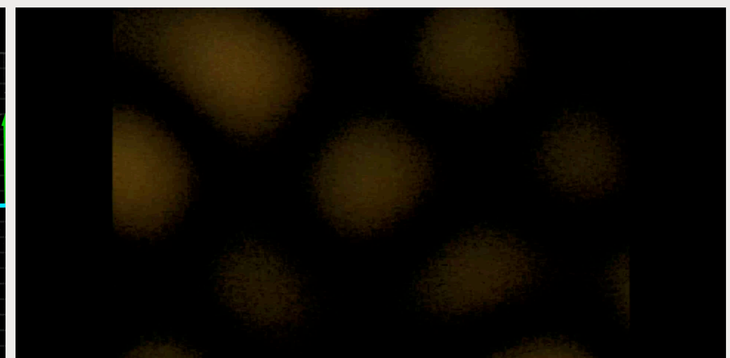
- Collisions weak or absent (high temperature, low density) or act differently on different species (low temperature)
  - Anisotropies, particle trapping, finite-Larmor radius effects, non-thermal heating, … (Howes, PoP, 2017; Matthaeus, ApJ, 2020; Alvarez Laguna et al., PoP, 2022)
- **How is plasma evolution described when the fluid model is not applicable?**
  - Need kinetic theory!



NASA's Scientific Visualization Studio



NASA's Scientific Visualization Studio



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Kinetic Theory - How does f_σ Evolve?

- Kinetic theory is a statistical theory of a plasma described by a phase space density f_σ
- We need a dynamical equation to describe how it evolves in time as a function of phase space coordinates $(\mathbf{r}, \mathbf{v})$
  - $\mathbf{r}$ is position coordinate, $\mathbf{v}$ is velocity coordinate
- The answer (non-relativistically, classically): the Boltzmann equation (1872)

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

  - m_σ is mass of constituent, $\mathbf{F}_\sigma$ is force
  - $C[f]$ 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.)

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} + \eta \frac{\partial f}{\partial y} + \zeta \frac{\partial f}{\partial z} + X \frac{\partial f}{\partial \xi} + Y \frac{\partial f}{\partial \eta} + Z \frac{\partial f}{\partial \zeta} + \qquad 44)$$

$$+ \int d\omega_1 \int b\,db \int d\varphi\, V (f f_1 - f' f'_1) = 0$$

Energy Conversion — Kinetic Approach

- One approach to study energy conversion using kinetic theory is to look at the associated bulk (fluid) properties of the system
  - For a system not in LTE described by its phase space density $f_\sigma(\mathbf{r}, \mathbf{v}, t)$, the velocity moments of f_σ give the bulk properties

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

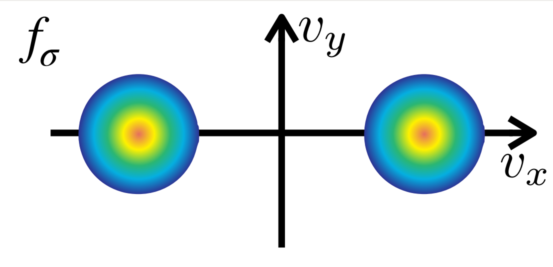
3rd moment: Tensor heat flux
$$Q_{\sigma,jkl} = \int d^3v m_\sigma (v_j - u_{\sigma j})(v_k - u_{\sigma k})(v_l - u_{\sigma l}) f_\sigma$$

… …

  - Analogous to moments of mass distributions (mass, center of mass, moment of interia)
- Note, there are in principle an infinite number of moments to describe the shape of f_σ!

Energy Conversion — Kinetic Approach

- Temperature T_σ is not well-defined for a system not in LTE! However, one can still define the internal (thermal) energy per particle $E_{\sigma,\mathrm{int}}$ as the average random kinetic energy:

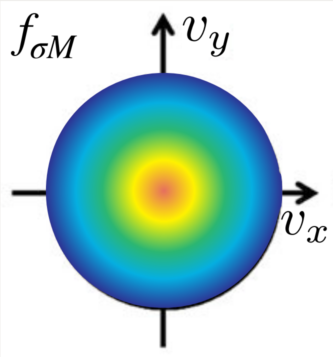


$$E_{\sigma,\mathrm{int}} = \frac{1}{n_\sigma} \int d^3v \left(\frac{1}{2} m_\sigma (\mathbf{v} - \mathbf{u}_\sigma)^2 \right) f_\sigma$$

- Can then define the "effective temperature" $\mathcal{T}_\sigma$ according to $E_{\sigma,\mathrm{int}} = (3/2) k_B \mathcal{T}_\sigma$

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

  - It is analogous to temperature in LTE; it is the temperature if the phase space density were changed to be a Maxwellian with the same internal energy



- For an arbitrary f_σ, the "Maxwellianized" distribution $f_{\sigma M}$ is (Grad, 1965)

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

Energy Conversion — Kinetic Approach

- Moments of the Boltzmann equation give kinetic theory generalizations of the fluid equations (Braginskii, 1965; Yang et al., 2017)

$$\frac{\partial n_\sigma}{\partial t} + \nabla \cdot (n_\sigma \mathbf{u}_\sigma) = 0$$ Continuity equation

$$m_\sigma n_\sigma \left[\frac{\partial \mathbf{u}_\sigma}{\partial t} + (\mathbf{u}_\sigma \cdot \nabla)\mathbf{u}_\sigma\right] = -\nabla \cdot \mathbf{P}_\sigma + q_\sigma n_\sigma \left(\mathbf{E} + \frac{\mathbf{u}_\sigma \times \mathbf{B}}{c}\right) + \mathbf{f}_{\mathrm{drag}}$$ Momentum equation

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

$$\ldots \qquad \ldots$$

  - An infinite number of fluid equations can be derived from the Boltzmann equations
    - The “closure problem” is that these equations do not close without assumptions
- The conversion of energy is studied using the internal energy density equation and the equations for other forms of energy density, namely bulk kinetic and electromagnetic:

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

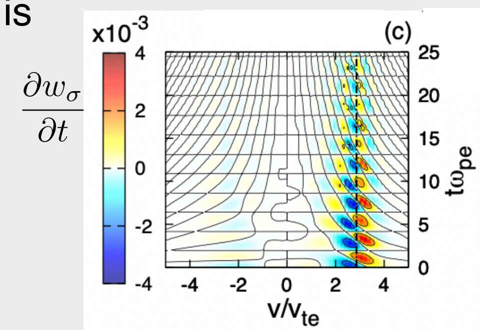
$$\frac{\partial \mathcal{E}_{EM}}{\partial t} + \nabla \cdot \mathbf{S} = -\mathbf{J} \cdot \mathbf{E}$$

  - These equations generalize the fluid equations presented previously

Energy Conversion — Particles $\leftrightarrow$ Fields

- The net energy conversion between particles and EM fields is simply related to $q_\sigma n_\sigma \mathbf{u}_\sigma \cdot \mathbf{E}$
- A kinetic theory measure of energy conversion is the "field-particle correlation" (Klein and Howes, ApJL, 2016); the particle energy per unit phase space volume w_σ is

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



Klein and Howes, ApJL, 2016

  - w_σ evolves according to

$$\frac{\partial w_\sigma}{\partial t} + \nabla \cdot \left(\frac{1}{2} m_\sigma v^2 \mathbf{v} f_\sigma \right) + \frac{q_\sigma v^2}{2 m_\sigma} \mathbf{E} \cdot \nabla_v f_\sigma = \frac{1}{2} m_\sigma v^2 C[f]$$

  - Integrating this over velocity space gives

$$\frac{\partial}{\partial t} \int w_\sigma d^3 v + \nabla \cdot \int \left(\frac{1}{2} m_\sigma f_\sigma v^2 \mathbf{v} \right) d^3 v \boxed{- q_\sigma n_\sigma \mathbf{u}_\sigma \cdot \mathbf{E}} = \int \frac{1}{2} m_\sigma v^2 C[f] d^3 v$$

    - Thus, w_σ evolution is related to conversion of energy between particles and fields
- Since w_σ is local in phase space, it can be used to distinguish between different energy conversion mechanisms, such as Landau damping and cyclotron damping in settings such as turbulence, shocks, and reconnection (Howes et al., JPP, 2017; Klein et al., JPP, 2017; Chen et al., Nat. Commun. 2019; Li et al., JPP, 2019; Klein et al., JPP, 2020; Juno et al., JPP, 2021; Verniero et al., JGR, 2021, Montag and Howes, PoP, 2022; McCubbin et al., PoP, 2022)

Energy Conversion — Bulk ↔ Internal

- The term that describes the conversion of energy between bulk kinetic energy and internal energy is the pressure-strain interaction, $-(\mathbf{P}_\sigma \cdot \nabla) \cdot \mathbf{u}_\sigma$ (Del Sarto et al., PRE, 2016; Yang et al., PoP, 2017)

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

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

  - In a closed collisionless system, the volume integrated pressure-strain interaction gives the net conversion into or out of internal energy; valid whether the system is in LTE or not
  - Commonly decomposed into pressure dilatation and “Pi-D”

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

  - Has been the subject of intense scrutiny (Yang et al., PRE, 2017; Del Sarto and Pegoraro, MNRAS, 2018; Sitnov et al., GRL, 2018; Chasapis et al., ApJ, 2018; Parashar et al., ApJL, 2018; Du et al., ApJ, 2018; Pezzi et al., PoP, 2019; Bandyopadhyay et al., PRL, 2020; Bandyopadhyay et al., PoP, 2021; Zhou et al., GRL, 2021; Fadanelli et al., JGR, 2021; Pezzi et al., MNRAS, 2021; Wang et al., JGR, 2021; Arró et al., A&A, 2022; Yang et al., MNRAS, 2022; Hellinger et al., ApJ, 2022; Yang et al., PoP, 2022; Cassak and Barbhuiya, PoP, 2022; Cassak et al., PoP, 2022; Barbhuiya and Cassak, PoP, 2022; Yang et al., ApJ, 2023)

Energy Conversion — Internal Energy

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

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

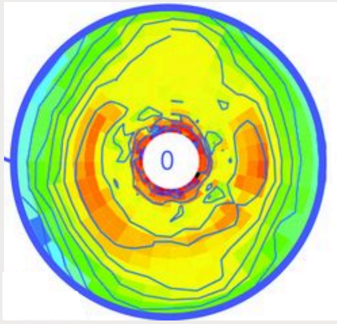
$$n_\sigma \frac{dE_{\sigma,\mathrm{int}}}{dt} = -\mathcal{P}_\sigma (\nabla \cdot \mathbf{u}_\sigma) - \Pi_{\sigma,jk} \mathcal{D}_{\sigma,jk} - \nabla \cdot \mathbf{q}_\sigma + n_\sigma \dot{Q}_{\sigma,\mathrm{coll,inter}}$$

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

- This is the **non-LTE generalization of the first law of thermodynamics**!
  - It is rigorously valid even when a scalar temperature is not well defined!

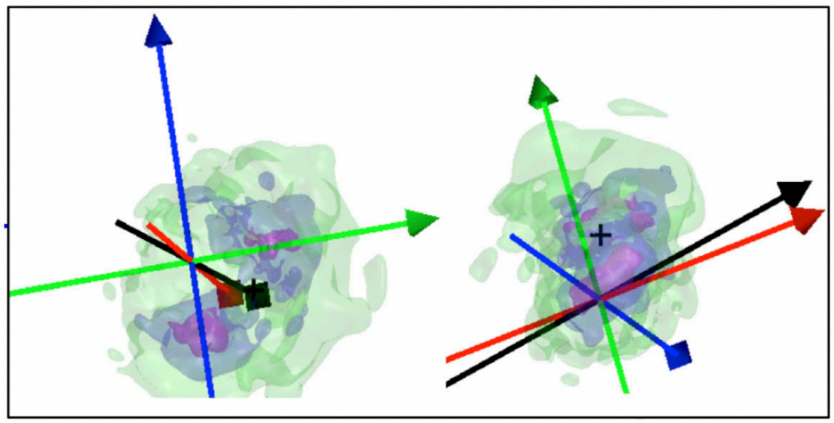
Going Beyond Energy?

- Energy evolution is described by the 2nd moment of f_σ
  - In LTE, it depends on the 0th moment of f_σ (the density)
- The fundamental quantity in kinetic theory is f_σ
  - When not in LTE, 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 <u>all</u> moments of f_σ



Goldman et al., JGR, 2020

Inspiration — the 2nd Law out of LTE

- The 2nd law of thermodynamics is $dS_\sigma/dt \geq 0$, where $dS_\sigma = dQ_\sigma/T_\sigma$
  - For non-LTE, one needs to define entropy in kinetic theory (“kinetic entropy”)
- In statistical mechanics, entropy S_σ is related to the number W_σ of microstates that are equivalent to a given macrostate, $S_\sigma = k_B \ln W_\sigma$
  - Systems tend to evolve towards more disordered states ⇒ higher entropy!
- Boltzmann showed that in kinetic theory, *i.e.*, in terms of f_σ, the kinetic entropy S_σ and kinetic entropy density s_σ for a system with N_σ particles are

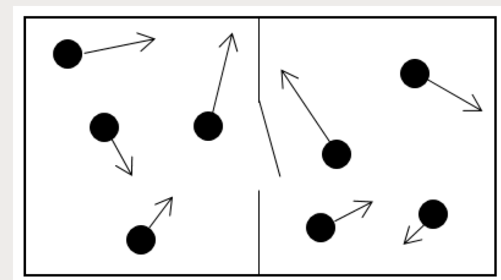
$$S_\sigma = \int s_\sigma d^3r, \qquad s_\sigma = -k_B \int f_\sigma \ln\left(\frac{f_\sigma \Delta^3 r_\sigma \Delta^3 v_\sigma}{N_\sigma}\right) d^3v$$

- Boltzmann (1877) directly calculated the time derivative of S_σ and used the Boltzmann equation for $\partial f_\sigma/\partial t$; from properties of a particular $C[f]$, he found

$$\boxed{\frac{dS_\sigma}{dt} \geq 0}$$

- This gives the kinetic theory (non-LTE) generalization of the second law of thermodynamics!

Photo taken by author



The Time Evolution of s_σ / n_σ

- Entropy contains information about all the "internal" moments of f_σ (moments of powers of $v_j - u_j$)
  - We argue its time evolution captures the time evolution of all internal moments (Cassak et al., PRL, 2023)

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

  - Kinetic entropy density satisfies a continuity-type equation (e.g., Eyink, PRX, 2018)

$$\frac{\partial s_\sigma}{\partial t} + \nabla \cdot \mathbf{J}_\sigma = \dot{s}_{\sigma,\mathrm{coll}}$$

- A trick — decompose s_σ into 2 terms, $s_{\sigma P}$ and $s_{\sigma V}$ (Mouhot and Villani, Acta Math, 2011):

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

- When written in terms of the kinetic entropy per particle s_σ / n_σ in the Lagrangian reference frame, the evolution equation is (Cassak et al., PRL, 2023; also Eu, JCP, 1995)

$$\boxed{\frac{d}{dt}\left(\frac{s_{\sigma P}}{n_\sigma}\right) + \frac{d}{dt}\left(\frac{s_{\sigma V}}{n_\sigma}\right) + \frac{\nabla \cdot \mathbf{J}_{\sigma,\mathrm{th}}}{n_\sigma} = \frac{\dot{s}_{\sigma,\mathrm{coll}}}{n_\sigma}}$$

The Time Evolution of s_σ / n_σ

- The first term directly gives rise to the generalized work term $\frac{d}{dt}\left(\frac{s_{\sigma P}}{n_\sigma}\right) + \frac{d}{dt}\left(\frac{s_{\sigma V}}{n_\sigma}\right) + \frac{\nabla \cdot \mathbf{J}_{\sigma,\mathrm{th}}}{n_\sigma} = \frac{\dot{s}_{\sigma,\mathrm{coll}}}{n_\sigma}$
- For the second term, decompose $s_{\sigma V}/n_\sigma$ into two terms (see also Grad, 1965):

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

  The resultant term is defined as "generalized internal energy," which contains internal energy and "relative energy"

$$dE_{\sigma,\mathrm{gen}} = dE_{\sigma,\mathrm{int}} + dE_{\sigma,\mathrm{rel}}$$

- Similarly the third term leads to a "generalized heat" which contains thermodynamic heat and "relative heat"

$$dQ_{\sigma,\mathrm{gen}} = dQ_\sigma + dQ_{\sigma,\mathrm{rel}}$$

- Then, the entropy per particle equation becomes

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

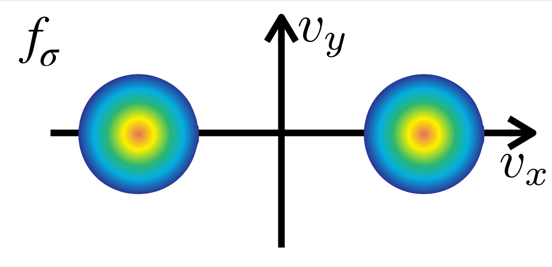
- This has the form of the first law of thermodynamics, but it is fully kinetic and captures all internal moments!
  - We call it "the first law of kinetic theory" (Cassak et al., PRL, 2023)
  - It is first principles with no assumptions, is valid arbitrarily far from LTE, and avoids "closure problem"

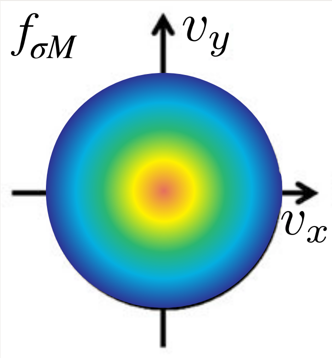
Higher Order Moments and "Relative Entropy"

- Consider the "relative entropy" term related to $s_{\sigma,\mathrm{rel}}$ (Grad, 1965)

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

  - Has its roots in the "Kullback-Leibler divergence" (Kullback and Leibler, 1951) in information theory
    - Extensively used in statistical mechanics, applied mathematics, chemistry, biology, quantum information theory, and economics
  - It is a scalar field that measures the statistical separation between a given probability distribution (f_σ here) and a reference probability distribution ($f_{\sigma M}$ here)





- $s_{\sigma,\mathrm{rel}} = 0$ if f_σ is Maxwellian and $s_{\sigma,\mathrm{rel}} < 0$ if it is not (Grad, 1965)
  - Related to, but different, from other non-Maxwellianity measures (Kaufmann and Paterson, JGR, 2009; Greco et al., PRE, 2012; Servidio et al., PRL, 2017; Liang et al., JPP, 2020)

Time Evolution of Relative Entropy

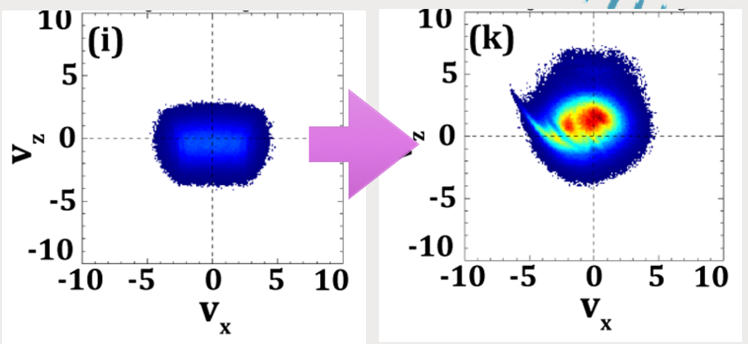
- Time derivative of $s_{\sigma,\mathrm{rel}}$ quantifies the rate at which the shape of f_σ changes (Cassak et al., PRL, 2023)

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

- Related to relative energy via $\dfrac{dE_{\sigma,\mathrm{rel}}}{dt} = \mathcal{T}_\sigma \dfrac{d(s_{\sigma,\mathrm{rel}}/n_\sigma)}{dt}$
- We defined "Higher ORder Non-Equilibrium Terms" (HORNET) $P_{\sigma,\mathrm{HORNET}}$ with dimensions of power density (Barbhuiya et al., PRE, 2024)

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

  - 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

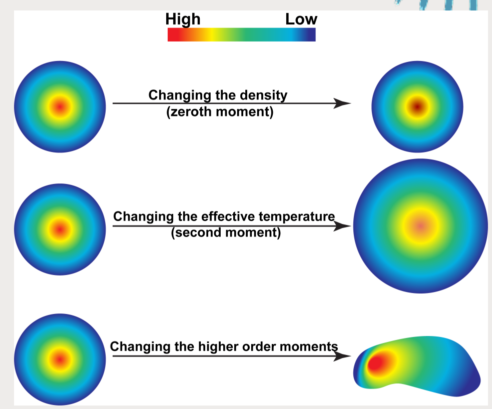

AP photo by Quinlyn Baine / Washington State Department

Interpretations In Context of First Law

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

$$\frac{dE_{\sigma,\text{rel}}}{dt} = \frac{dQ_{\sigma,\text{rel}}}{dt} + \dot{Q}_{\sigma,\text{coll,rel}}$$

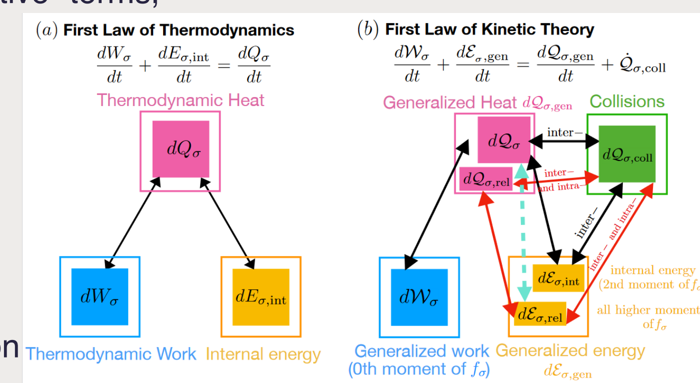
  - In this interpretation, the first law of thermodynamics describes energy conversion (relating the second moment to the zeroth); the above equation supplements the first law for non-LTE systems, describing the time evolution of the shape of f_σ



- Interpretation 3: In terms of the total of the non-LTE thermodynamic plus "relative" terms, $dE_{\sigma,\text{gen}} = dE_{\sigma,\text{int}} + dE_{\sigma,\text{rel}}$ and $dQ_{\sigma,\text{gen}} = dQ_\sigma + dQ_{\sigma,\text{rel}}$:

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

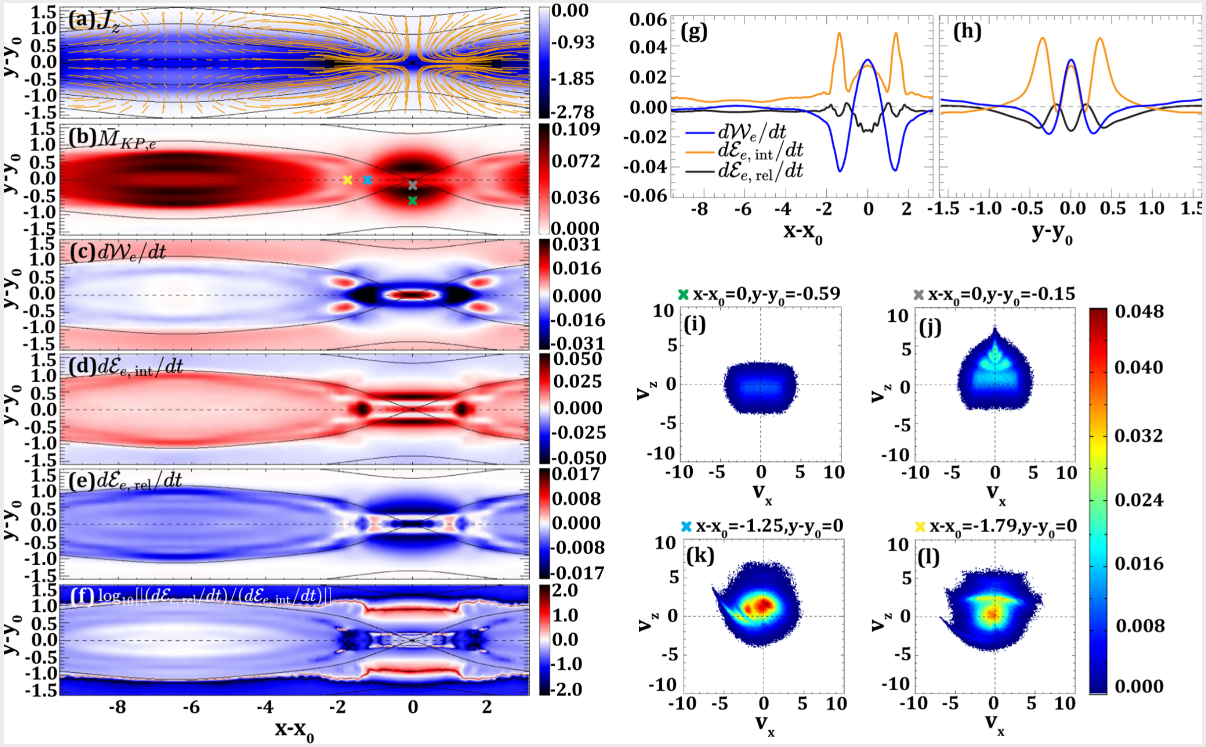
  - Interpret the first law of thermodynamics in LTE as linking the evolution of all the internal moments necessary to describe the system ($n_\sigma \leftrightarrow dW_\sigma$, $T_\sigma \leftrightarrow dE_{\sigma,\text{int}}$); then this expression generalizes the first law of thermodynamics for non-LTE systems by relating the evolution of all the infinite number of internal moments that can evolve in time



Cassak et al., PRL, 2023

Accounting of Evolution of All Moments in PIC Simulations of Magnetic Reconnection

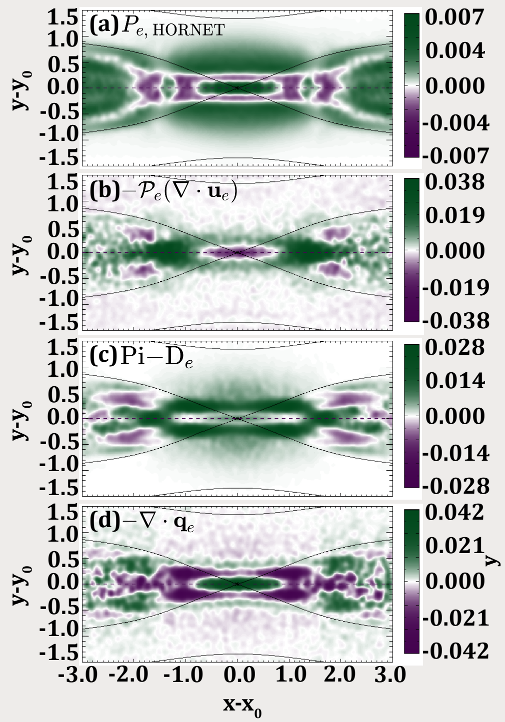
- P3D particle-in-cell (PIC) code (Zeiler et al., 2022)
- Domain size = 12.8 x 6.4
- Mass ratio m_i/m_e = 25, speed of light = 15
- **Particles per grid = 25,600**
- At a time during onset when the reconnection rate is increasing most rapidly
- Plots –
  (a) out-of-plane current density
  (b) non-Maxwellianity
  (c) rate of work per particle
  (d) rate of internal energy change per particle
  (e) rate of relative energy change per particle
  (f) log (relative / internal)
  (g, h) horizontal, vertical cuts
  (i-l) phase space densities
- **Relative energy term can be dynamically significant!**



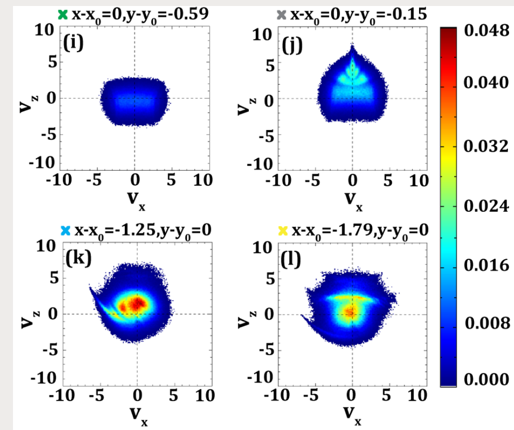
Cassak et al., PRL, 2023

Examples - Reconnection & Turbulence

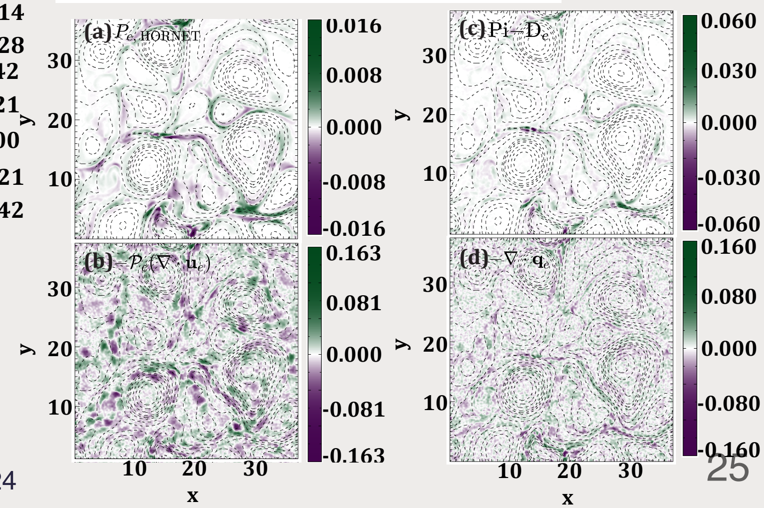
- 2D collisionless particle-in-cell simulations of magnetic reconnection and decaying plasma turbulence (Barbhuiya et al., PRE, 2024)
- Results:
  - In reconnection, HORNET has the sign expected from knowledge of evolution of f_σ
    - HORNET can be locally important, but the net is small when integrated 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, 2024



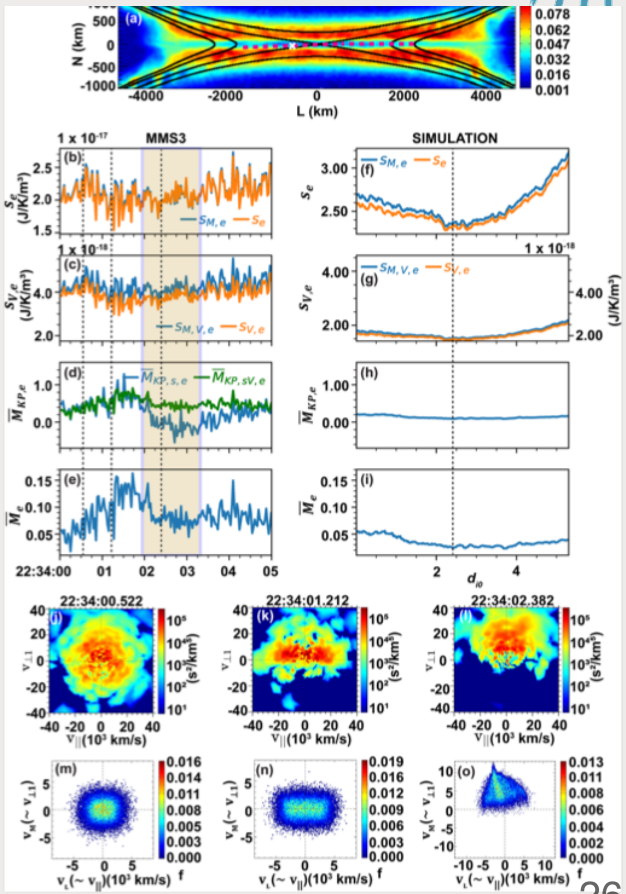
Cassak et al., PRL, 2023



Barbhuiya et al., PRE, 2024

Satellite Observations of Kinetic Entropy

- Amazingly, satellites on NASA's Magnetospheric Multiscale (MMS) mission have sufficient spatio-temporal resolution to directly measure kinetic entropy reasonably accurately (Argall et al., PoP, 2022; Lindberg et al., Entropy, 2022)
  - Allows for comparisons between numerical simulations and *in situ* observations
- Recent observations of magnetic reconnection (Argall et al., PoP, 2022)
  - MMS was used to calculate two non-Maxwellianity measures, kinetic entropy density, velocity space kinetic entropy density, and the phase space density
    - Reasonably good agreement with PIC simulations
    - Shows that simulations with periodic boundary conditions can give reasonable local values even though it is a closed system and naturally occurring reconnection is in open systems
  - We are pursuing further comparisons presently

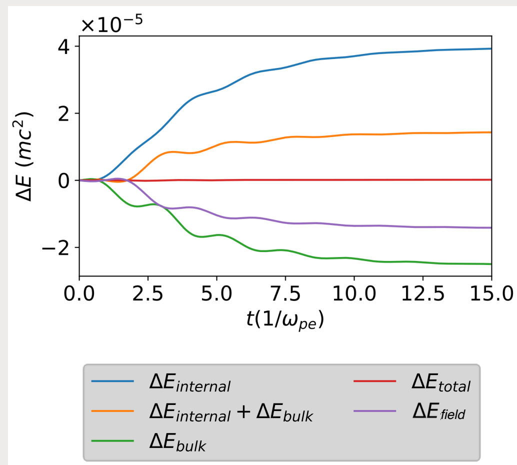


Argall et al., Phys. Plasmas, 2022

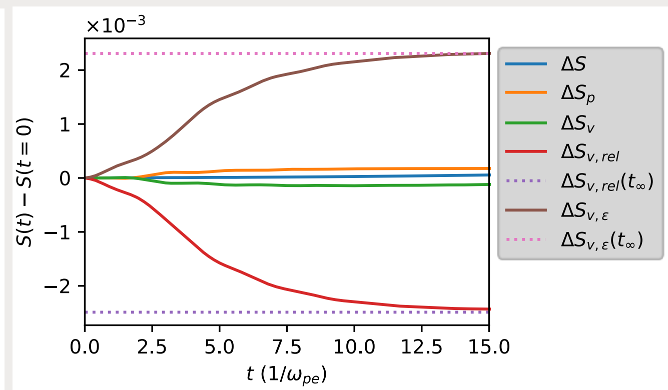
Example - Landau Damping

- 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

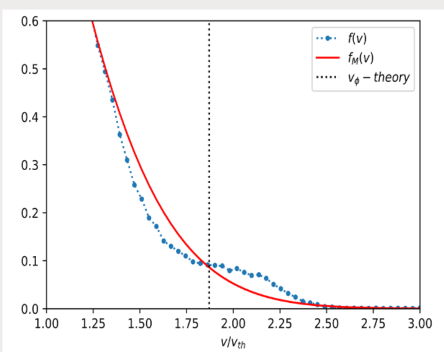
Conservation of energy

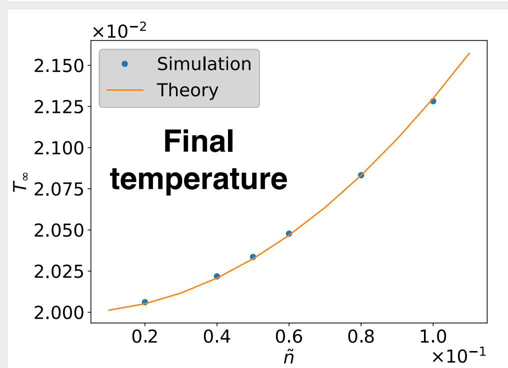


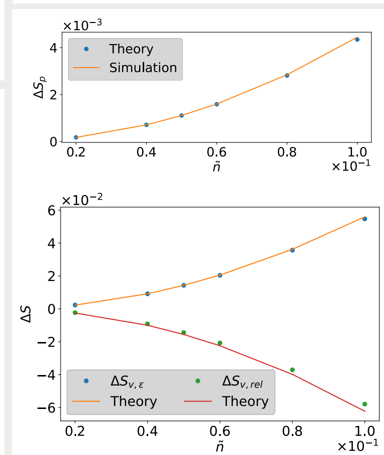
Conservation of entropy



Phase Space Density







Final position space entropy

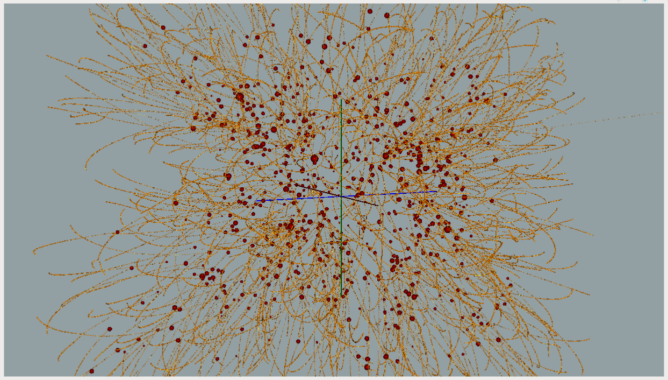
Final velocity space entropy

Final relative entropy

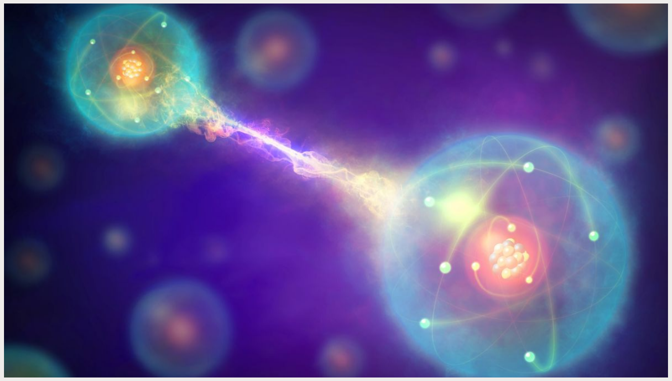
Perera et al., in prep

Potential Applications

- The theory should be useful for any plasma simulation tool that includes the full phase space density, such as particle-in-cell, Vlasov/Boltzmann, and hybrid simulations, plus satellite observations
  - Applications – magnetic reconnection, turbulence, collisionless shocks, wave-particle interactions, low temperature plasmas, …
  - Could be useful for identifying closures in plasma systems, such as through machine learning
- The theory should be applicable to other systems outside plasma physics that employ kinetic theory
  - Neutrino physics, dark matter, etc.
- Theory can be directly applied to any numerical technique that outputs the phase space density
  - Molecular dynamics simulations of micro- and nano-fluids for chemical and biological systems
- Could be useful for an analogous result for quantum statistical mechanics for applications to entanglement (Floerchinger and Haas, Phys. Rev. E, 2020)



http://philippos.info/nbody/



MARK GARLICK/SCIENCE PHOTO LIBRARY via Getty Images

Conclusions

- Energy conversion is often studied using the language of equilibrium thermodynamics, but many plasmas are out of local thermodynamic equilibrium (LTE) and need an infinite number of moments to describe them
- Here, we derive a closed-form expression quantifying the evolution of *all* non-LTE physics (Cassak et al., *Phys. Rev. Lett.*, **130**, 085201, 2023)
  - First-principles; no approximations
  - Non-perturbative, *i.e.*, valid arbitrarily far from LTE and avoids the “closure problem”
  - Related to “kinetic entropy”
- It augments or generalizes the first law of thermodynamics for systems not in LTE
  - We call it the “the first law of kinetic theory”
- We introduce a measure called HORNET with dimensions of power density describing the non-LTE evolution, which can be useful for quantitative comparison to standard power densities, $\mathbf{J} \cdot \mathbf{E}$ and pressure-strain interaction (Barbhuiya et al., *Phys. Rev. E*, **109**, 015205, 2024)
- The theory could be useful for any plasma simulation tool that includes the full phase space density, such as particle-in-cell, Vlasov/Boltzmann, and hybrid simulations, plus satellite observations
  - Applications – reconnection, turbulence, collisionless shocks, wave-particle interactions, low temperature plasmas, …
  - Could be useful for identifying closures in plasma systems, such as through machine learning
  - May have applications in other systems, including astronomy/cosmology, biology, chemistry, and quantum mechanics

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