KINETIC ENTROPY AS A DIAGNOSTIC IN PARTICLE-IN-CELL SIMULATIONS OF THE VLASOV EQUATION

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OUTLINE

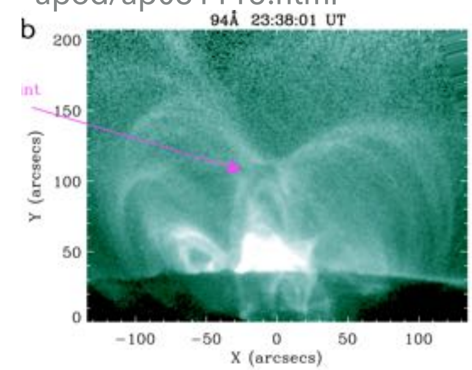
- “Dissipation” in Plasmas
- Kinetic Entropy as a Diagnostic of Plasma Dissipation
- Implementation and Validation of Kinetic Entropy into Fully-Kinetic Particle-in-Cell (PIC) Simulations
- Decomposition of Kinetic Entropy into Position Space and Velocity Space Kinetic Entropies
- Entropy-Based Non-Maxwellianity Measure and Uses
- Towards Comparisons with Observational (MMS) Data

Boltzmann’s gravestone

DISSIPATION IN (COLLISIONAL) FLUID PLASMAS

- Dissipation is a critical feature of shocks, reconnection, and turbulence
- In the (collisional) fluid description, the dissipation mechanism is relatively straight-forward: viscosity and/or resistivity dissipate energy in boundary layers
    - Turbulence is interesting - boundary layer physics is not likely straight diffusion; reconnection happens instead (Servidio et al., 2009, 2010, 2011; Donato et al., 2012, Haggerty et al., 2017; Shay et al., 2018)
    - Models of this are being developed (Mallet et al., 2017; Loureiro and Boldyrev, 2017; Cerri et al., 2018)
- All these dissipation processes are completely *irreversible!*

Shock: https://apod.nasa.gov/apod/ap031115.html

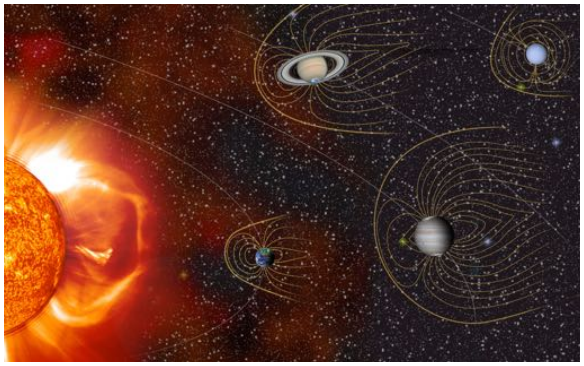


Reconnection: https://aasnova.org/2016/05/18/reconnection-on-the-sun/

Turbulence: Dobbie et al., 2009

"DISSIPATION" IN KINETIC THEORY

- Many heliospheric, planetary, and astrophysical systems are "nearly collisionless" - what takes the place of viscosity and resistivity in a such systems?
  - What does dissipation mean in collisionless systems? *Not* just an increase in temperature! Does it have to be **irreversible**?
- A number of collisionless energy conversion/dissipation mechanisms have been discussed (e.g., Vaivads et al., 2016):
  - Resonant wave-particle interactions (Landau damping, cyclotron damping)
  - Non-resonant wave-particle interactions (stochastic heating)
  - Coherent structures (direct acceleration, reconnection, magnetic islands)
  - Diffusive shock acceleration

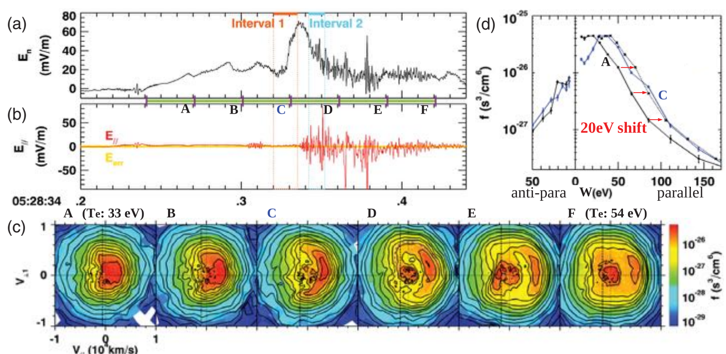


https://magnetospheres.sciencesconf.org/resource/page/id/1

https://www.plasmas.org/space-astrophys.htm

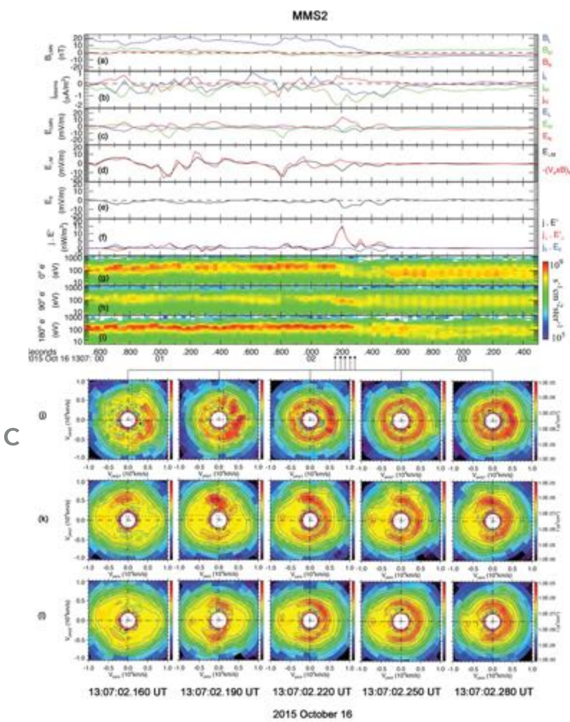
KINETIC PHYSICS IN MMS OBSERVATIONS

- Kinetic scale dissipation is now accessible to MMS satellite observations

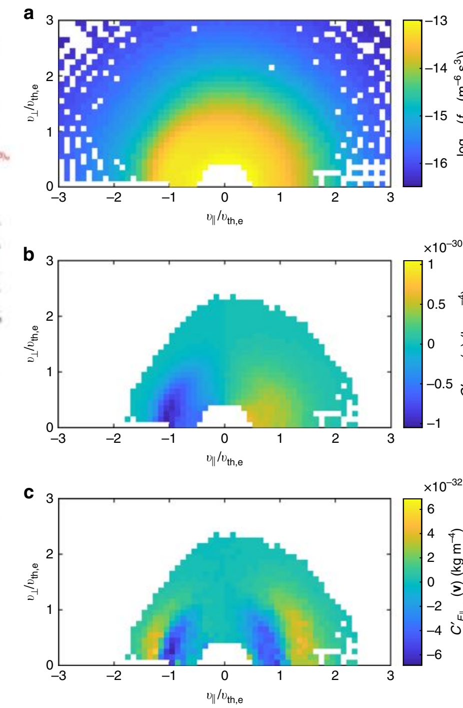


Chen et al., 2018

- Shock (Chen et al., 2018) - Electrons accelerated by electric field in whistler, thermalize via current-driven instability
- Reconnection (Burch et al., 2016) – Electrons accelerated by out-of-plane electric field at dayside magnetopause
- Turbulence (Chen et al., 2019) – Landau damping of kinetic Alfvén wave turbulence in magnetosheath



Burch et al., 2016



Chen et al., 2019

WHAT QUANTITIES ARE USED TO IDENTIFY DISSIPATION/ENERGY CONVERSION?

- Recent examples
  - Zenitani "dissipation" parameter, $D_e = \vec{J} \cdot (\vec{E} + \vec{v}_e \times \vec{B})$ (Zenitani et al., 2011)
  - Agyrotropy: Scudder and Daughton (2008) $A\O_e = 2\frac{|P_{\perp e1} - P_{\perp e2}|}{P_{\perp e1} + P_{\perp e2}}$; Aunai et al. (2013) D_{ng}; Swisdak (2016) $\sqrt{Q} = \sqrt{\frac{P_{12}^2 + P_{13}^2 + P_{23}^2}{P_\perp^2 + 2P_\perp P_\parallel}}$
  - The pressure-strain rate term in energy equation *Pi-D*$_e$ (Yang et al., 2017) or the negative of it (Sitnov et al., 2018) $P_{ij} = p\delta_{ij} + \Pi_{ij}, D_{ij} = S_{ij} - \frac{1}{3}\delta_{ij}\nabla \cdot \mathbf{v}$
  - Greco et al. (2012) – mean squared deviation between the distribution function *f* and the "Maxwellianized" distribution function f_M, $\frac{1}{n}\sqrt{\int d^3v(f - f_M)^2}$
  - Servidio et al. (2017) – Expand distribution function in Hermite polynomials, then take mean square deviation from Maxwellian $f(\boldsymbol{v}) = \sum_m f_m \psi_m(\boldsymbol{v})$ $\psi_m(v) = \frac{H_m(\frac{v-u}{v_{\rm th}})}{\sqrt{2^m m! \sqrt{\pi} v_{\rm th}}} e^{-(v-u)^2/2v_{\rm th}^2}$, $\Omega(t) \equiv \int_{-\infty}^{\infty} \delta f^2(\boldsymbol{v}, t) d^3v = \sum_{m>0} [f_m(t)]^2$
  - Conversion of electric field energy to particle energy through the relevant term in the Vlasov equation (Klein and Howes, 2016); energy density $w_s = ½mv^2 f$ evolves according to $\frac{\partial w_s}{\partial t} = -\mathbf{v} \cdot \nabla w_s - \frac{q_s v^2}{2}\mathbf{E} \cdot \frac{\partial f_s}{\partial \mathbf{v}} - \frac{q_s v^2}{2}(\mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f_s}{\partial \mathbf{v}}$.

CAN ANY QUANTITY UNIQUELY IDENTIFY DISSIPATION?

- All these quantities can be non-zero for perfectly reversible systems!
- Question - Is there a quantity that uniquely is associated with irreversible dissipation?
- Answer - Maybe! The (kinetic) entropy $S = -k_B \int d^3r d^3v f \ln f$
  - The Boltzmann H-theorem: start with the Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f + \frac{q(\vec{E} + \vec{v} \times \vec{B})}{m} \cdot \nabla_v f = C(f)$$

C(f) = collision operator

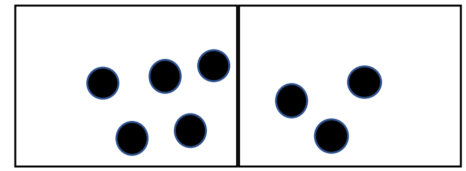
  - Use it to calculate dS/dt: $\frac{dS}{dt} = -k_B \int d^3r d^3v C(f) \ln f$
    - Thus, if there are no collisions, entropy is perfectly conserved (for a closed system)
  - For a suitably defined collision operator, $\frac{dS}{dt} \geq 0$
- Entropy is used regularly in gyrokinetics, but is underutilized for *fully kinetic* (PIC) studies
  - Important because weakly collisionless systems can have strongly non-Maxwellian *f*'s
  - Entropy and dissipation *only linked in a closed system;* real systems are not closed!

"Now, in the *second* law of thermodynamics . . ."

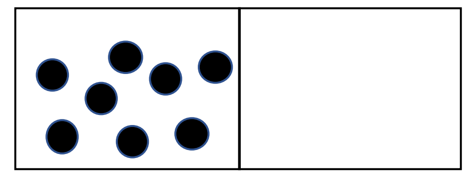
PHYSICAL INTERPRETATION OF ENTROPY IN KINETIC THEORY

- Follows from Boltzmann's description
  - "Combinatorial" kinetic entropy $\boxed{\mathcal{S} = k_B \ln \Omega}$

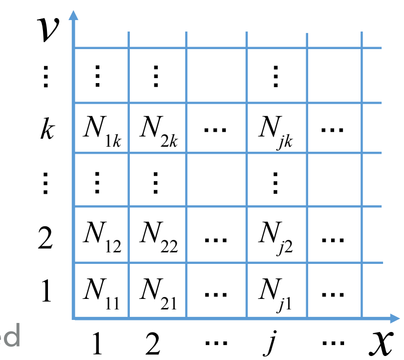
    where Ω = "permutation number" = $\dfrac{N!}{\Pi_{jk} N_{jk}!}$
- As in statistical mechanics, Ω is the number of ways to arrange the "microstate" to produce a given "macrostate"
  - Macrostates with more microstates are more likely; associated with higher entropy
    - More evenly distributed systems have higher entropy
  - In kinetic theory, permutations are not in *position space*, they are in *phase space*
  - Letting $N_{jk} = f(\mathbf{r}_j, \mathbf{v}_k) d^3r d^3v$, massaging and assuming $N_{jk} \gg 1$, and using the Stirling approximation gives $\boxed{S = -k_B \int d^3r d^3v f \ln f}$, the "continuous" kinetic entropy
    - When f is a Maxwellian, the kinetic description reproduces the fluid entropy $\dfrac{s}{n} \propto \ln\left(\dfrac{p}{\rho^\gamma}\right)$



$$\mathcal{S} = k_B \ln \frac{8!}{5!3!} \simeq 4k_B$$



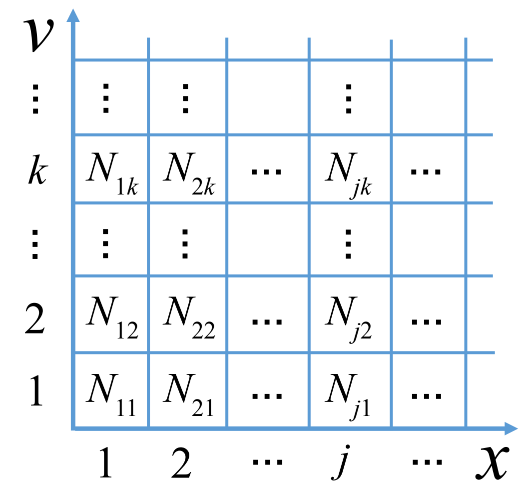
$$\mathcal{S} = k_B \ln \frac{8!}{8!0!} = 0$$



Liang et al., submitted

IMPLEMENTATION AS A DIAGNOSTIC IN PIC SIMULATIONS

- Goal – study entropy in closed numerical systems; apply knowledge to real systems
- We implement (Liang et al., submitted) both the “continuous” and “combinatorial” forms of the *non-relativistic* kinetic entropy into a particle-in-cell code (P3D, Zeiler et al., 2002)
  - At each time step, find $\mathcal{N}_{jk}$, the number of *macroparticles* in each phase space bin with velocity space grid Δv, using the algorithm’s shape function and particle weight
    - For combinatorial kinetic entropy, one needs to define number of *real particles* per macro-particle a; then $N_{jk} = a\mathcal{N}_{jk}$
    - For the continuous kinetic entropy, this is not necessary at run-time; can take $f \rightarrow af$ at the end to convert it to real units
  - Δv should be slightly less than the thermal speed, Δx should be sub-Debye scale
  - Finally, calculate $S = -k_B \int d^3r d^3v f \ln f$ and $\mathcal{S} = k_B \left[\ln[\Gamma(N+1)] - \Sigma_{jk} \ln[\Gamma(N_{jk}+1)]\right]$



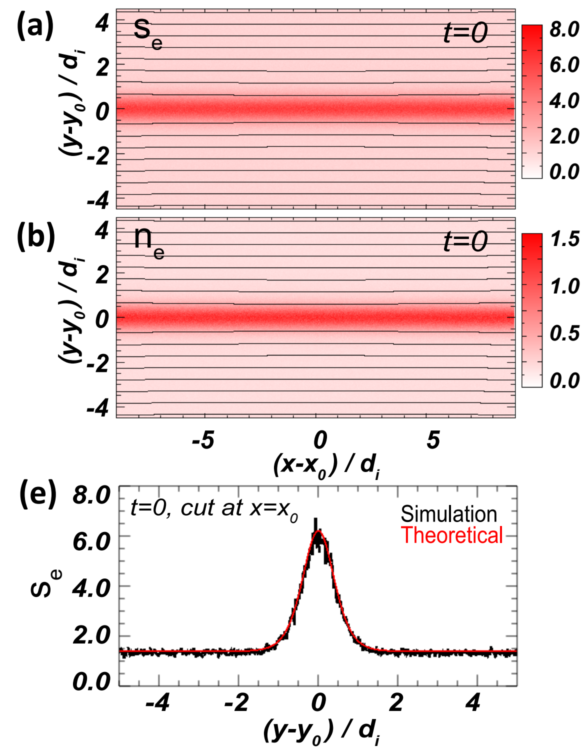
Liang et al., submitted

VALIDATION OF ENTROPY DIAGNOSTIC IN PIC SIMULATIONS

- We initialize a 2.5D collisionless antiparallel reconnection simulation with multiply periodic boundary conditions and two sech^2-profile current sheets (Liang et al., submitted)
- Initially plasmas have drifting Maxwellian distributions with uniform temperatures (upstream β = 0.2) and T_i / T_e = 5
  - At *t* = *0*, the entropy density is exactly solvable

$$s(\vec{r}) = -k_B \int d^3v f(\vec{r},\vec{v})[\ln f(\vec{r},\vec{v})] \xrightarrow[\text{when } f = f_M]{} s_M(\vec{r}) = \frac{3}{2}k_B n(\vec{r}) \left[1 + \ln\left(\frac{2\pi k_B T(\vec{r})}{m n^{2/3}(\vec{r})}\right)\right]$$

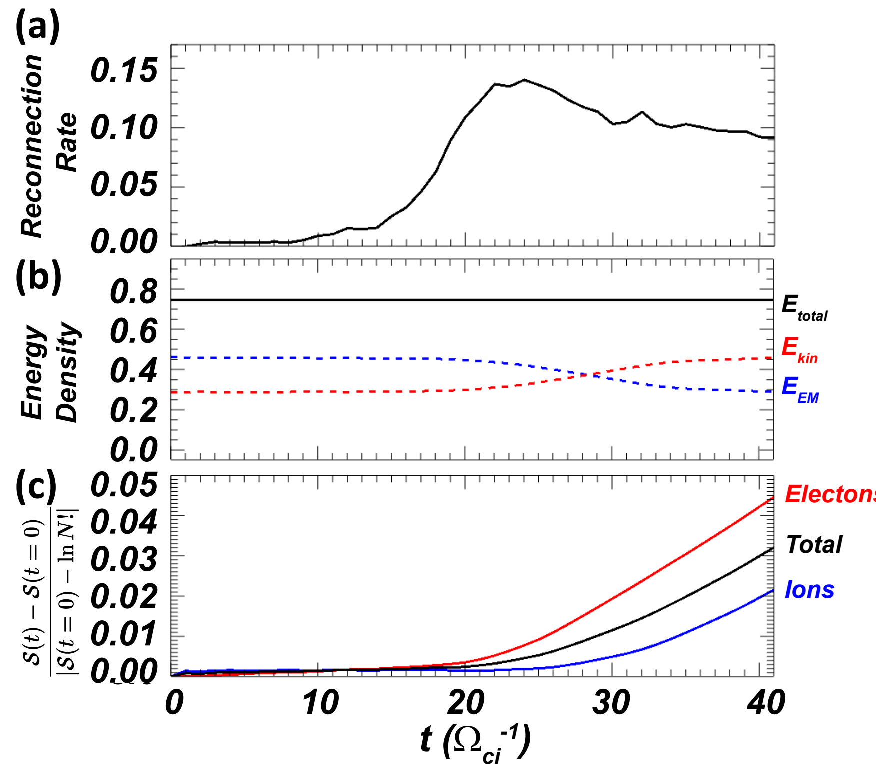
    - Can use to confirm numerics!
    - At *t* = *0*, kinetic entropy profile (a) looks similar to density profile (b)
- (c) Plot confirms combinatorial kinetic entropy is calculated properly; continuous kinetic entropies also agree in appropriate limit (not shown)
  - $\boxed{\text{Important - agreement at } t = 0 \text{ does not imply agreement at later times!}}$



Liang et al., submitted

CONSERVATION AND CONVERSION OF ENTROPY

- (a) Reconnection rate as a function of time, showing typical evolution to a steady-state
- (b) Total / kinetic / electromagnetic energy evolution; total is conserved well, conversion from magnetic to kinetic occurs during reconnection
- (c) Evolution of combinatorial kinetic entropy $\mathcal{S}$
  - Total entropy is conserved quite well (~3%)
    - Increases slowly due to numerical effects
  - Electrons gain higher fraction of entropy
- Not shown - If one uses few particles per grid cell, can get reasonable reconnection rate but entropy goes bad; important for studies of heating and acceleration!



Liang et al., submitted

DECOMPOSITION OF ENTROPY INTO POSITION AND VELOCITY SPACE ENTROPIES

- Kinetic entropy can be decomposed into position and velocity space entropies (Liang et al., submitted; also discussed in *Mouhot and Villani*, 2011)
  - Add and subtract a common term in the combinatorial kinetic entropy

$$\mathcal{S} = k_B \left[\ln N! - \sum_j \ln N_j! \right] + k_B \sum_j \left[\ln N_j! - \sum_k \ln N_{jk}! \right]$$

  - Each bracketed term has the same structure as total kinetic entropy

$$\mathcal{S}_{\rm position} = k_B \left[\ln N! - \sum_j \ln N_j! \right] \qquad \mathcal{S}_{\rm velocity} = \sum_j k_B \left[\ln N_j! - \sum_k \ln N_{jk}! \right]$$

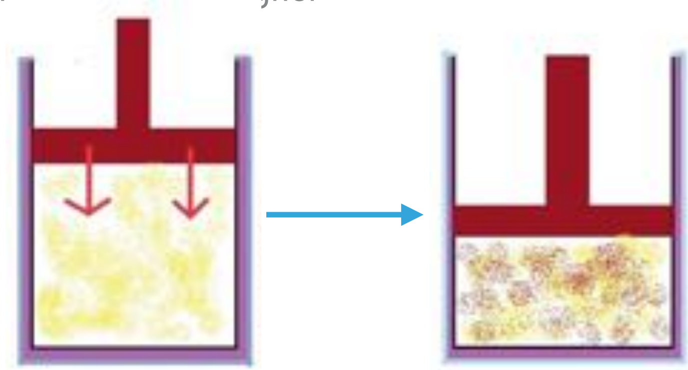
  - As before, can write continuous forms of position and velocity space entropy

$$\boxed{S_{\rm position} = k_B \left[N \ln\left(\frac{N}{\Delta^3 r} \right) - \int d^3 r\, n(\vec{r}) \ln n(\vec{r}) \right]}$$

$$\boxed{\begin{aligned} S_{\rm velocity} &= \int d^3 r\, s_{\rm velocity}(\vec{r}) \\ s_{\rm velocity}(\vec{r}) &= k_B \left[n(\vec{r}) \ln\left(\frac{n(\vec{r})}{\Delta^3 v} \right) - \int d^3 v\, f(\vec{r},\vec{v}) \ln f(\vec{r},\vec{v}) \right] \end{aligned}}$$

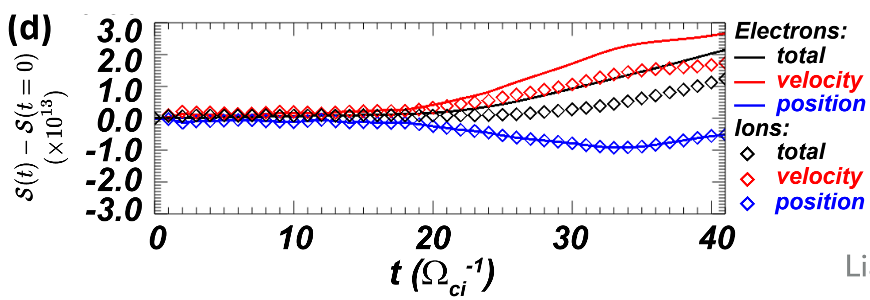
PHYSICAL INTERPRETATION OF POSITION AND VELOCITY SPACE ENTROPIES

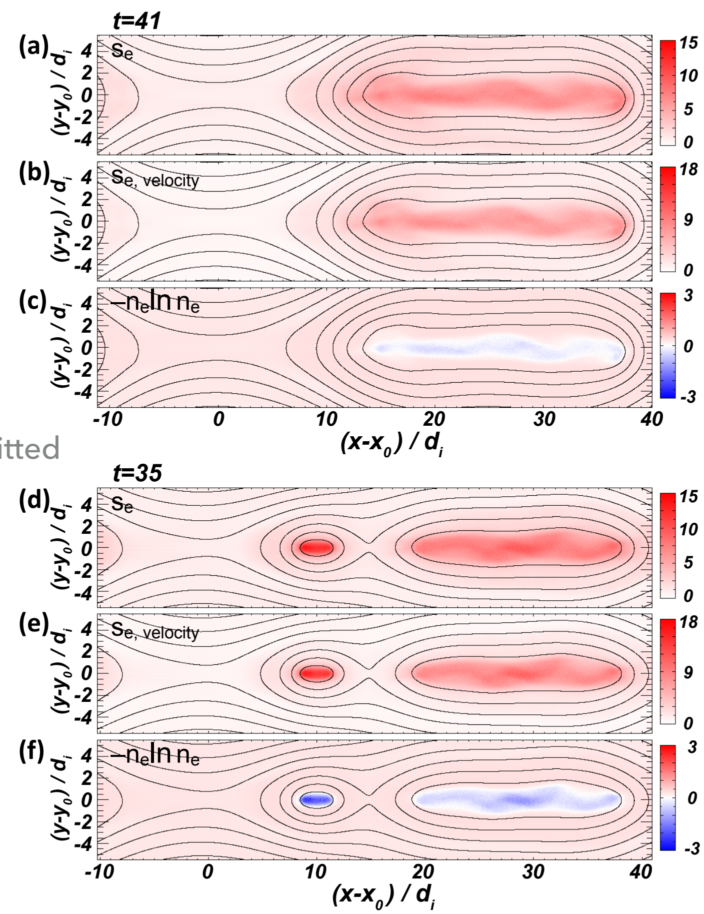
- The physics of the combinatorial position space kinetic entropy $\mathcal{S}_{\text{position}} = k_B \left[\ln N! - \sum_j \ln N_j! \right]$ is due to interchange of particles in space without regard to velocity
- The physics of the combinatorial velocity space kinetic entropy $\mathcal{S}_{\text{velocity}} = \sum_j k_B \left[\ln N_j! - \sum_k \ln N_{jk}! \right]$ is due to interchanging velocities of particles in a particular spatial grid, then summing over all space
    - Note, the entropy density $s(\vec{r}) = -k_B \int d^3v f(\vec{r},\vec{v})[\ln f(\vec{r},\vec{v})]$ and the velocity space kinetic entropy density $s_{\text{velocity}}(\vec{r}) = k_B \left[n(\vec{r}) \ln \left(\frac{n(\vec{r})}{\Delta^3 v} \right) - \int d^3v f(\vec{r},\vec{v}) \ln f(\vec{r},\vec{v}) \right]$ are not the same!!!
- Physical interpretation - when particles are more evenly distributed, combinatorial kinetic entropy is higher
    - Position space entropy - compression decreases it, expansion increases it
    - Velocity space entropy - heating increases it, cooling decreases it
        - E.g., heating due to adiabatic compression - position space entropy decreases and velocity space entropy increases; sum is conserved for an adiabatic process
- $\boxed{\text{Can be useful in interpreting kinetic entropy in plasma systems!}}$



CONSERVATION AND CONVERSION OF POSITION AND VELOCITY SPACE ENTROPIES

- Conversion (d, below) between position and velocity entropy is observed for each species





Liang et al., submitted

- Snapshots at *t = 41* (a-c) and *t = 35* (d-f) shown to the right
  - Reveal decrease of position space kinetic entropy occurs in magnetic islands due to compression, as expected

ENTROPY-BASED MEASURE OF NON-MAXWELLIANITY

- Find the local continuous kinetic entropy density based on the distribution function f:

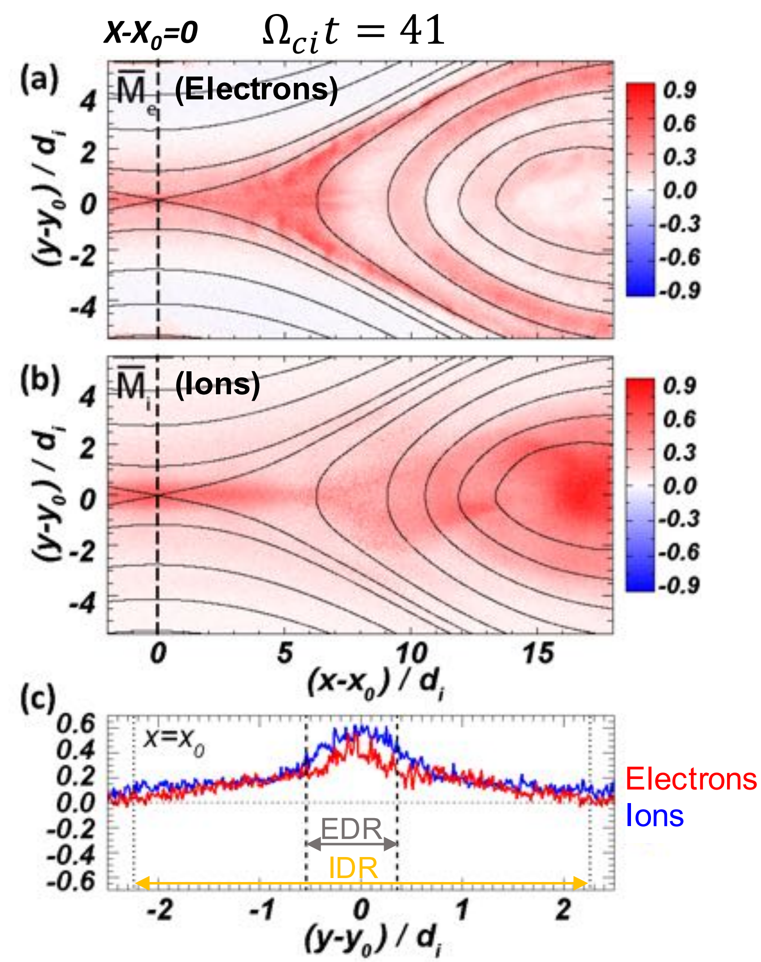
$$s(\vec{r}) = -k_B \int d^3v f(\vec{r},\vec{v})[\ln f(\vec{r},\vec{v})]$$

  - The Maxwellianized f_{M} has the same local density n, bulk flow u, and temperature T as f; calculate the associated $s_M(\vec{r}) = \frac{3}{2}k_B n(\vec{r})\left[1+\ln\left(\frac{2\pi k_B T(\vec{r})}{mn^{2/3}(\vec{r})}\right)\right]$

- Dimensional normalized form: $\boxed{\bar{M}(\vec{r}) = \frac{s_M(\vec{r}) - s(\vec{r})}{n(\vec{r})}}$
  - This form was used by *Kaufmann and Paterson* (2009) in studies of the plasma sheet and Cerri et al. (2018) in the study of plasma turbulence
- Dimensionless normalized form (Liang et al., in prep): $\boxed{\bar{\mathcal{M}}(\vec{r}) = \frac{s_M(\vec{r}) - s(\vec{r})}{s_M(\vec{r})}}$

ENTROPY-BASED NON-MAXWELLIANITY IN PIC

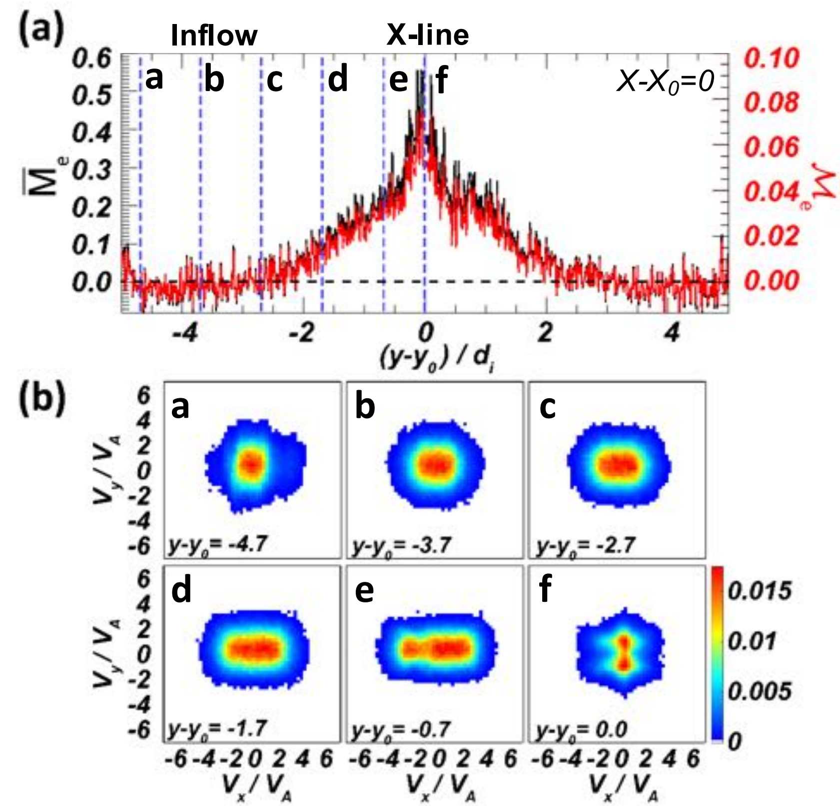
- Investigation of non-Maxwellianity $\bar{M}$ in PIC simulation using 2D plots (*Liang et al.*, in prep)
- As can be seen in a vertical cut through the X-line (c), for both species, $\bar{M}$ is non-zero in the ion diffusion region (IDR) [between the dotted lines] and become appreciably bigger in the electron diffusion region (EDR) [between the dashed lines]



Liang et al., in prep

SHOWING NON-MAXWELLIANITY FINDS NON-MAXWELLIAN DISTRIBUTIONS

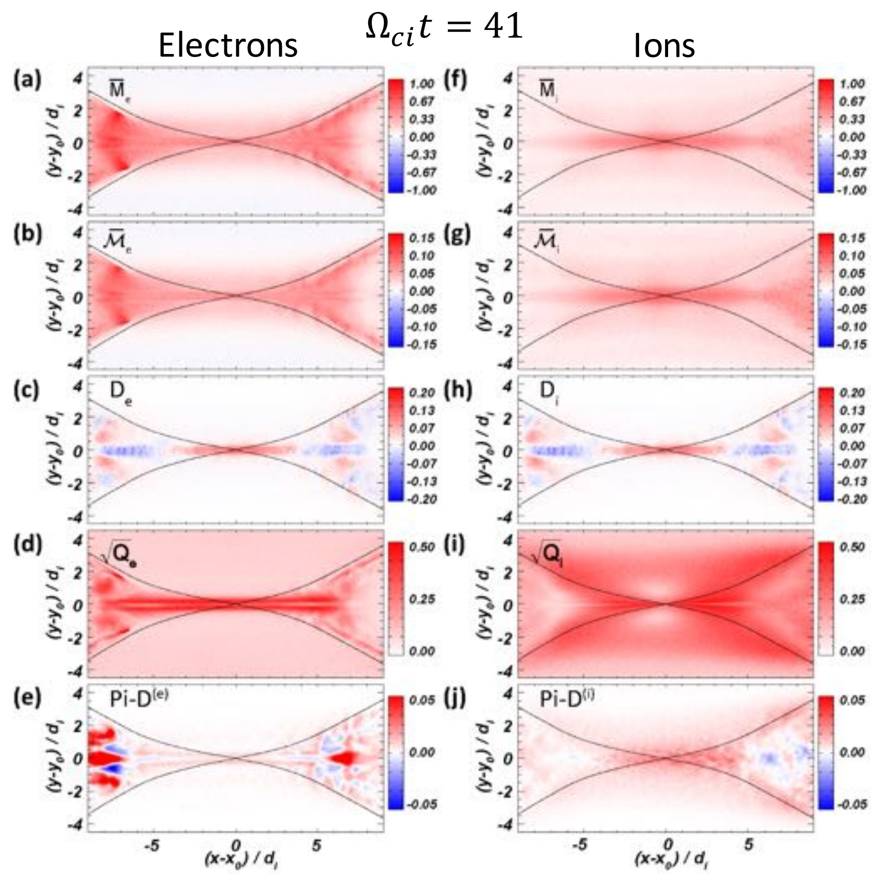
- Cut in inflow direction through X-line:
  - Dimensionless $\bar{\mathcal{M}}_e$ is quite similar to dimensional $\bar{M}_e$
  - (a) and (b) – mostly Maxwellian
  - (c), (d), and (e) – elongated distributions in parallel (x) direction
    - Due to trapped electrons (*Egedal et al.,* 2013)
  - (f) – at X-line, meandering orbits
  - Has the maximum departure from a Maxwellian at this cut
  - Result - Entropy-based non-Maxwellianity successfully identifies non-Maxwellian distributions



Liang et al., in prep

NON-MAXWELLIANITY AND ITS COMPARISON WITH DIFFUSION REGION INDICATORS

- Dimensional non-Maxwellianity $\bar{M}_e$
- Dimensionless non-Maxwellianity $\bar{\mathcal{M}}_e$
- Dissipation parameter *D (Zenitani et al.,* 2011)
- Nongyrotropy parameter $\sqrt{Q}$ *(Swisdak,* 2016)
- Pressure-strain rate *Pi-D (Yang et al.,* 2017; *Sitnov et al.,* 2018)
    - Result - As with the other measures, the entropy-based non-Maxwellianity does a reasonable job of indicating diffusion regions
    - Entropy can be bigger in the exhaust, where thermalization takes place (e.g., Drake et al., 2006)

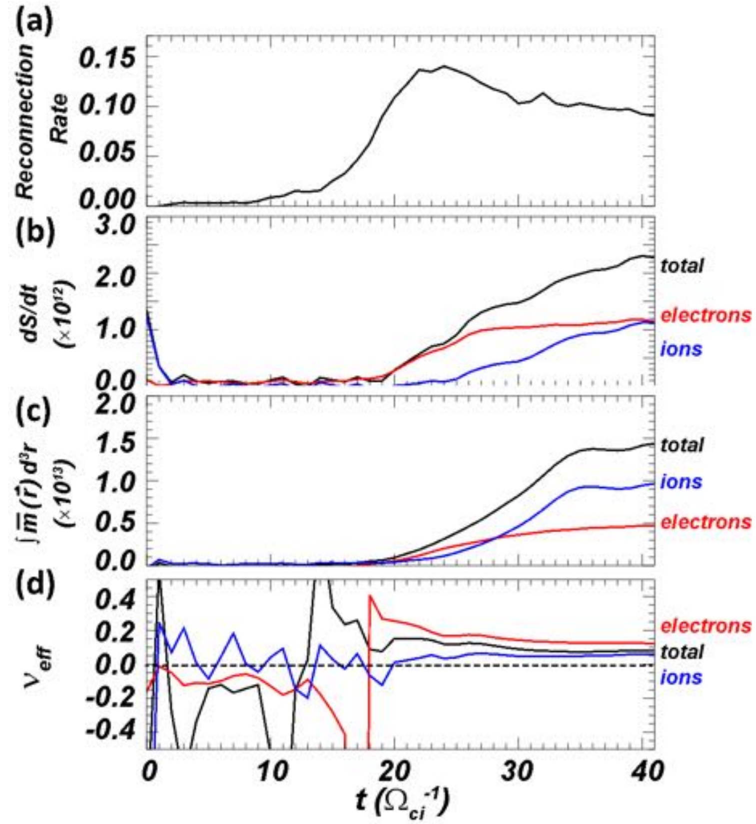


Liang et al., in prep

RELATING NON-MAXWELLIANITY TO DISSIPATION AND APPLICATIONS TO PIC SIMULATIONS

- $\bar{M}$ is related to dissipation when collisions are present (not if collisions are absent!)
  - The Boltzmann equation df/dt = C(f) implies $\frac{dS}{dt} = -k_B \int d^3r d^3v C(f) \ln f$
  - For weak non-Maxwellianity, a typical assumption is the relaxation-time approximation (RTA), $C(f) = -\nu_{\rm eff}(f - f_0)$, where $\nu_{\rm eff}$ is the effective collision frequency and f_0 is the equilibrium (Maxwellian) distribution
    - To second order in $f - f_0$, we get $\frac{dS}{dt} = 2\nu_{\rm eff} \int d^3r \bar{m}(\vec{r})$

      where $\bar{m}(\vec{r}) = s_M(\vec{r}) - s(\vec{r}) = n(\vec{r})\bar{M}(\vec{r})$
    - This implies $\nu_{\rm eff} = \frac{1}{2}\frac{dS}{dt} \Big/ \int d^3r \bar{m}(\vec{r})$
  - This can easily be calculated in PIC simulations to estimate $\nu_{\rm eff}$
- Effective collision frequency $\nu_{\rm eff}$ is steady during steady reconnection (t > 28)
  - Ions have 0.05, electrons have 0.12, total has 0.07 (in units of $1/\Omega_{ci}$)
- This result will be useful to determine the level of explicit collisionality required to overcome numerical effects in future *collisional* PIC simulations

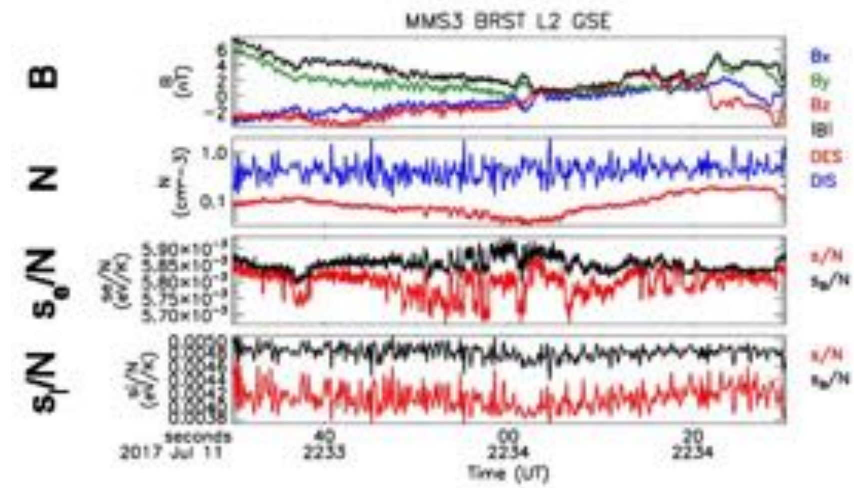


Liang et al., in prep

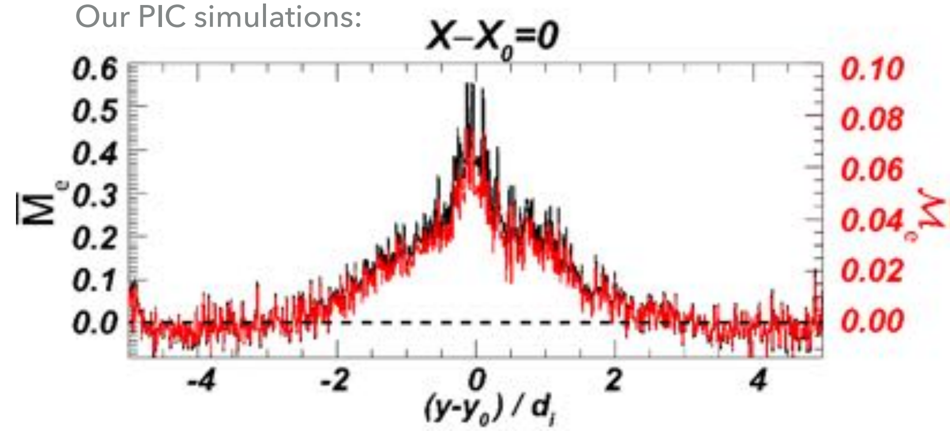
TOWARDS COMPARISONS WITH MMS

- Using MMS data to calculate the kinetic entropy and using the non-Maxwellianity as a diagnostic is currently being undertaken (*Argall et al.*)
- Very preliminary results from the 2017 July 11 magnetotail event (*Torbert et al.*, 2018)
  - **Observation:** electron non-Maxwellianity $\bar{M}_e$ has maximal value of ~2.0 x 10^{-4} eV/K
  - **Simulation:** $\bar{M}_e$ peak value at X-line is ~0.5, corresponding to ~0.43 x 10^{-4} eV/K
- Suggests simulations can be used for direct comparison of kinetic entropy in MMS data

MMS Observations (Torbert et al., 2018) with kinetic entropies (courtesy of Matt Argall)



Our PIC simulations:



CONCLUSIONS

- The use of kinetic entropy to diagnose kinetic dissipation in PIC simulations is explored (Liang et al., submitted)
  - Our collisionless PIC simulation demonstrates good conservation of total entropy (approximately 3%)
    - Since the code is collisionless, all entropy production is due to numerical effects
    - Entropy should be a useful diagnostic to ensure proper numerics in studies of heating and particle acceleration
  - The total kinetic entropy can be decomposed into position space and velocity space entropies
    - During reconnection, position space entropy decreases because plasma is compressed, while velocity space entropy increases because particles are heated
- Kinetic entropy can be used to define a non-Maxwellianity parameter (Liang et al., in prep)
  - It is an effective indicator of regions where dissipation is prone to occur, which may be more in exhausts and islands than in diffusion regions; future collisional simulations are necessary
  - Can be used to estimate effective collision frequency in collisionless PIC simulations
  - Capable of direct comparison with MMS data (*Argall et al.*)
- Techniques should be useful not just in reconnection – but in turbulence and shocks too!