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Analysis of particle spectra and the treatment of uncertainties and bias with applications to photons, charged particles, and neutrals

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Detectors that count things

- Spectro-imager: measures brightness from a range of arrival directions (2D) across a range of wavelengths: **3D dataset: (φ,θ,λ)**.

- Particle detector: measures flux of particles from a range of arrival directions (2D space) across a range of energies : **3D dataset: (φ,θ,E)**.

- Measurement space broken into smaller elements (**pixels**): **(Δφ, Δθ, Δλ)** or **(Δφ, Δθ, ΔE)**.

- For each pixel the count rate is proportional to the flux of particle/photons seen by that pixel. The mean count rate (**λ**) related to the flux by:
  - A factor that accounts for the instrument design/optics/geometry (**G**).
  - An efficiency factor (**ϵ**).

- The counts in an observation period (accumulation time or integration time) is obtained from **τ** x **λ**.

Phase space

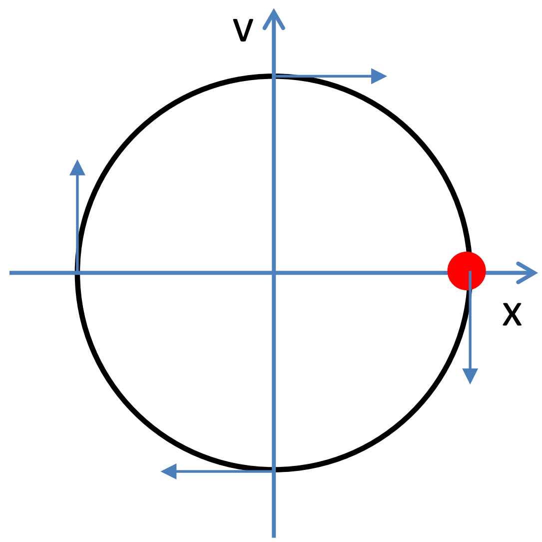
- Particle datasets we are looking to understand the distribution of particles in velocity space.

- Related to idea of phase portrait for a pendulum.

- Various analytical distributions: Maxwell-Boltzmann distribution, Kappa distribution.

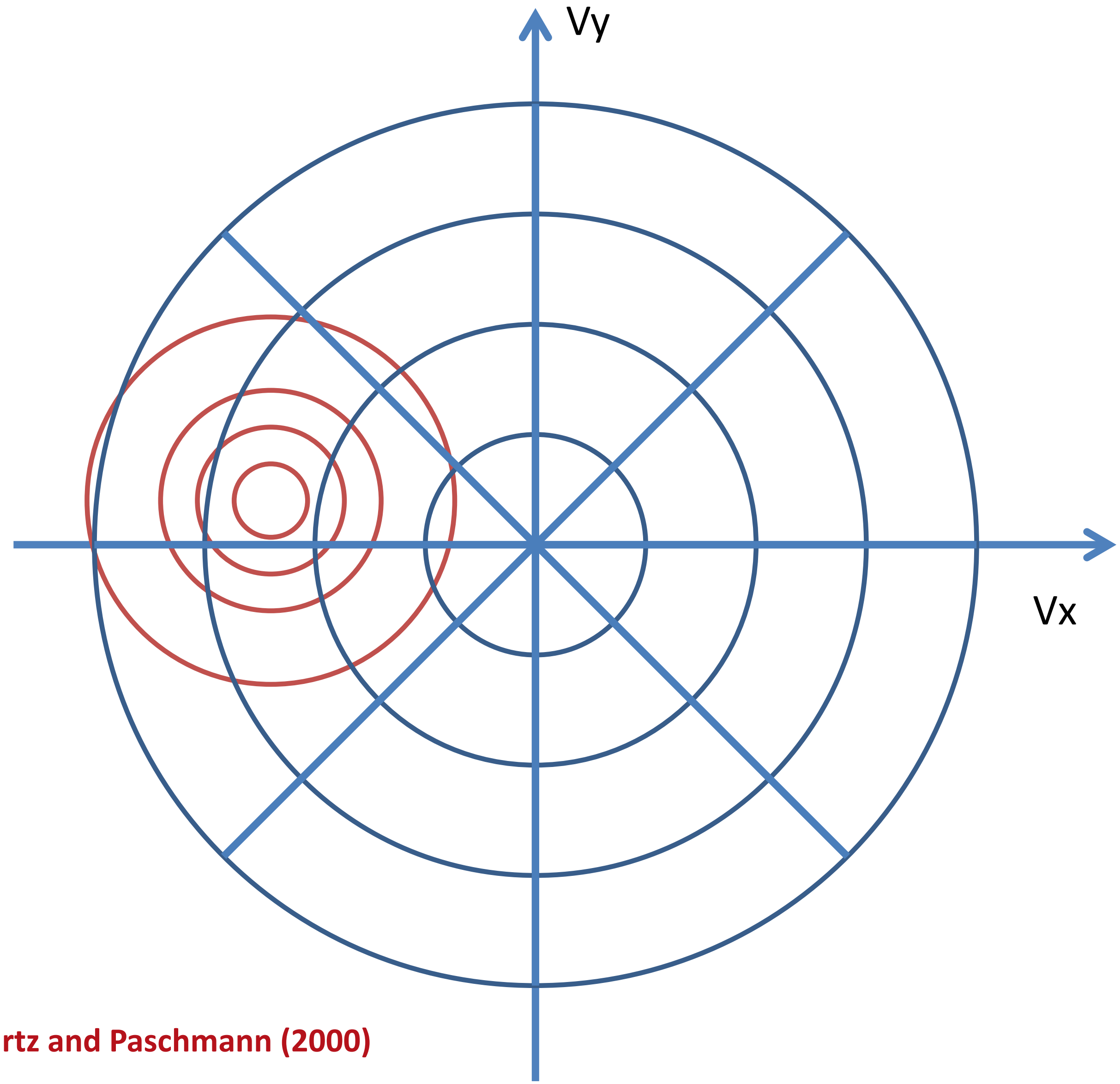
- Almost every particle population in a (collisionless) plasma is not a Maxwellian; they have significant power-law tails.

- Number of particles in an infinitesimal volume: (r,v,θ,φ) to (**r**+d**r**, v+dv, θ+dθ, φ+dφ). The idea of a phase space density.



$$f\,d\mathbf{r}d\mathbf{v} = f\,d\mathbf{r}v^2dv\sin\theta\,d\theta d\varphi$$

Phase space



After Fazakerley, Schwartz and Paschmann (2000)

Anatomy of a particle detector

- Many different types of particle detector depending on the nature of the particle and the energy range of interest.

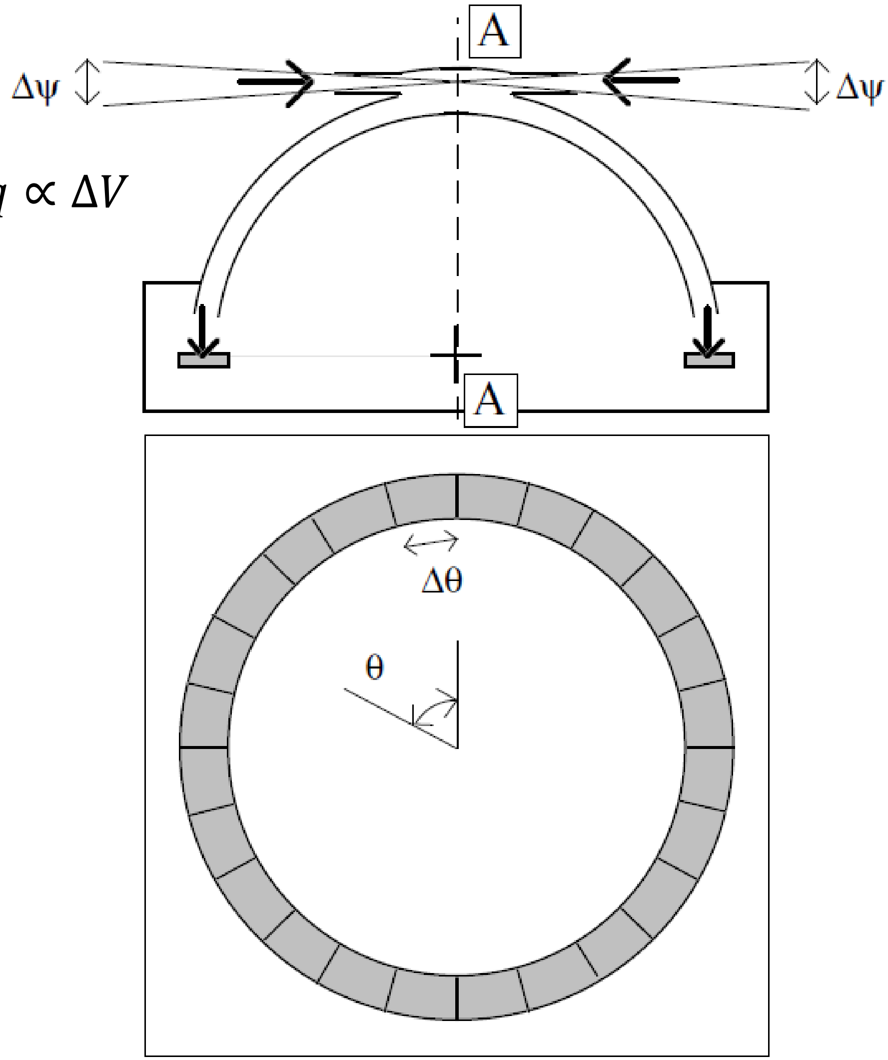
- Electrostatic analysers: charged particle optics to select velocity space volume, some sort of detector to count particles, e.g., microchannel plate (MCP) or silicon detector.
  - Two main types: curved plate analysers and retarding potential analysers (only cover the first type).

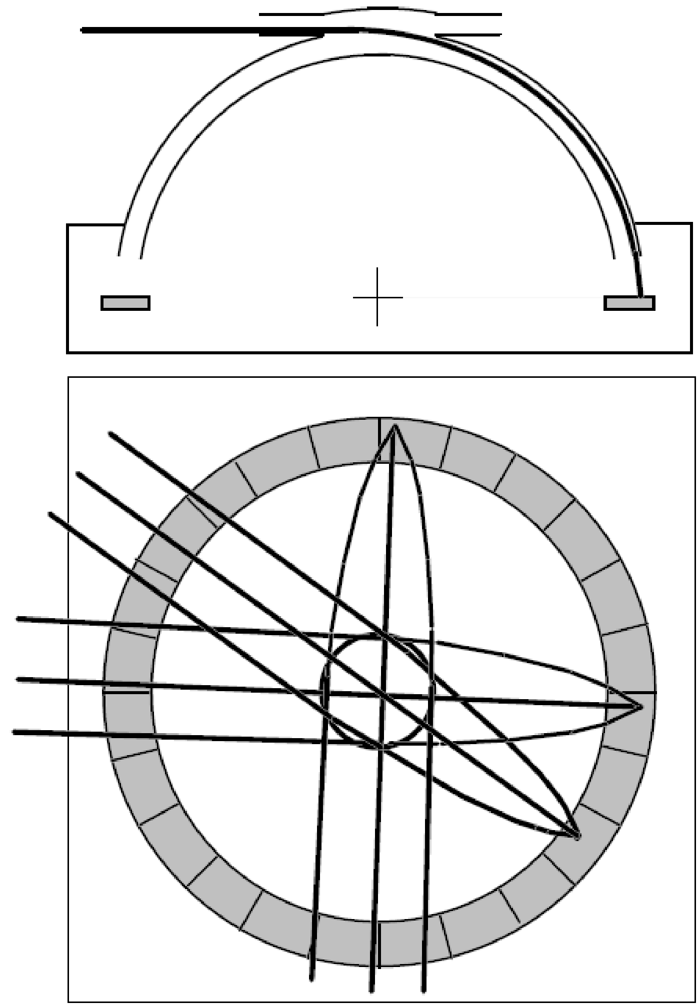
- Neutral detectors usually ionise the neutral before detection using an electrostatic analyser.

- Energetic particle detectors: particles go through a stack of silicon detectors. Which detectors they travel through, and which one they stop in determines their energy (channel logic).

Curved plate electrostatic analyser

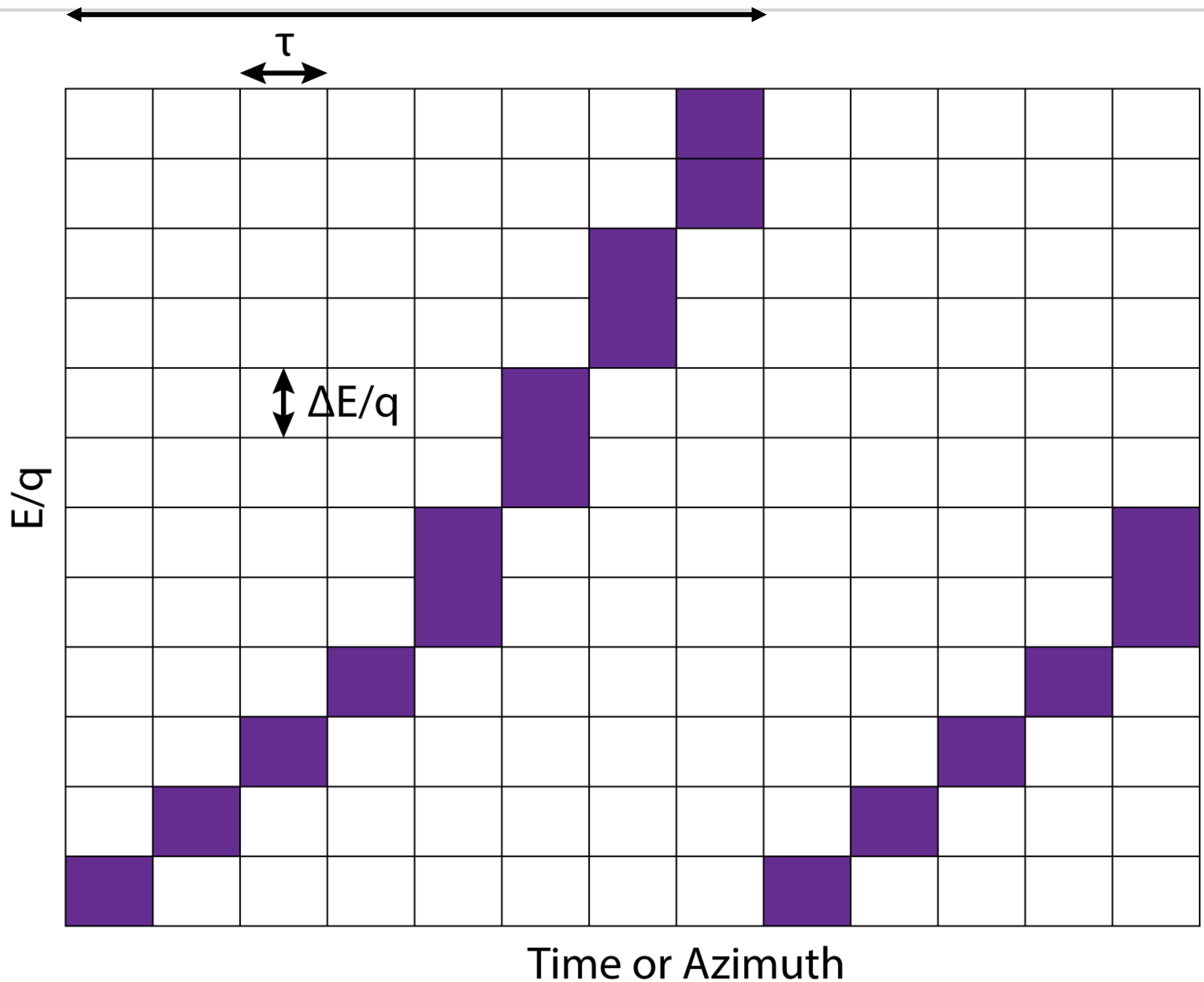
$E/q \propto \Delta V$





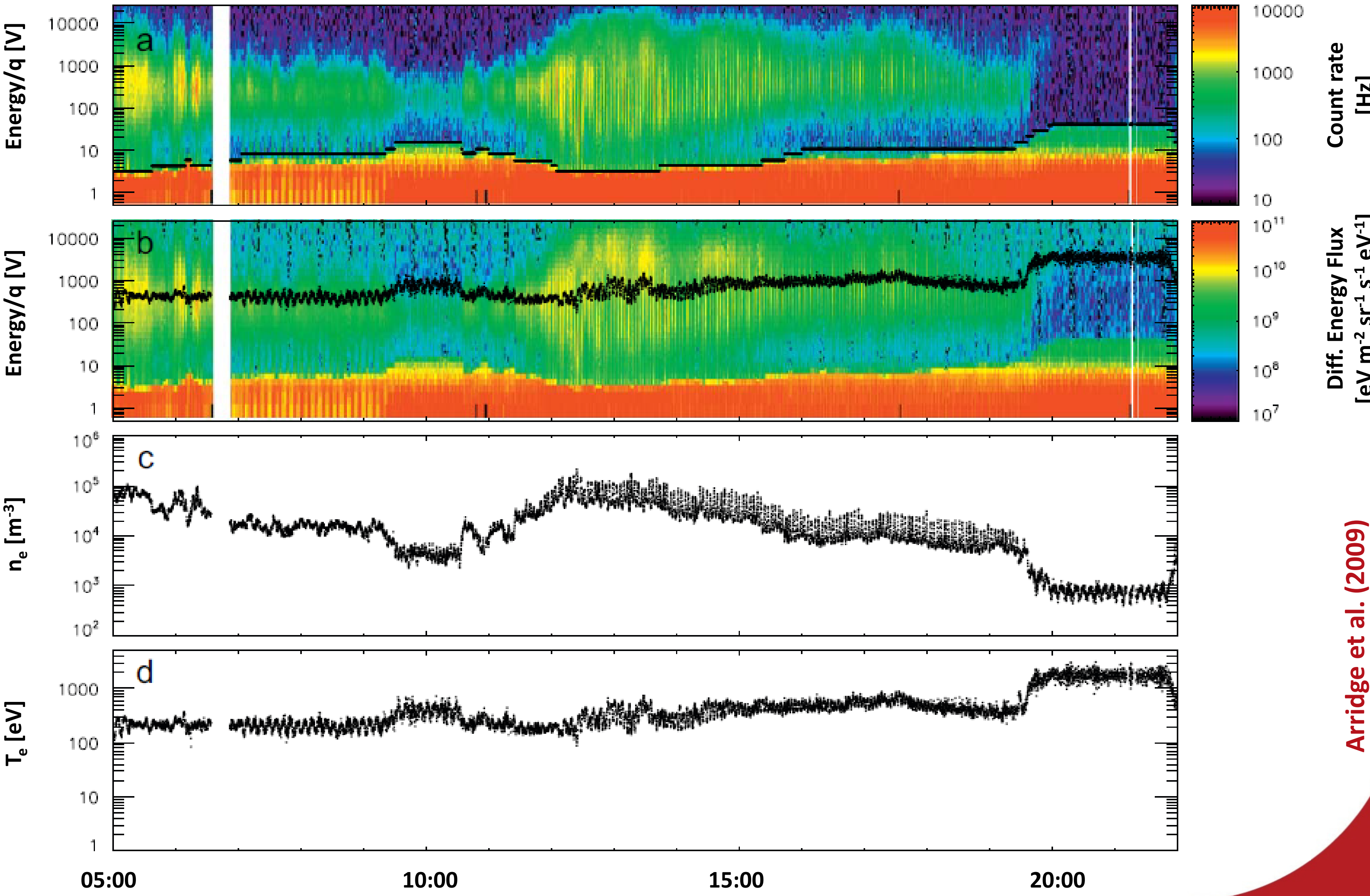
Fazakerley, Schwartz and Paschmann (2000)

Coverage of energy and azimuthal space



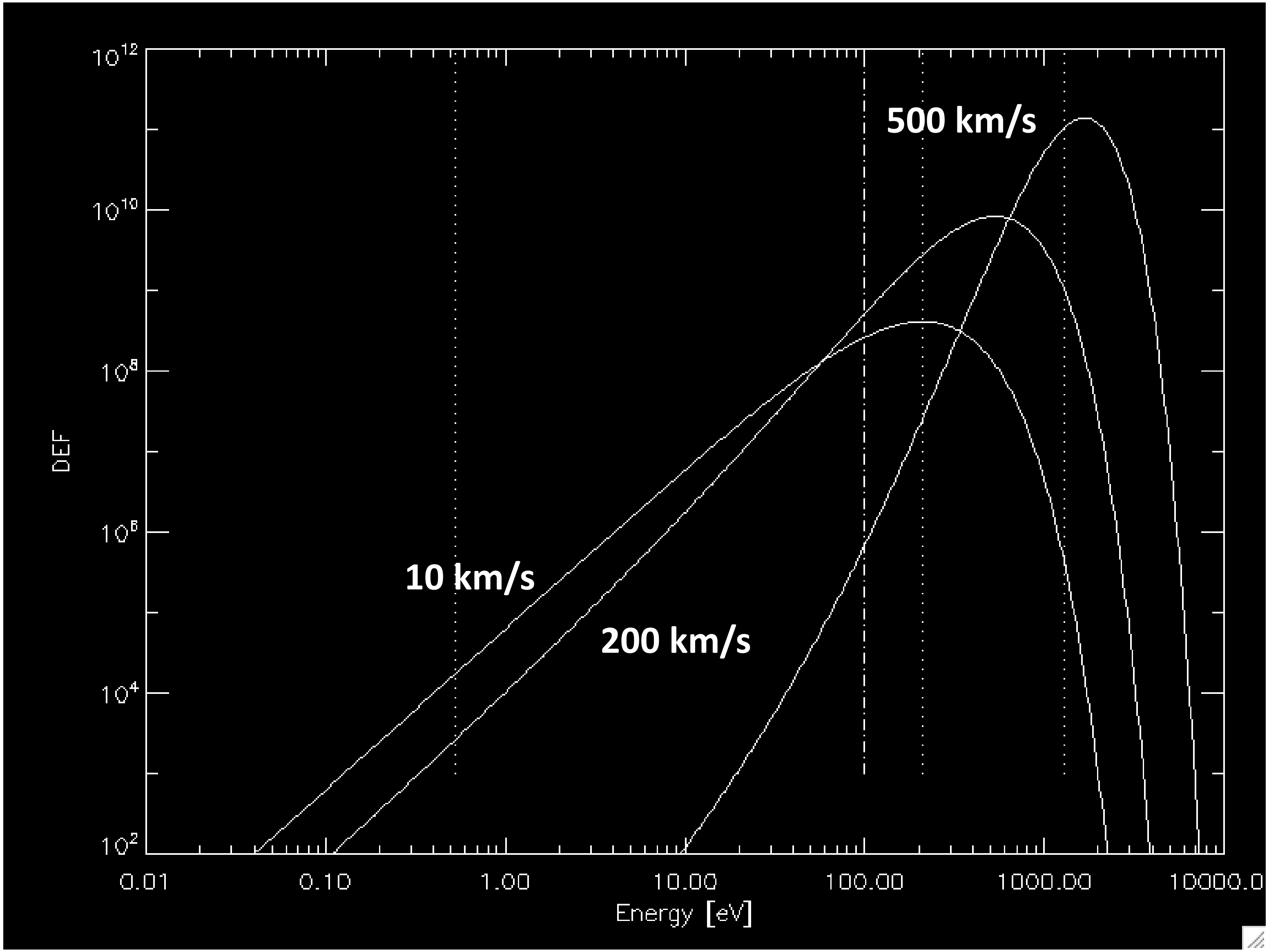
After Fazakerley, Schwartz and Paschmann (2000)

Some data from Cassini



Arridge et al. (2009)

Supersonic/subsonic distributions: v_b/v_{th}



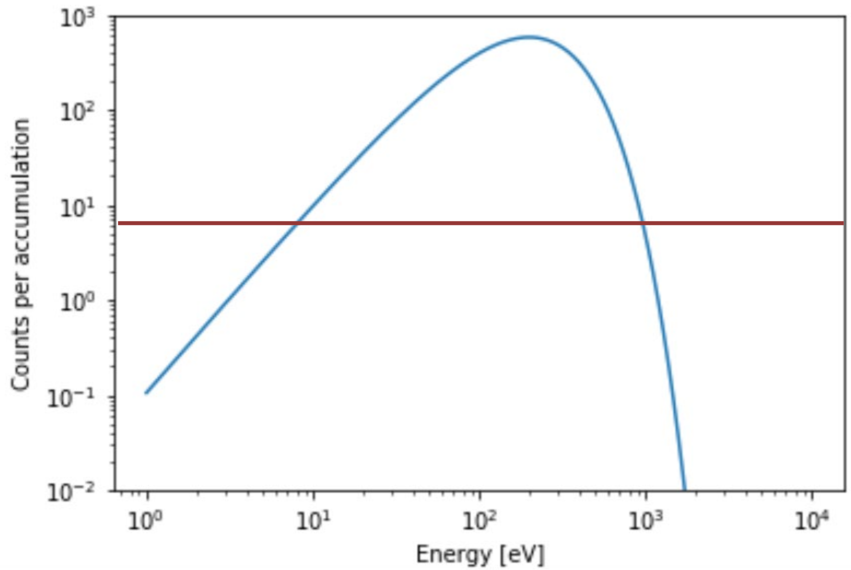
Sources of error/uncertainty

- **Noise**:
  - Radiation sources.
  - Cosmic rays.
  - Penetrating radiation.
  - Electronics.
- **Random error:** statistical, not an "error"
  - Poisson or shot noise.
- Subsequent processing, e.g., model fitting, numerical integration..
- **Systematic**: inaccuracies/problems in the measurement method
  - Coverage: e.g., detector blocked in certain directions, not measuring certain combinations of energy and azimuth.
  - Resolution – under-resolving structures in wavelength, energy, space.
  - Gain depression – can't count fast enough.
  - Cross-talk
  - Aliasing
  - Quantisation
  - Compression.

Noise sources – background counts

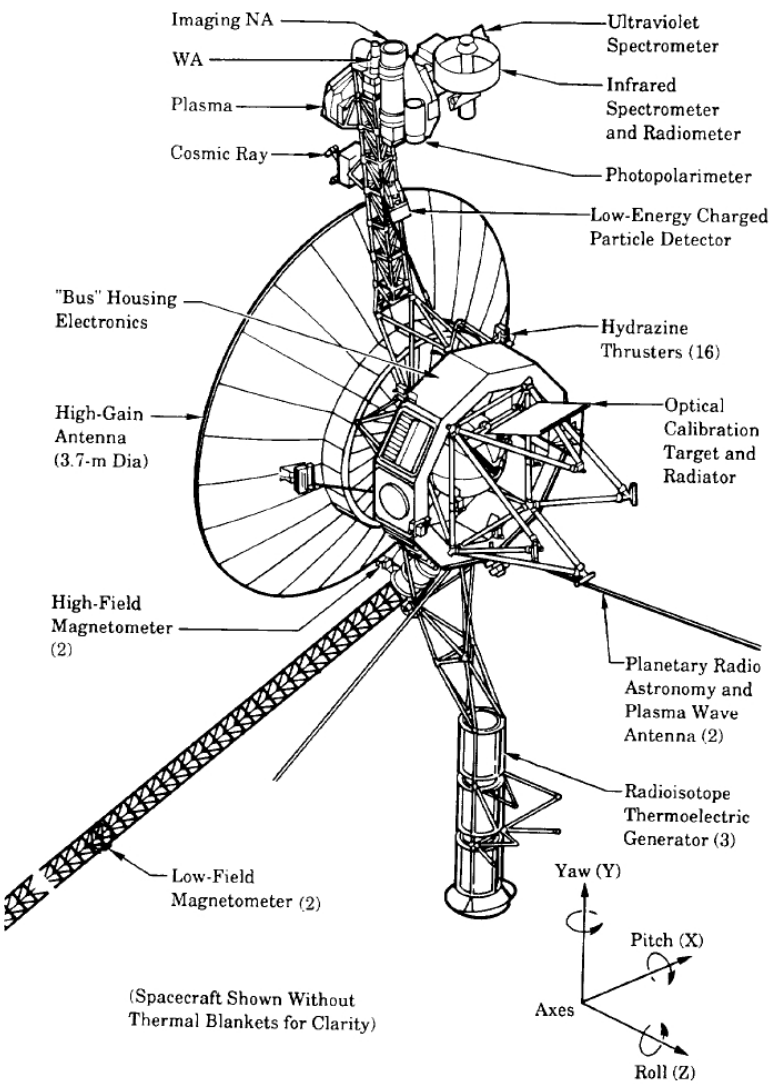
What do we mean by noise?

- Measurement: signal+noise (foreground+background).
- For ESA background is independent of E/q; hasn't been velocity space-filtered. May vary with azimuth/pixel.



- Low background: mean may be <~ 1 count/acc. Lots of Poisson noise.
- High background: mean may be very high compared to the foreground and so hard to fully remove/treat.
- Mitigation: subtract, parameterised, calculate signal-to-noise (S/N or SNR) ratios and reject low S/N measurements, averaging, longer integration, include background channel (pre-flight), coincidence measurements.

Radiation sources



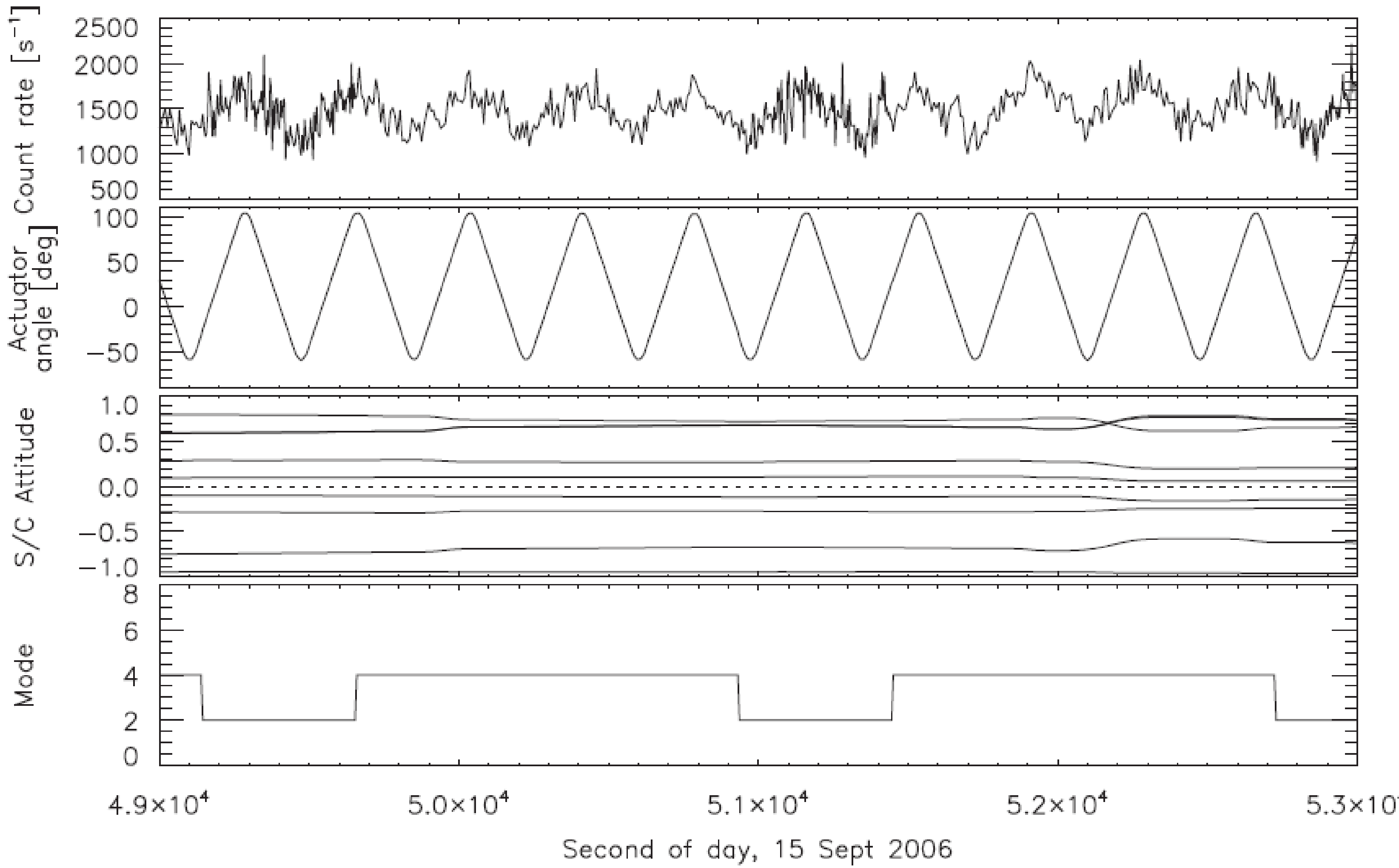
NASA

- Many deep space missions use nuclear power and/or heat sources due to large heliocentric distances.
- Pu-238 is the typical radionuclide.
- Gamma rays from alpha decay; also some neutrons from spontaneous fission.
- Can trigger MCPs with a few % efficiency.
- Need to know the radiation field around the spacecraft: spacecraft can partially shield the instrument.

Noise from the detector itself

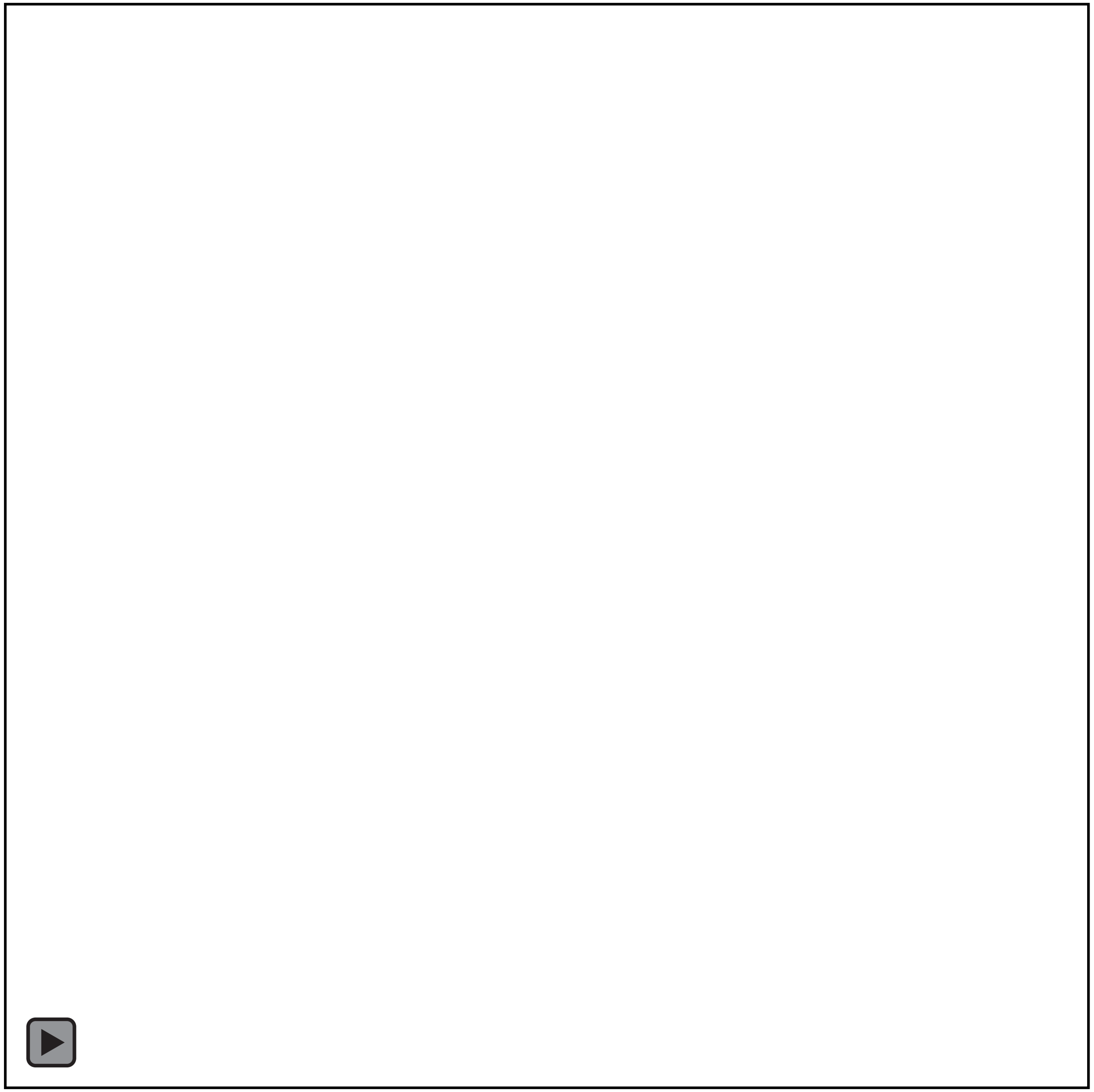
- MCPs are made from ceramics that contain radioactive impurities.
- For example, U-238, Th-232 and K-40 in glass.
- Some detectors (e.g., fundamental physics) use very high purity glass to reduce the radionuclide content and so reduce the noise level.

Electron detector noise: Cassini RTGs



Arridge et al. (2009)

Cosmic rays and penetrating radiation



SOHO (ESA and NASA)

- Charged particles with sufficient energy can penetrate inside an instrument.
- Trigger detector and produce a background.
- Examples: Cosmic rays, Solar Energetic Protons, Electrons in radiation belts.

Cosmic rays and penetrating radiation

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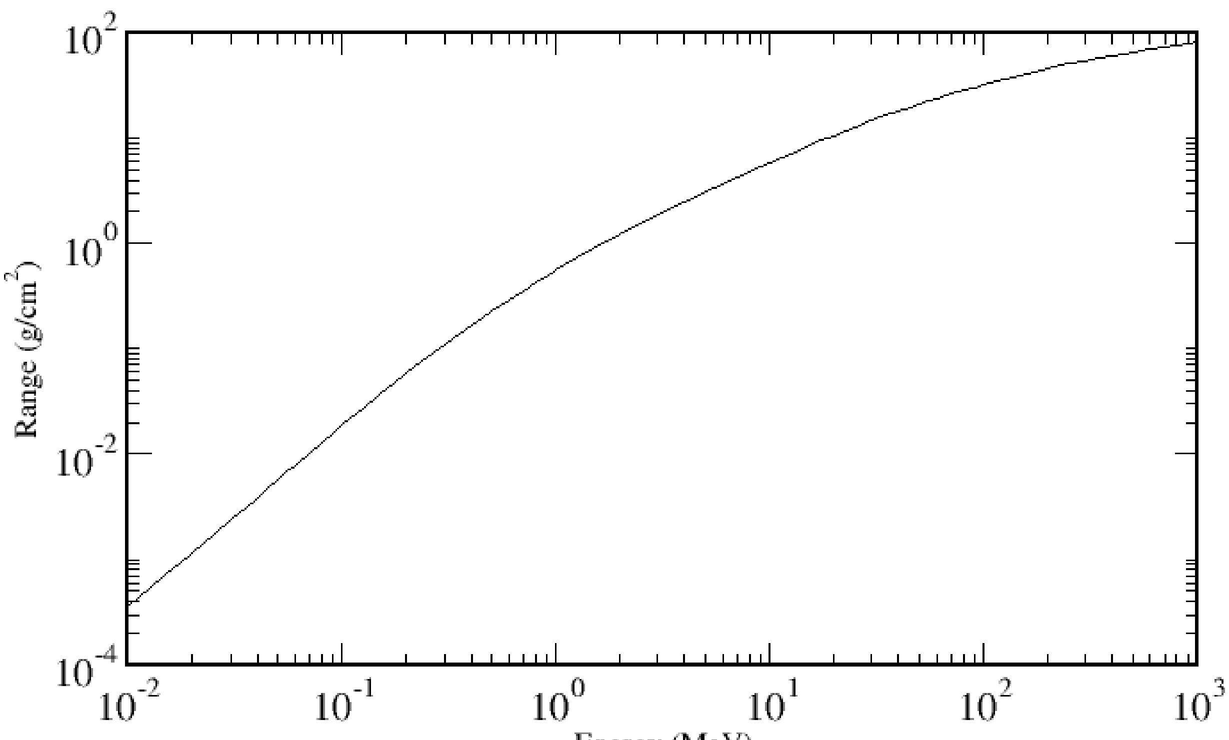
- A given material and thickness will be able to stop particles up to a given energy: stopping distance.

- Calculations for electrons hitting aluminium. Units are slight unusual, need to divide by density to get the depth. For example, 1 g/cm^2 divided by 2.7 g/cm^3 = 0.37 cm: <2 MeV electrons will be stopped by 0.37 cm f aluminium.



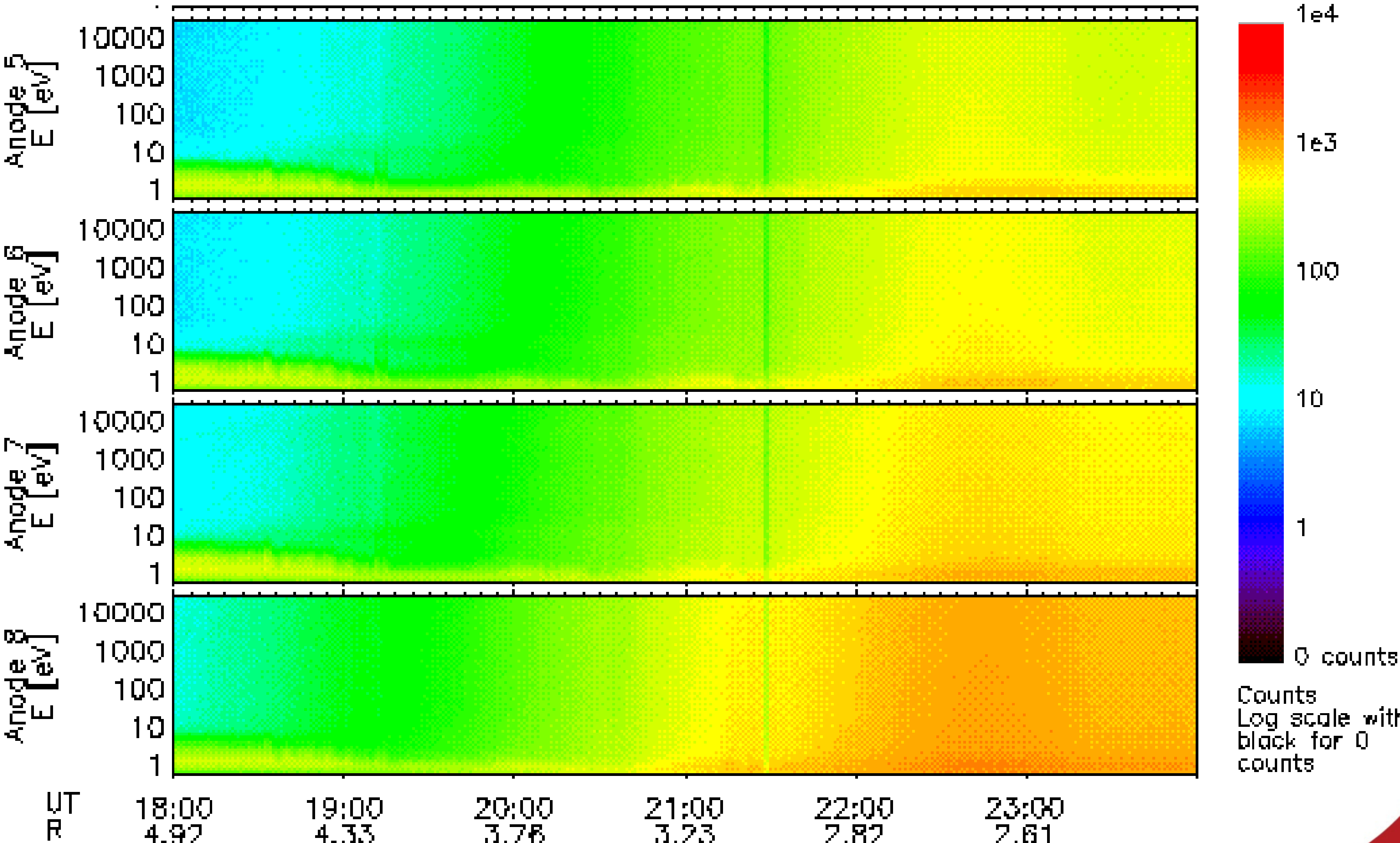
For example:

1 g/cm^2 / 2.7 g/cm^3 = 0.4 cm

So electrons with energy <2 MeV will be stopped by 0.4 cm of aluminium.

https://www.nist.gov/pml/stopping-power-range-tables-electrons-protons-and-helium-ions

Penetrating radiation in radiation belts



Systematic and Random error

Random variables and Poisson statistics

- Random errors are not mistakes or something that gives you a wrong result. They are statistical: errors that in a measurement that will give a different value each time.

- In general, the counts recorded by a pixel are **random variables** that follow a **Poisson distribution**.

$$C \sim \mathrm{Pois}(\lambda) \qquad P(C) = \exp(-\lambda)\frac{\lambda^{C}}{\lambda!} \qquad E(C) = \lambda \qquad Var(C) = \lambda$$

- Poisson distribution: discrete probability distribution
  - Events occur at random with a constant mean rate.
  - The probability of an event doesn't change with time since the last event.

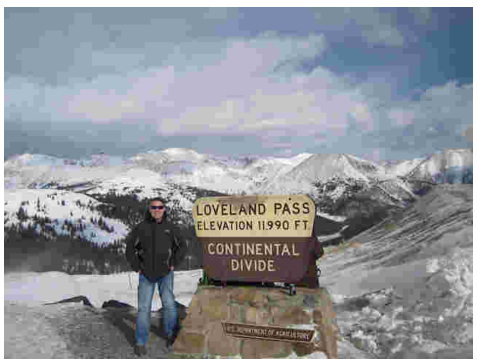
Compression

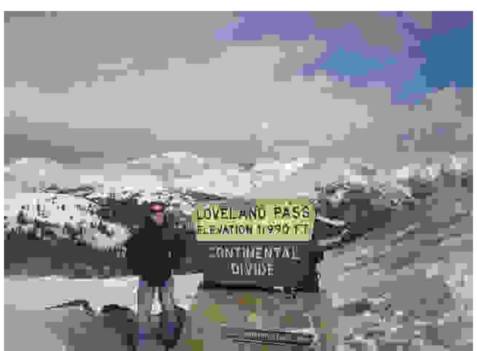
- Two main types of technique.

- **Lossless**:
  - Data can be recovered exactly – exact inverse operation.
  - Examples: DEFLATE algorithm used in ZIP files (LZ77/Huffman encoding) and RLE (used in Windows PCX files and fax machines).

- **Lossy**:
  - Some information is lost but usually performed in a way that the human sensory system can't **perceive** the reduction in information.
  - Examples: JPEG, MP3, G.729 used in VOIP, GSM-FM used in mobile telephones, simple averaging, number compression.

Lossy compression





- Compression is **irreversible**: information is **lost**.

- For example: simply resizing and averaging an image:
  - Resize image: e.g., $512 \times 512 \rightarrow 256 \times 256$ ($4\times$ smaller).
  - Every block of 4 pixels is averaged to produce the intensity of a single pixel in the resized image.
  - Can’t get the intensities of the original 4 pixels back.

- Better techniques which preserve the information content whilst reducing the data volume.

- Remove **imperceptible** information or **predicting** the signal → compression algorithm needs to be matched to human perception.

Lossy compression of particle data

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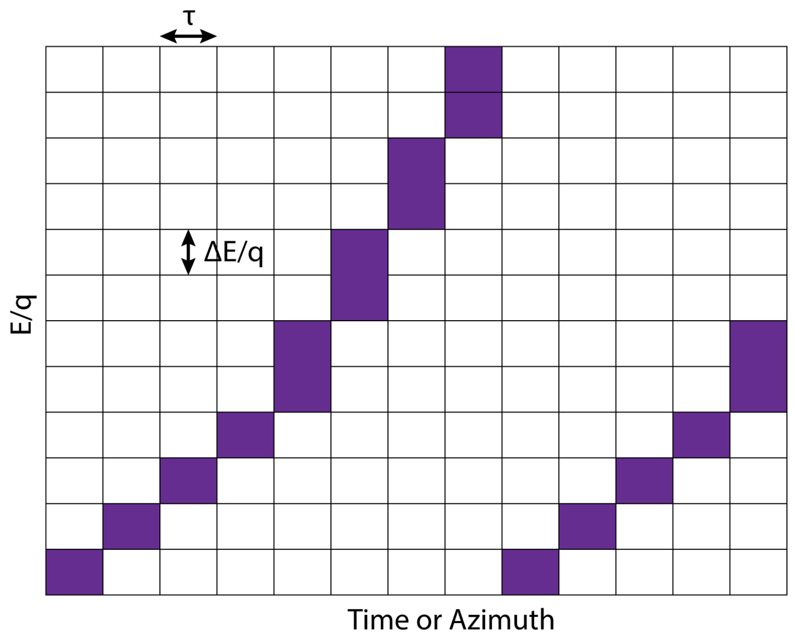
- One technique for averaging particle data is to average adjacent energy bins, or average adjacent azimuths or pixels.

- Important to recognise that this does not simply take data away, it also changes how the data has been sampled in velocity space.



- One technique is to compress the numbers themselves: if the counts are stored in 16 bits, we can compress that into 8 bits and reduce the data volume by a factor of two.

- Issues with lower SNR points.

Quasi-log compression

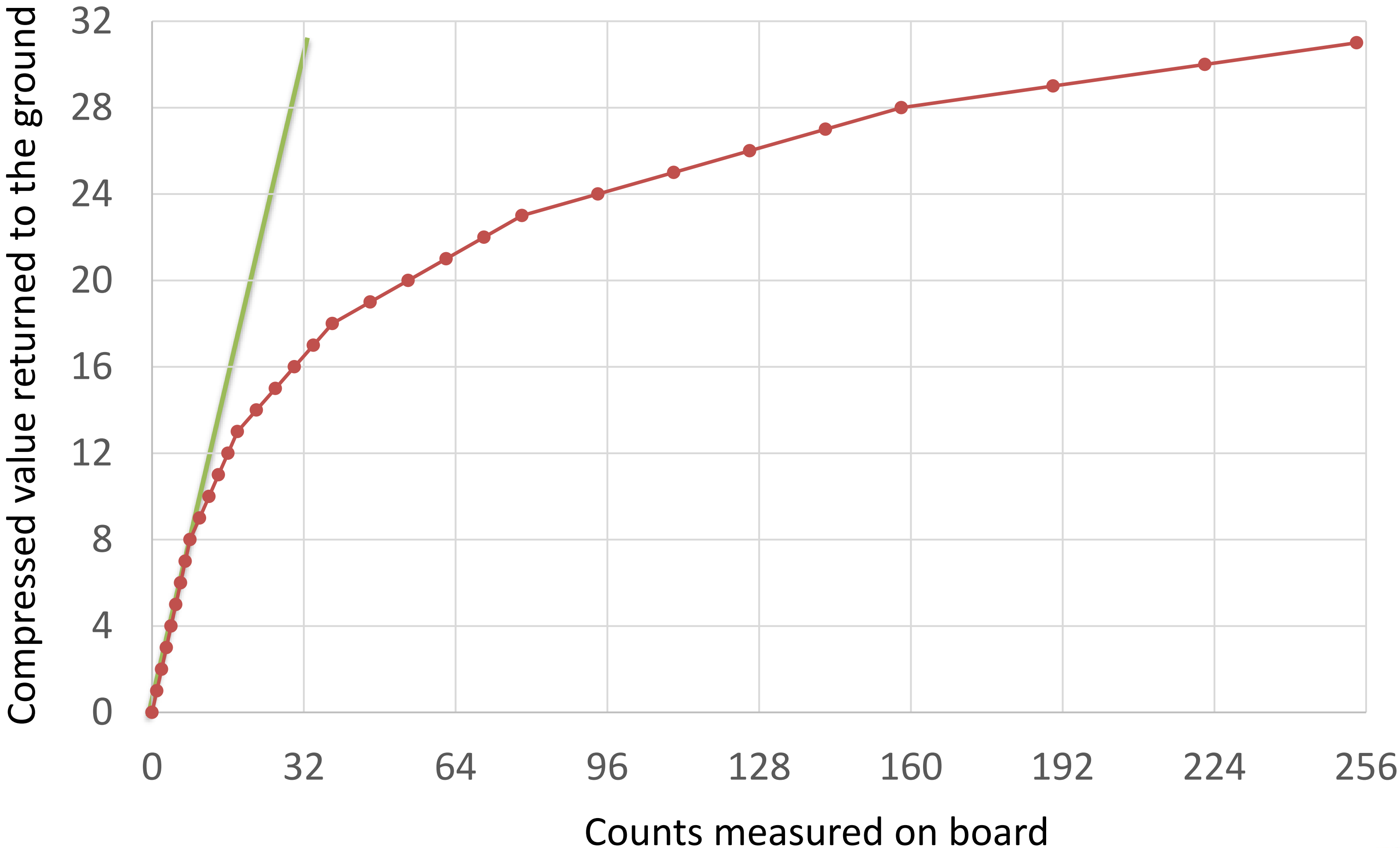
- Basic idea: up to some value we return the actual number of counts, above that we return the counts only in steps of 2, 4, 8…

Measured	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Compressed	0	1	2	3	4	5	6	7	8	8	9	9	10	10	11	11	12	12	13	13
Decompressed	0	1	2	3	4	5	6	7	8	8	10	10	12	12	14	14	16	16	18	18

Measured	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
Compressed	13	13	14	14	14	14	15	15	15	15	16	16	16	16	17	17	17	17	17	17
Decompressed	18	18	22	22	22	22	26	26	26	26	30	30	30	30	34	34	34	34	34	34

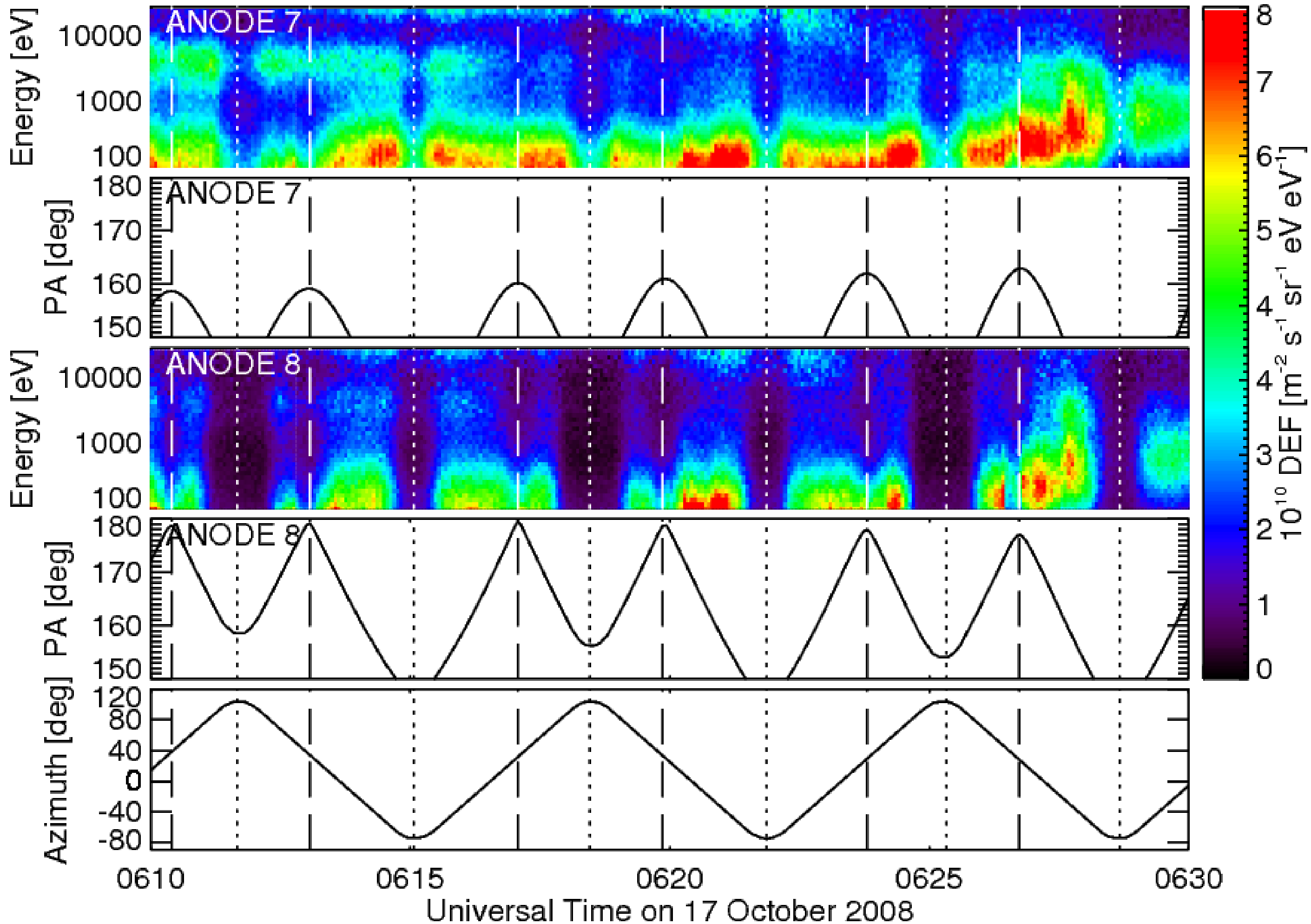
Quasi-log compression

- Basic idea: up to some value we return the actual number of counts, above that we return the counts only in steps of 2, 4, 8…

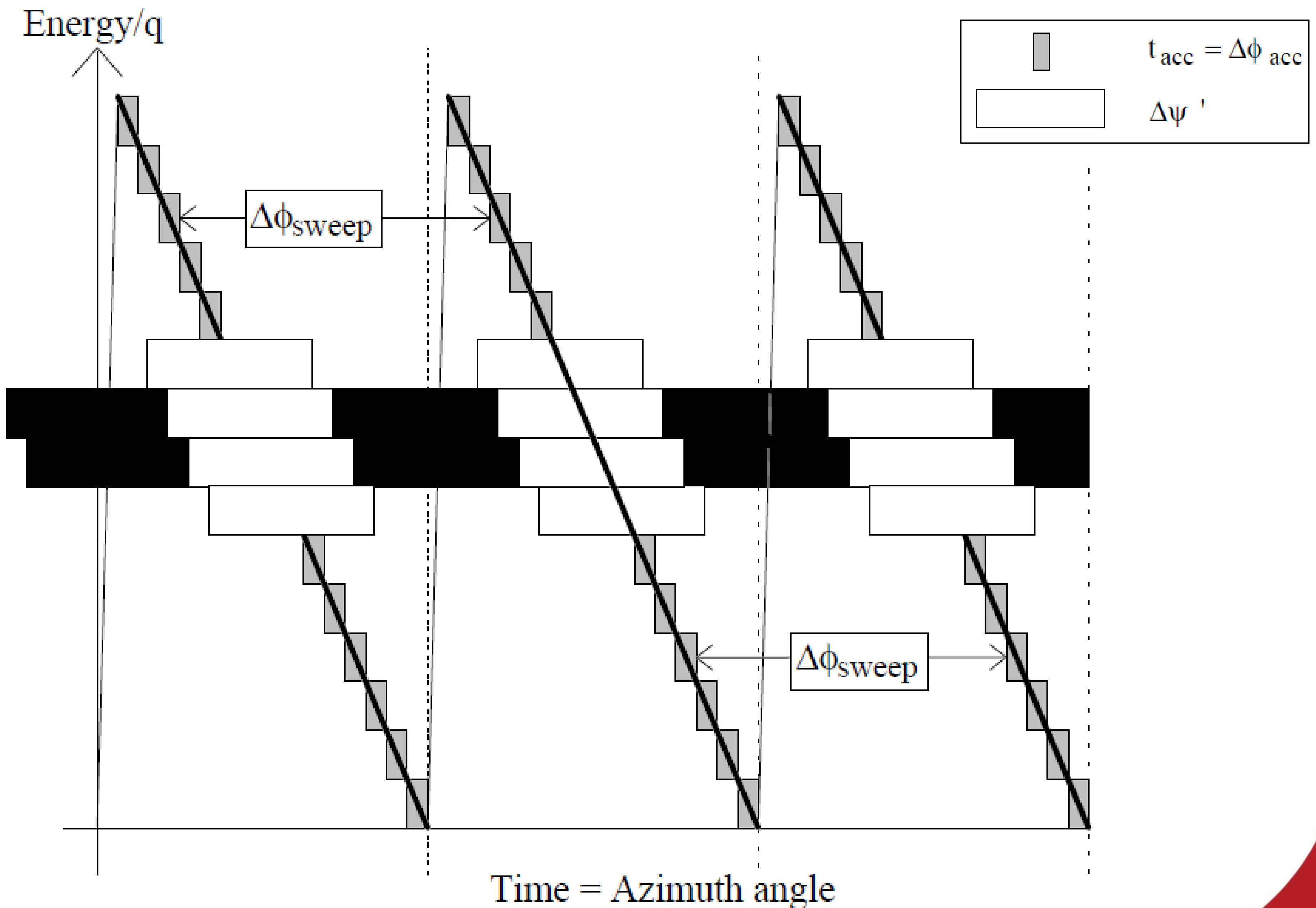


Detector coverage

- Some pixels can be blocked by different parts of the spacecraft.

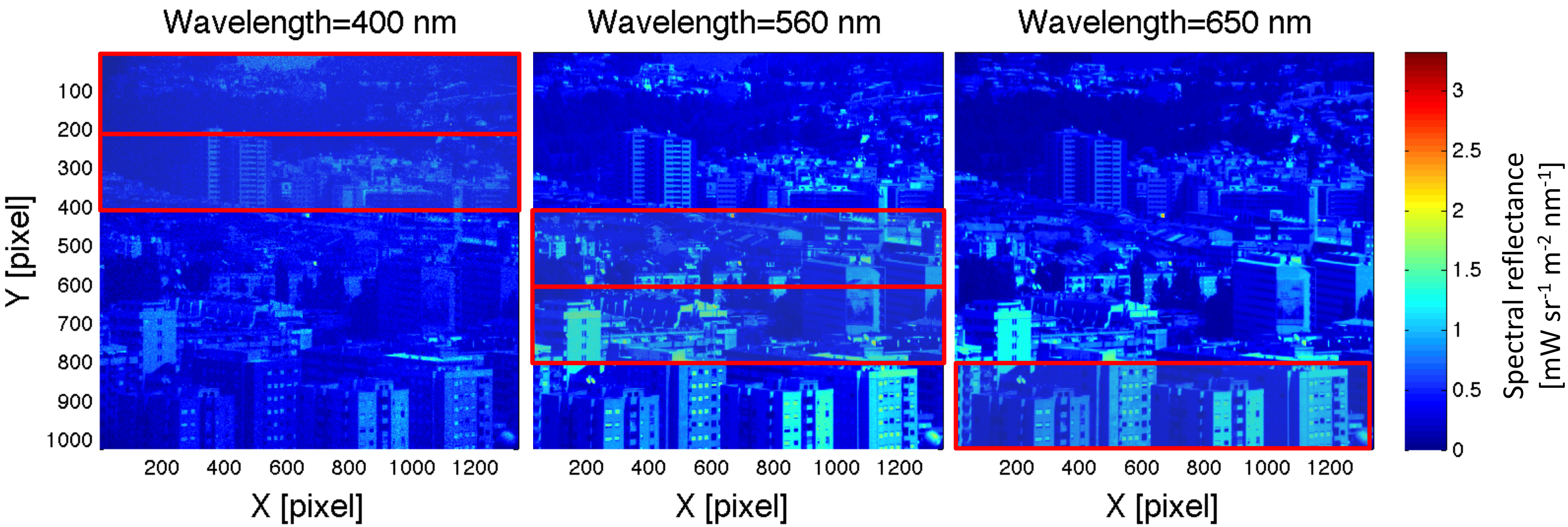


Unsampled regions in velocity space



Fazakerley, Schwartz and Paschmann (2000)

Unsampled regions in space-wavelength



Foster et al. (2006)

4π steradian coverage

- Ideally want to cover all 4π steradians around the spacecraft to observe as much of velocity space as possible.
- Possible on three-axis stabilised spacecraft, but need multiple sensor heads.
- Usually you don't get 4π sr, often less than 2π sr.

Mitigation for missing detector coverage

- Filling.
- Symmetry: assume isotropy (distribution is uniform over 4π sr) or anisotropy (distribution is mirror symmetric about a pitch angle of 90 degrees).
- Analytical distributions and fit – but take into account missing data by weighting appropriate to avoid biasing the fit.

Under-resolving features in the velocity distribution

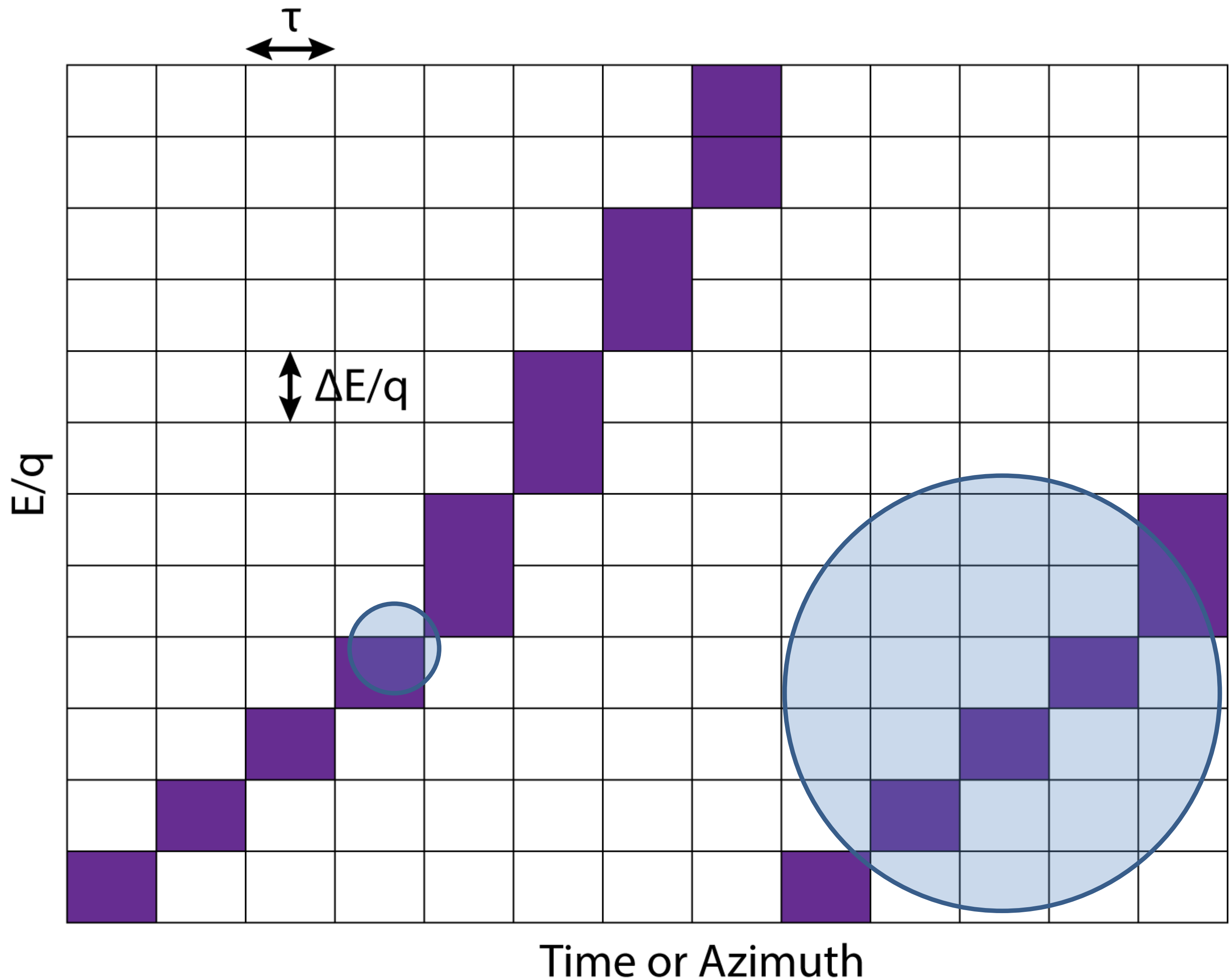
- The design of the instrument is a trade space; given expected fluxes in the target mission environment(s) we need to tune the angular resolution, accumulation time, dynamic range and energy resolution against data volume and aliasing issues.

- Generally won't be optimal in every environment; for example the ion beam and electron strahl in the solar wind. Properties vary with heliocentric distance.

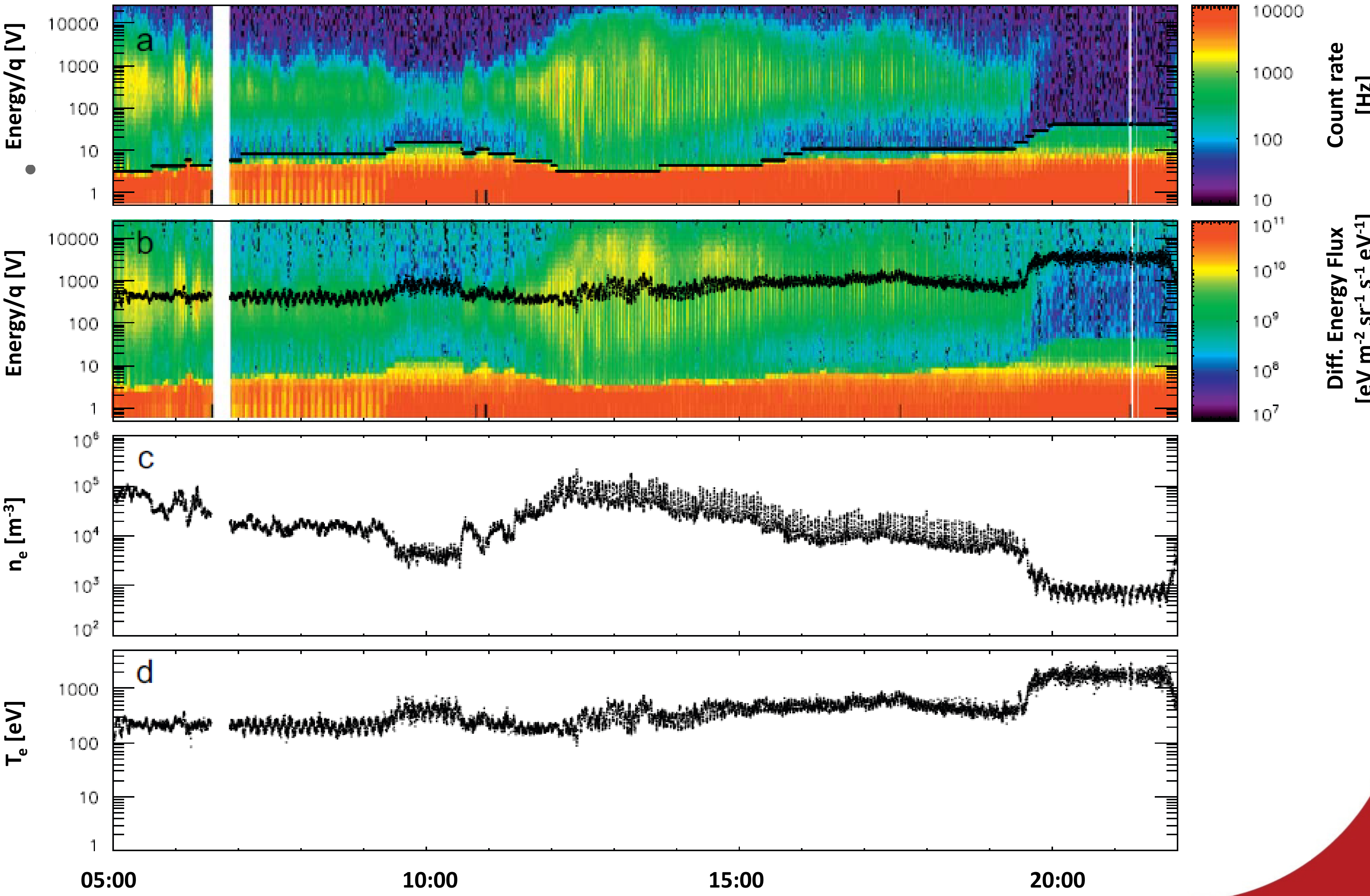
- Major issue is under-resolving features (e.g., loss cones and beams) in the velocity distribution. Can greatly affect derived products.

- Similar issue arises in spectroscopy where spectral lines are under-resolved and appear in a single wavelength bin.

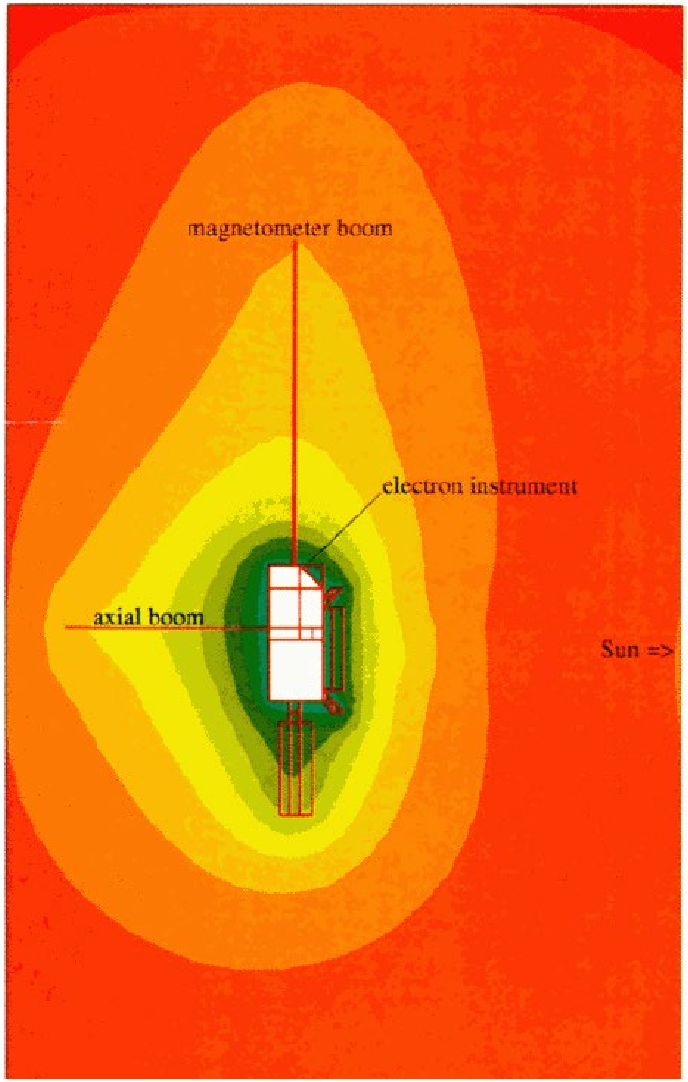
Under-resolving features in the velocity distribution



Spacecraft charging



Spacecraft charging and wake effects



Scime, Phillips and Bame (1994)

- Since electrons have been accelerated through a potential drop V_{sc}, gaining energy eV_{sc}, this is a known trajectory in phase space.

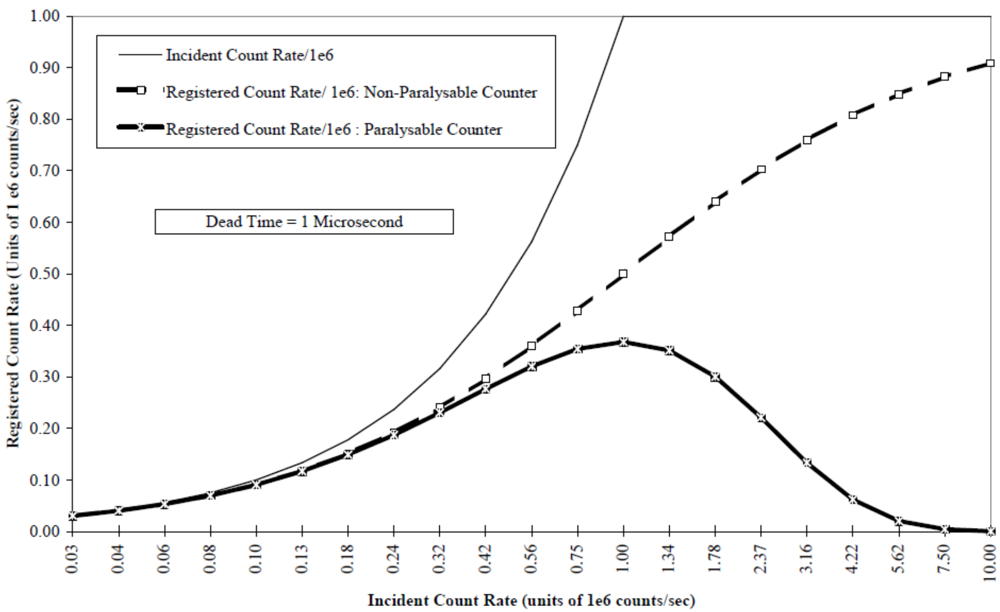
- The undisturbed electron distribution can be recovered using Liouville's Theorem (phase space density is constant along trajectories).

- However, the potential is non-uniform around a spacecraft. At low measurement energies the ambient electrons do not follow straight paths to the instrument – deforms velocity space measurement volume.

Gain depression: can't count fast enough

- Detector: at very high count rates the efficiency of an MCP can drop. Usually this isn't a problem as the detector is designed for an environment and such high count rates will be avoided.

- Electronics: all counters need a finite amount of time to respond to an event – this is dead time.

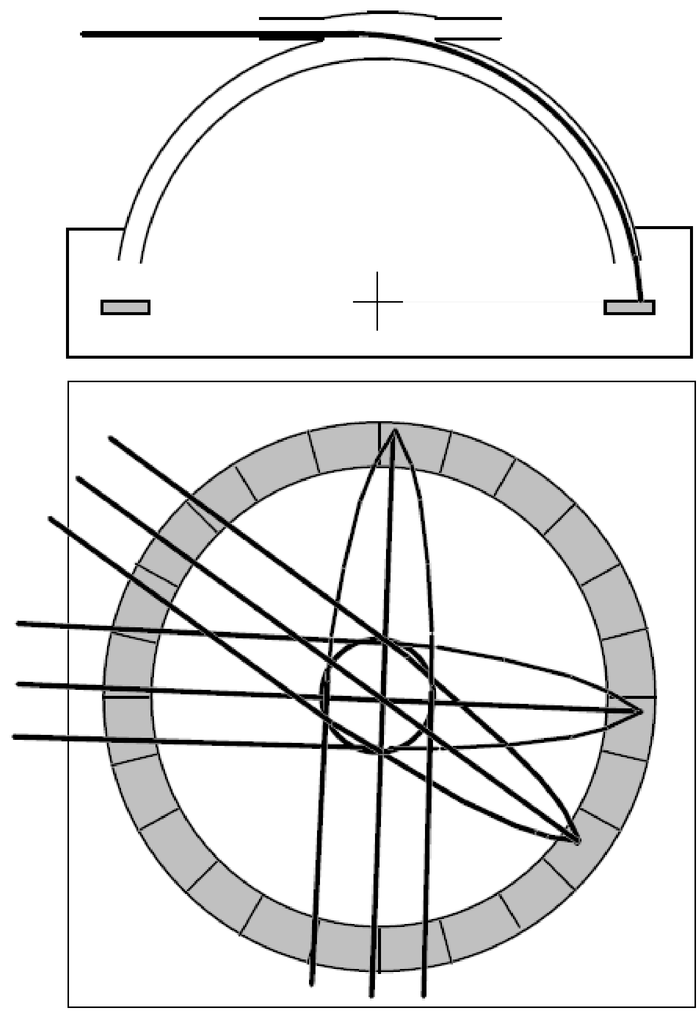


- The actual number of counts can sometimes be recovered (depends on the details of the electronics).

Fazakerley, Schwartz and Paschmann (2000)

Cross-talk

- Can be produced by scattering within the optical part of the analyser.
- Can also be produced in the counter electronics.
- Need to apply a correction matrix.
- Also related to resolution issues – but a separate effect.



Fazakerley, Schwartz and Paschmann (2000)

Aliasing

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- Measurement time<real variability – what we are measuring doesn't change during accumulation/integration.
- Effect on moments. Fake velocities, currents, anisotropies.
- Doesn't matter if you are studying data with a 5 minute or 1 ms sampling interval. If the phenomenon of interest is going to vary at a shorter period then there are issues.
- Particularly relevant for wave-particle interactions – waves have modified the particle distribution faster than it can be measured.
- Mitigation: simulation,

Calibration

- Ground calibration can give an estimate of the uncertainty that can be propagated through an analysis.
- Also a need for in-flight calibration because the instrument changes with time: materials out-gas, thermal cycling, radiation damage.
- In-flight calibration might use another reference, e.g., calibrating against a density measurement from a plasma wave instrument. But that had uncertainties in its measurement that should then affect the uncertainty in the calibration.

Higher order products

What is a higher order product?

- Collapsing spectral information into a small set of numbers that characterise the distribution in more/less meaningful ways, e.g.:
  - Total emitted power.
  - Red shift.
  - Colour ratio.
  - Density.
  - Temperature.
  - Energy flux.

Moments

- Numbers that characterise the shape of a function:

$$\mu_i = \int_{-\infty}^{\infty} (x-c)^i f(x) dx$$

- Each "i"th moment has a specific meaning

i	Probability distribution	Velocity distribution
0	=1	Number density
1	Mean	Number flux
2	Standard deviation	Momentum flux
3	Skew	Energy flux

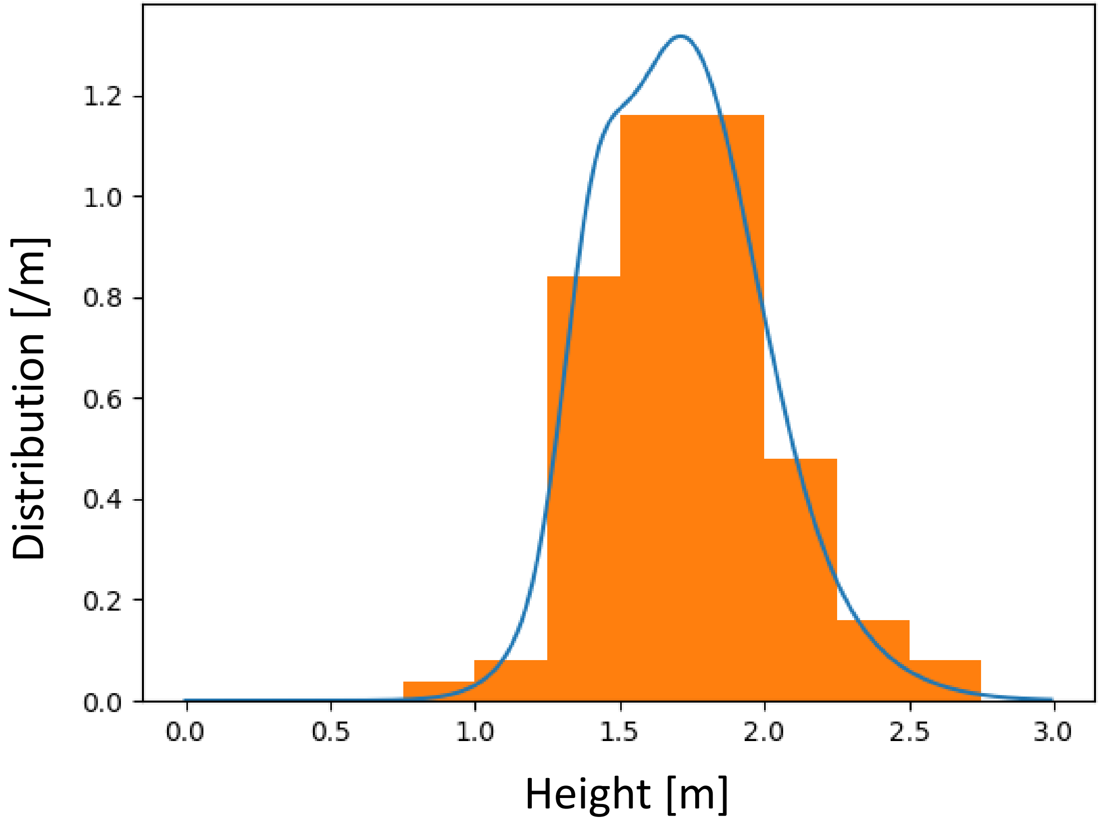
- Higher order moments are more susceptible to errors due to their velocity space weighting.

Plasma moments

i	Moment	R	Centred	Non-centred moment
0	Number density	S (0)	$n = \int f(\mathbf{v}) d\mathbf{v}$	
1	Number flux	V (1)	$n\mathbf{u} = \int f(\mathbf{v})\mathbf{v} d\mathbf{v}$	
2	Momentum flux /pressure	T (2)	$\Pi = m \int f(\mathbf{v})\mathbf{v}\mathbf{v} d\mathbf{v}$	$\boldsymbol{P} = \frac{m}{2} \int f(\mathbf{v})(\mathbf{v} - \mathbf{u})(\mathbf{v} - \mathbf{u}) d\mathbf{v}$
3	Energy flux / heat flux	V (1)	$\boldsymbol{Q} = \frac{m}{2} \int f(\mathbf{v}) v^2 \mathbf{v} d\mathbf{v}$	$\boldsymbol{Q} = \frac{m}{2} \int f(\mathbf{v})(v - u)^2 (\mathbf{v} - \mathbf{u}) d\mathbf{v}$

Probability distribution example

- We might draw an analogy with trying to estimate the population mean and standard deviation of the heights of adults.



Numerical integration

$$n = \int f(\mathbf{v}) d\mathbf{v}$$

$$n\mathbf{u} = \int f(\mathbf{v})\mathbf{v} d\mathbf{v}$$

Density:

$$N = \sum_k \frac{1}{V(E)} \sum_\phi \sum_\theta \; C(\theta, \phi, E)$$

Number flux density vector:

$$N V_x = \sum_E \sum_\phi \cos\phi \; \sum_\theta \cos\theta \; C(\theta, \phi, E)$$

$$N V_y = \sum_E \sum_\phi \sin\phi \; \sum_\theta \cos\theta \; C(\theta, \phi, E)$$

$$N V_z = \sum_E \sum_\phi \sum_\theta \sin\theta \; C(\theta, \phi, E)$$

- Numerically integrate moment equations, e.g., using the Trapezium rule.
- Errors can be propagated through – but rarely are.
- Fine if you have data over 4π sr.

Paschmann, Fazakerley and Schwartz (2000)

Forward modelling and fitting

- Construct a forward model of the instrument:
  - Model velocity distribution, e.g., drifting Maxwellian, Kappa, loss-cone.
  - Convert to count rate, account for resolution and obscuration.
  - Convert to counts/accumulation, add noise sources.

- Adjust the parameters of the model velocity distribution to minimise the difference between the data and the result of the forward model.

$$\chi^2 = \frac{1}{N-\nu}\sum_i \frac{(C_i - M(\mathbf{x}, i))^2}{\sigma_i^2}$$

- Non-linear fitting algorithms (Levenberg-Marquardt, Downhill simplex, particle swarm optimisers) also Bayesian and Maximum Likelihood methods.

- Uncertainties: the Hessian matrix, covariance matrix, a direct (qualitative and quantitative) examination of the χ^2 space, or Monte-Carlo methods. Do you believe the error? Are the errors correlated (off-diagonal terms in covariance matrix)?

- Also, is the fit significant? Significance test the value of χ^2 to accept/reject the fit.

Advantages and disadvantages

	Advantages	Disadvantages
Numerical integration	• Model independent. • Uncertainties are derived directly from data. • Fast. • Uncertainties due to finite resolution directly contribute to error.	• Limited handling of under-resolved features. • Need to fill gaps in the distribution. • Harder to extract sub-populations.
Fitting analytical distributions	• Using a forward model provides the ability to handle resolution issues. • Potentially better at handling low S/N distributions. • Can extract multiple populations from the same spectrum.	• Suitability of the model and ability to find local minima/maxima contributes to uncertainties. • Need to fill gaps or suitably weight the fit. • How do we know that there isn't a better analytical distribution? • Potentially slow.

Thoughts, critiques and future directions

Critiques

Analysis and presentation

- Many many papers in the literature that do not quote any uncertainties on derived parameters – in many cases this could easy invalidate a result.
- Use of isotropy (or other symmetry assumption) without further justification/checking.
- Use of standard data products without any understanding about how they have been measured and processed.
- No evidence when claiming “significant differences”.
- Chi-by-eye.
- Where are the error bars?

Workflow

- Over-reliance on standard GUI-driven tools that don’t capture meta-data associated with analysis.
- Lack of clarity in workflows – essentially impossible to reproduce when handling/reducing complex data sets.
- Incomplete documentation provided with data.

Reproducibility

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- Interest in reproducibility: reproduce results – not necessarily bit-for-bit.
- Lots of interest from numerical computing side, but I think it applies equally in data analysis.
- Reproducibility concepts have been considered on a spectrum, starting with replicability by yourself as a floor level, increasing through to replicability by others: more work, but increasing community value [Ivie and Thain, 2018].
- *"Reproducible research needs to be perceived by all involved as a more effective contribution to science rather than an inconvenient and unachievable ideal."* Ivie and Thain (2018)
- Trying to build into my workflows –including development roadmaps.

Analysis

- Moments are not always necessary; other measures and techniques. What is the question we want to answer?

- Spectra are super-interesting and can be used for kinetic calculations.

- Missions like MMS and Solar Orbiter are doing detailed science – lots of assumptions simply can’t be made, or should be validated (e.g., gyrotropy).

- Let’s bring the data closer to the analysis: opportunities to exploit the data
  - Quite often one needs a density or temperature for an analysis.
  - Are we comparing apples-with-apples? The data reduction may have produced a “temperature” (a measure of thermal kinetic energy) [from a non-Maxwellian distribution, and we might compare this with the result of an MHD calculation.
  - A time-series of 3D spectra can be hard to deal with conceptually – but there are methods that we can use – we can collapse to a 2D (pitch angle and energy) distribution – we can use machine learning or Bayesian methods.
  - **Over-reliance on moments**.

Commoditisation

- There is a reason why data on PSA/PDS isn't always in a plug-and-play format and why the manuals are extensive. Avoid reducing data analysis to a qualitative analysis: "the density gets bigger", "the temperature is hotter here".

- Example of user guides:
  - https://pds-ppi.igpp.ucla.edu/search/view/?f=yes&id=pds://PPI/CO-E_J_S_SW-CAPS-3-CALIBRATED-V1.0
  - https://www.cosmos.esa.int/web/csa/documentation

- Publish or perish is having a deleterious impact on quality of science: caveats do not get read or heeded – we just want the thing that allows us to continue doing the thing we're doing.

- Not about impeding science.

- Empowerment to do good science with high quality data; rather than providing pre-reduced simplistic numbers.

Further reading

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- Press et al. "*Numerical Recipes*" [http://numerical.recipes/]
- Bevington and Robinson "Data Reduction and Error Analysis for the Physical Sciences"
- "Analysis Methods for Multi-Spacecraft Data" (Ch. 5-7) [http://www.issibern.ch/PDF-Files/analysis_methods_1_1a.pdf]
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