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In Conference Materials if you want to follow along!

Implications of Radial Diffusion Ensemble Models for Forecasting

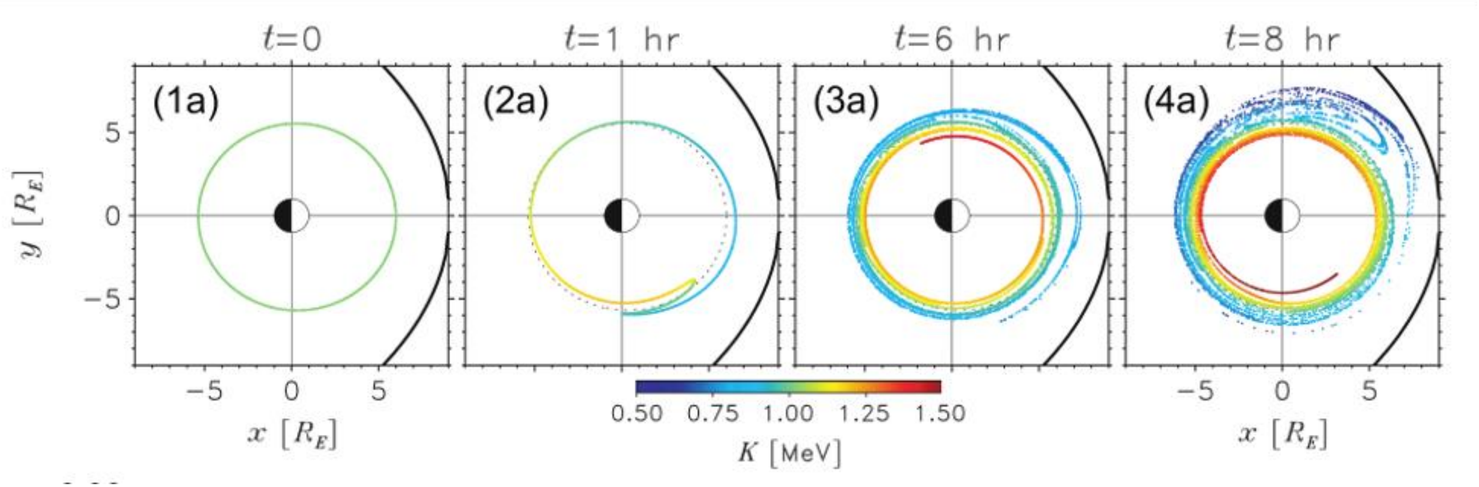
S. N. Bentley[1,2], J. R. Stout[2], R. L. Thompson[2], D. J. Ratliff[1], C. E. J. Watt[1,2]

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Bentley et al. 2024, Physics of Plasmas; https://doi.org/10.1063/5.0217268

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Background: Radial diffusion



Numerical simulation, radial diffusion via ULF waves, Ukhorskiy & Sitnov 2008.

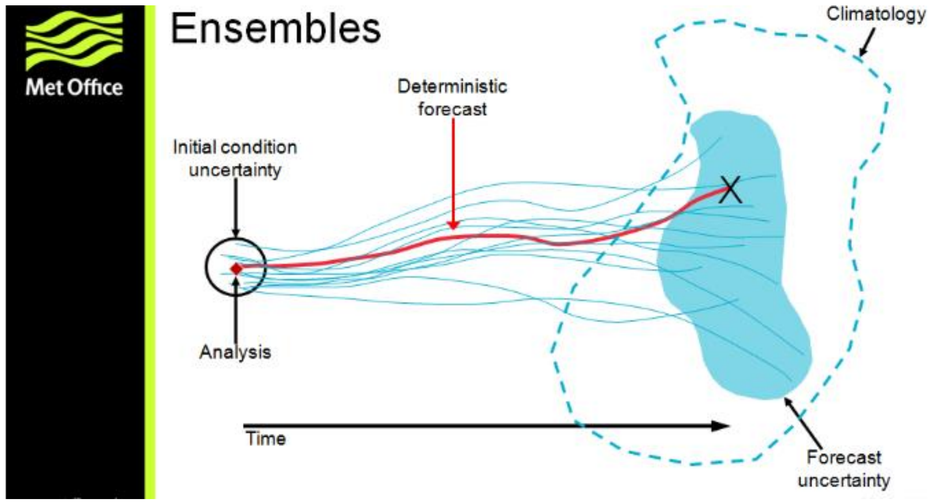
- Timescales longer than bounce and gyromotion.
- Use diffusion across drift paths to represent bulk behaviour towards / away from the Earth.
- Use to investigate large scale processes before adding to full models.

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Background: Ensemble modelling

Why should we capture uncertainty, variability?

- Estimate forecast uncertainty.
- Identify where to improve modelling.
- Represent inherent variability due to radiation belt physics and observations.
  - *We know that variability in diffusion coefficients affects radiation belt distributions, e.g. Watt et al. 2022; Thompson et al. 2019*

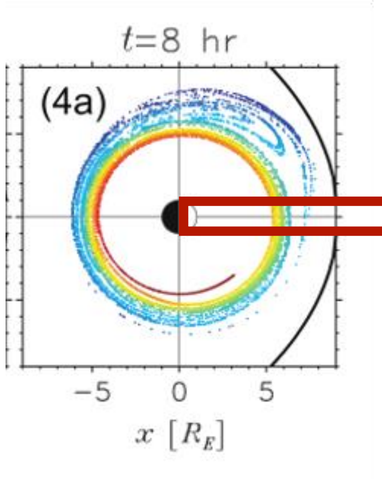


(Met Office) Ensembles can be used to capture uncertainty that reflects physical reality.

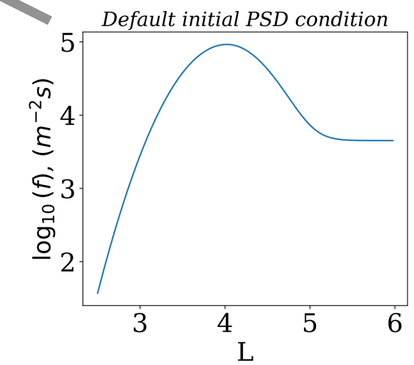
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Reduced radiation belt diffusion model

$$\frac{\partial f}{\partial t} = +L^2 \frac{\partial}{\partial L}\Big|_{\mu,J} \left(\frac{D_{LL}}{L^2} \frac{\partial f}{\partial L}\Big|_{\mu,J} \right) - \mathcal{L}f$$



Azimuthal variation is collapsed onto a radial co-ordinate *L*; we average over each drift.



Numerical simulation, radial diffusion via ULF waves, Ukhorskiy & Sitnov 2008.

- Radial diffusion only, plus pitch angle loss term
- Remember that physics determining diffusion is almost all in diffusion coefficient D_{LL}
- Note that D_{LL} depends on L^*;

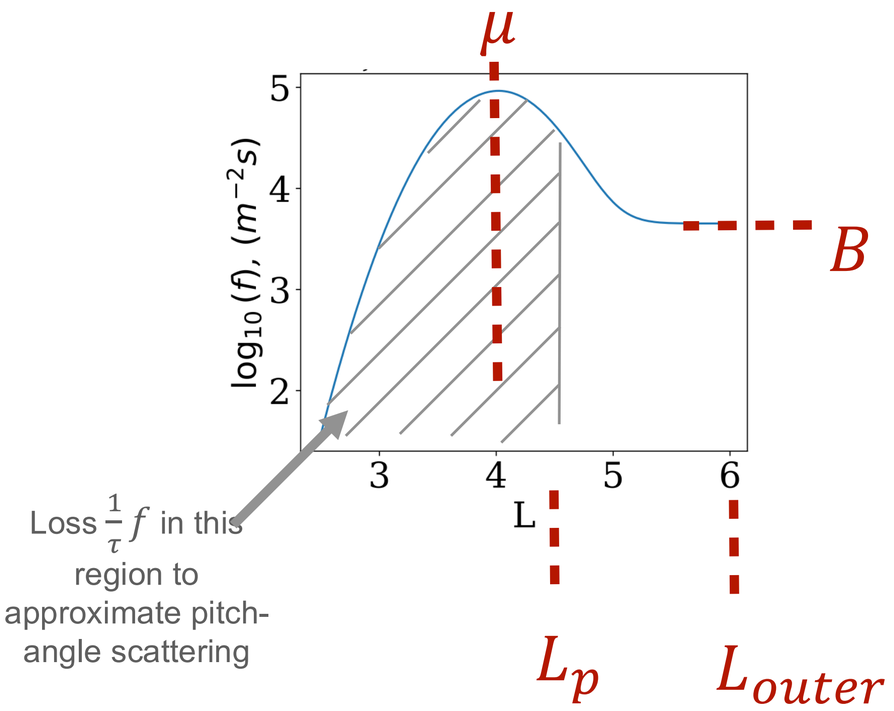
$$D_{LL} \propto L^n$$

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How much do initial model settings affect the ensemble?

- ? Will they bias any ensemble if we just choose a random spread?
- ? How can we measure this?
- ? What is the effect of model settings on the final distribution?

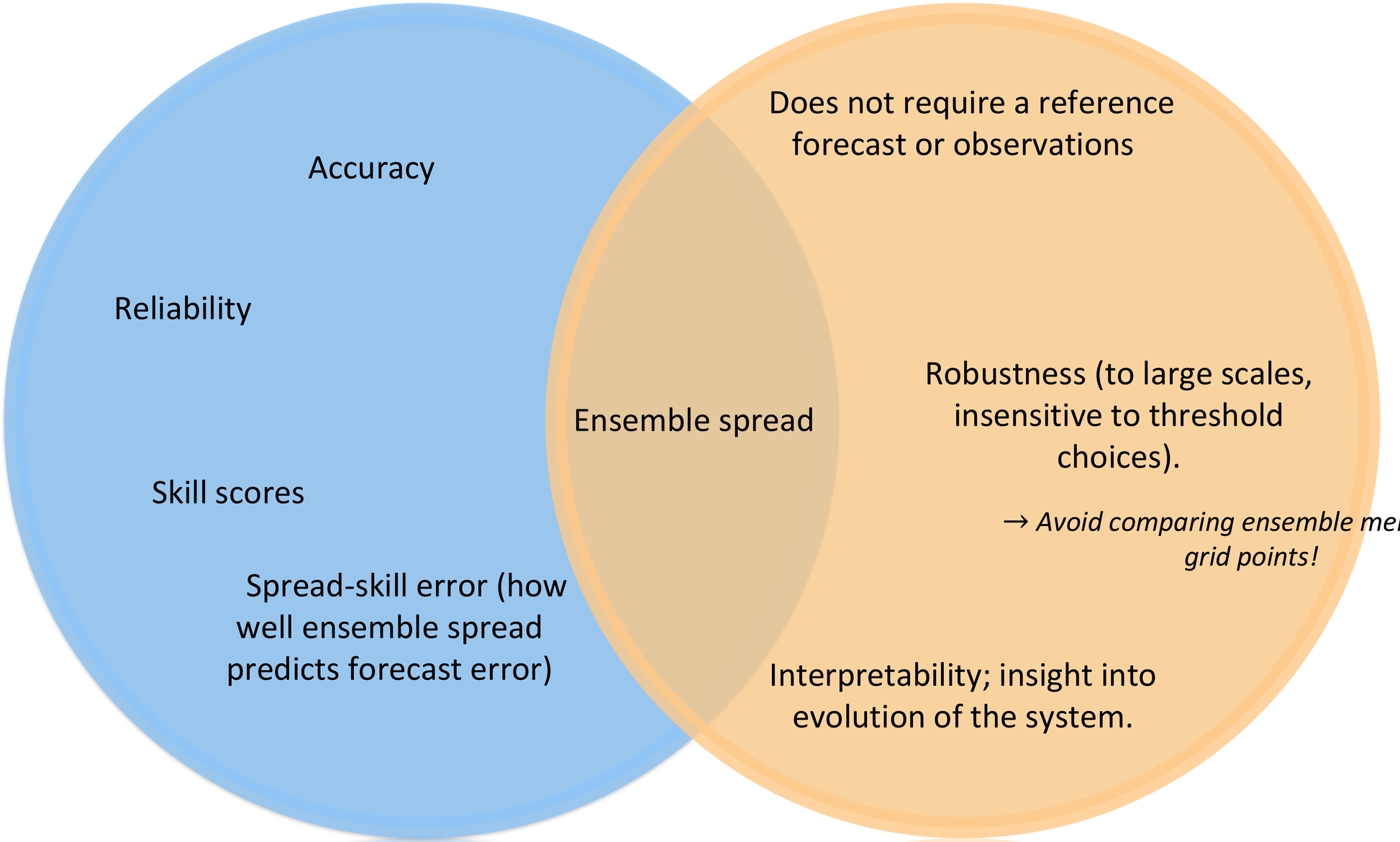
- To answer these, for a simplified model we:
  - Completed and interpreted a parameter scan (a “tester ensemble”)
  - Found suitable metrics



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Ensemble metrics

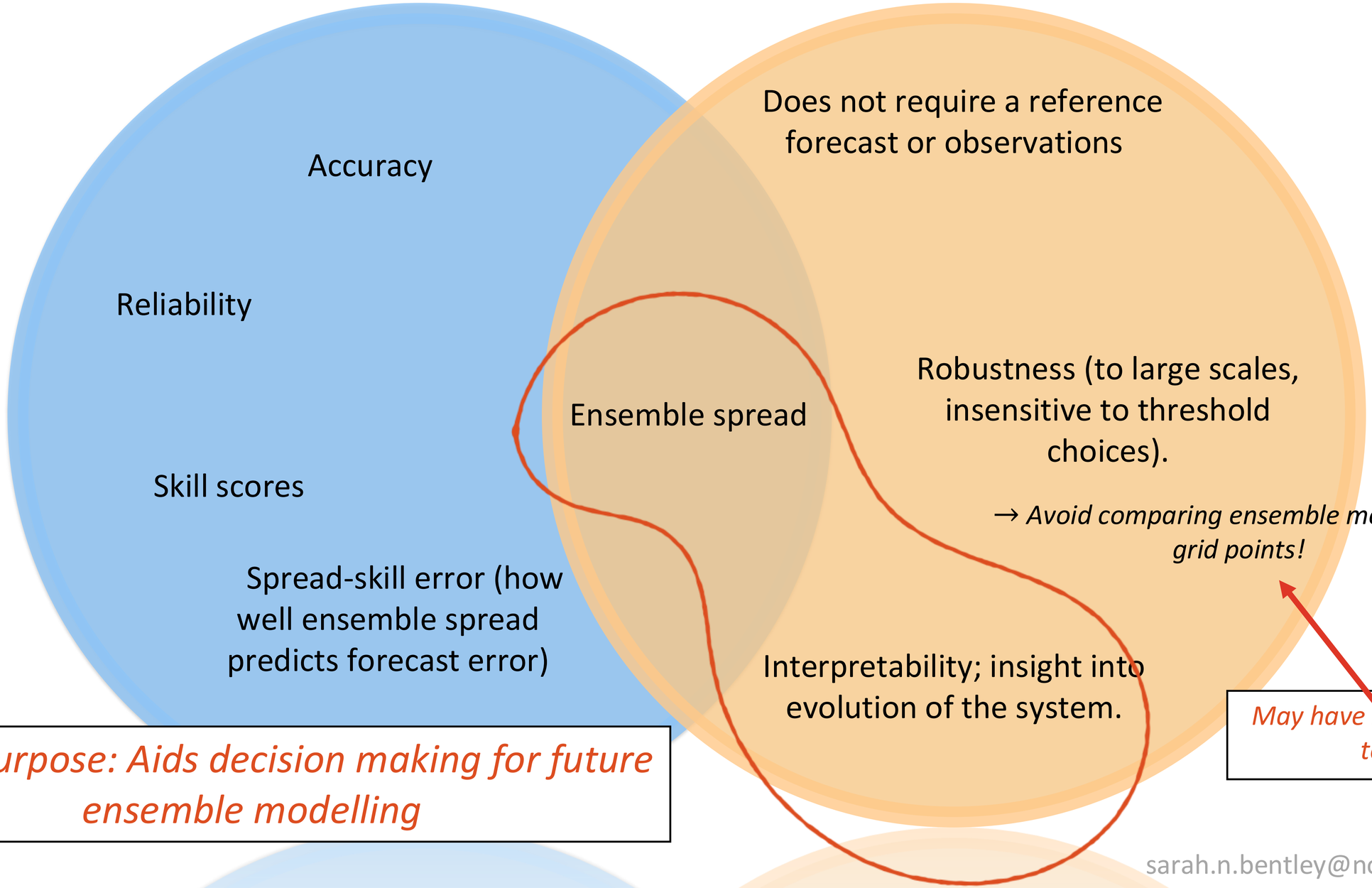
Our requirements



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Ensemble metrics

Our requirements



Metric purpose: Aids decision making for future ensemble modelling

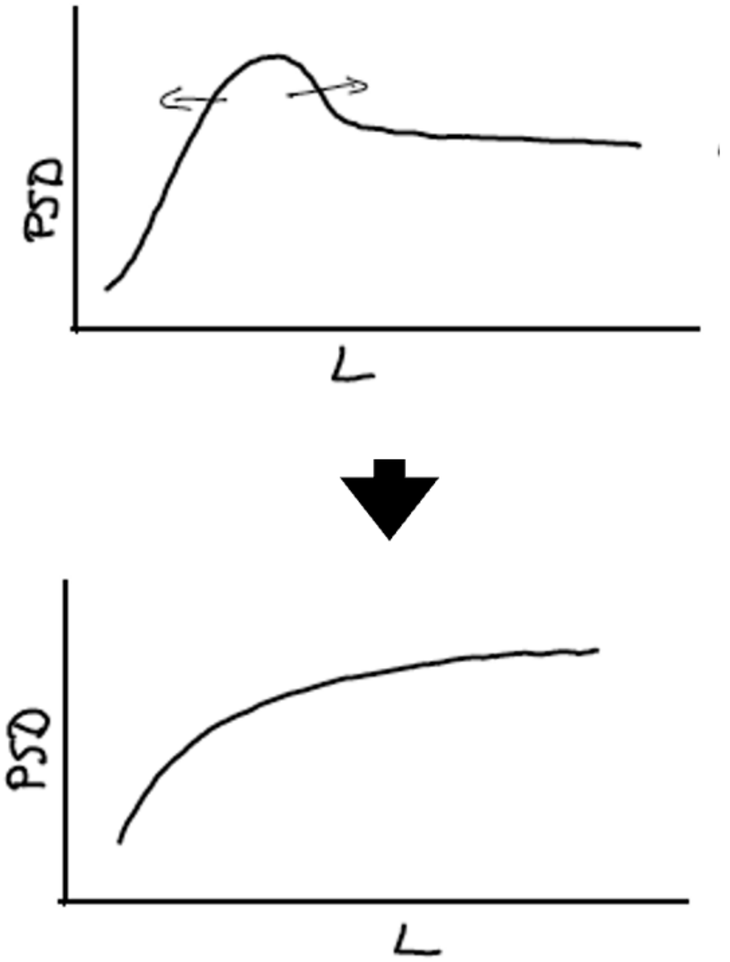
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t_m, "Time to monotonicity"

- Time until the distribution is monotonic.
- Answers the physics question:

  "How long until the enhancement has diffused away?"

- Gives us a timescale for each simulation, which we can compare across the ensemble.

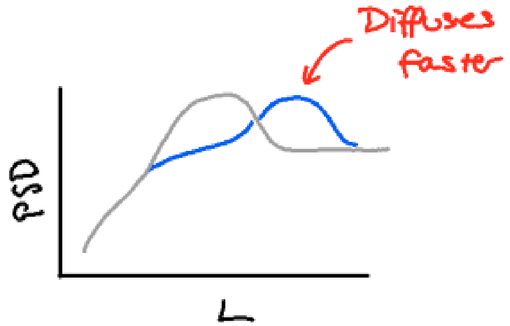


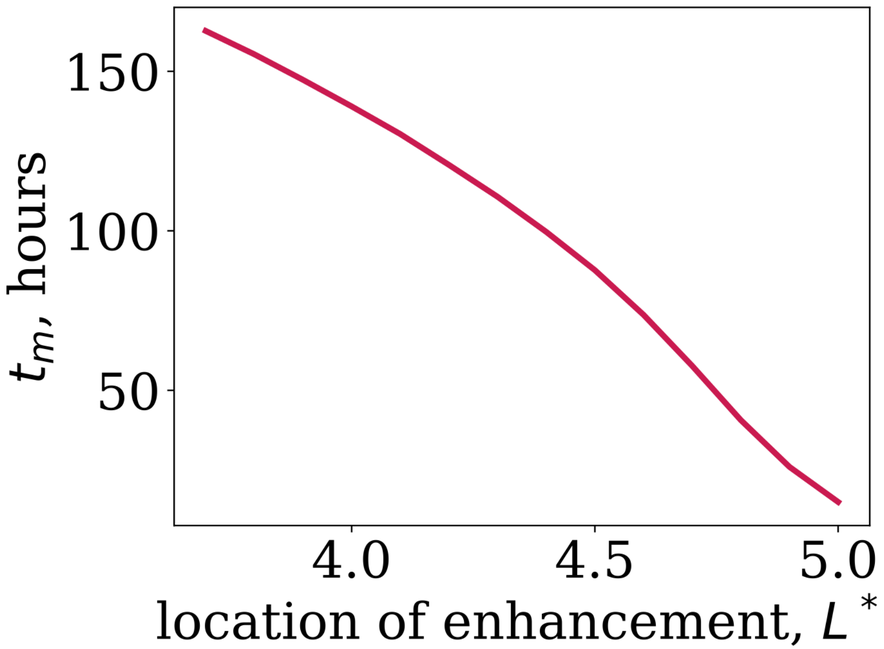
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Result: features in L* affect ensemble outcomes

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- Example: for a set Kp, an enhancement at higher L^* diffuses away more quickly.
- Consequence: Evenly spread ensemble members may result in bias.
- Why does this happen: D_{LL} depends on L^*, e.g. $D_{LL} \propto L^8 10^{aL+bKp^2+cKp}$. Diffusion is faster at higher L^*.





Simulation results: monotonicity reached sooner if the initial enhancement starts farther out (Dirichlet outer boundary, Kp=7)

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Analytic metrics: Mass- and energy-like moments $\mathcal{N}, \mathcal{E}$

- Total mass and “energy” in the simulation. $\mathcal{E}$ is minimised when the distribution stops evolving; the simulation will evolve to a low $\mathcal{E}$ state.

$$\mathcal{N} = \int \frac{f}{L^2} dL$$

Mass in experiment

$$\mathcal{E} = \frac{1}{2c_\epsilon} \int \frac{f^2}{L^2} dL$$

How close the distribution is to a zero state / a state not changing with time

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How close the distribution is to a zero state / a state not changing with time

- We can see how these are evolving ($\mathcal{N}_t, \mathcal{E}_t$) by choosing $D_{LL} = D_0 L^n$ and substituting in our 1-D radial diffusion equation.

$$\mathcal{E}_t = \left[\frac{D_{LL}}{L^2} f f_L\right]_{IB}^{OB} - \int \frac{D_{LL}}{L^2} (f_L)^2 dL$$

We can explicitly see how f, D_{LL}, boundaries etc affect evolution to a "diffused away" state.

Note: for simplicity, the loss term is not shown here

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Result 2: to improve models, should we improve f_L or D_{LL}?

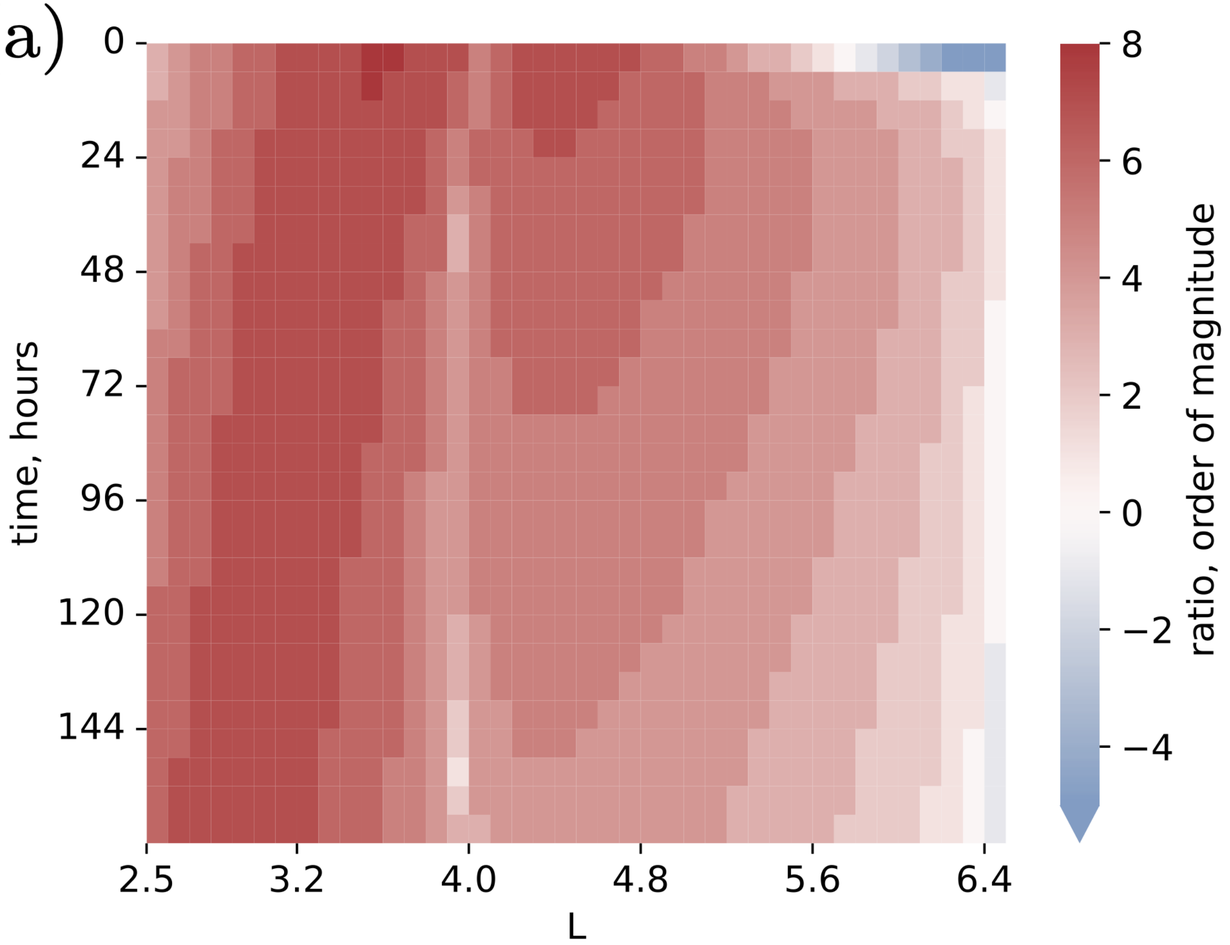
$$-\int \frac{D_{LL}}{L^2}(f_L)^2 dL$$

- Part of $\mathcal{E}_t$ tells us what dominates evolution
- For constant diffusion: “diffusion acts against gradients” (i.e. f_L)
- For us: Either f_L or D_{LL}. Let’s look at the ratio of these?

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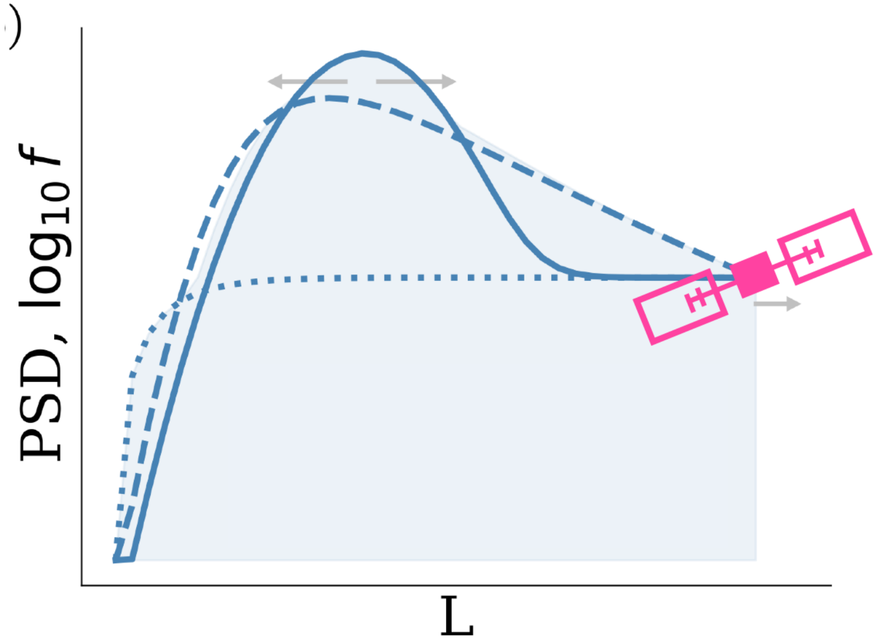
- Part of $\mathcal{E}_t$tells us what dominates evolution
- For constant diffusion: “diffusion acts against gradients” (i.e. f_L)
- For us: Either f_L or D_{LL}. Let’s look at the ratio of these?
- Suggests gradients, rather than diffusion coefficients. Needs verification!



Order-of-magnitude ratio $(f_L)^2 : D_0 L^{n-2}$; the gradient term dominates everywhere, for both boundary conditions

Combining metrics gives questions about the outer boundary

- Reminder: operationally, use a curtailed data driven outer boundary, e.g. at GOES ($L = 6.6R_E$), not the actual last closed drift shell (8-11 R_E)
- Reminder: anything at higher L* means more diffusion total
- So…Any consequences to different domain lengths?



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Combining metrics gives questions about the outer boundary

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Metric 1 (t_m) :

Both outer boundary conditions are unphysical.

Some transport across the boundary is needed.

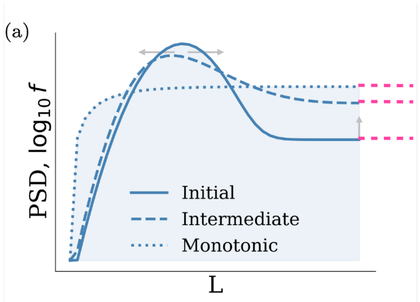
Metric 2 ($\mathcal{N}, \mathcal{E}$):

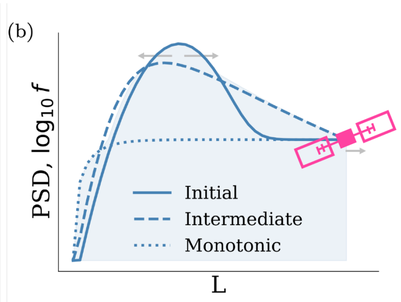
Longer domains reduce this boundary condition effect.

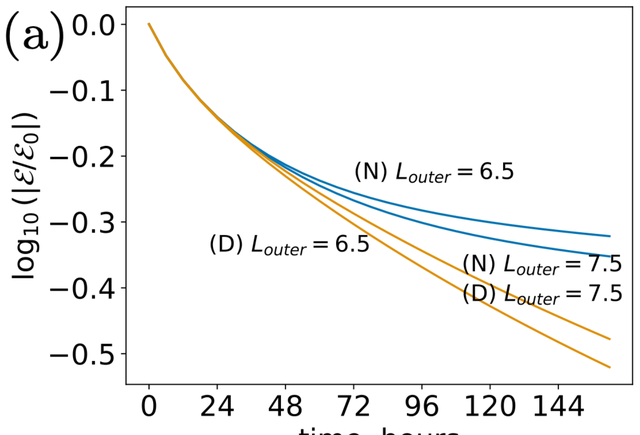
Longer domains are effectively a different system.

Together:

1. Longer domains are more physical.
2. Both fixed flux, value boundary conditions aren't quite physical.







Current models have a shortened, data-driven value boundary. Is this OK?

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Is a curtailed, data-determined boundary a problem?

- Not a problem:
  - Pitch-angle loss (in our simple pilot) is greater than this effect.
  - Experiments (Lee et al. 2024) indicate that a shorter domain using data is better than the alternatives.

- Yes, a problem:
  - This fix only works when data is available - e.g. not for forecasting.
  - In future, we need mixed boundary conditions to allow transport across the boundary.

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Summary

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Two metrics:

Metric 1 (t_m) "*How long for an enhancement to diffuse away?*".
Depends on initial and boundary conditions - but mostly on loss.

Metric 2 ($\mathcal{N}$, $\mathcal{E}$) *"What dominates the diffusion?"*
Quantify how model components contribute to movement of mass and evolution to a lower energy ("most diffused") state.

Three main results for ensemble modelling:

1. Size of domain (i.e. how far out we model) changes the physics, because diffusion is more rapid farther out (D_{LL} depends on L^*!) Data constrains this where available.

2. The distribution gradient f_L may affect diffusion more than the diffusion coefficient D_{LL}. Verify this.

   If yes - we need to shift our study focus as a field.

   If no - stop using 1D radial diffusion toy models.

3. Future metrics: use co-ordinate transformations for grid point comparisons, MSE etc. (i.e. a $\frac{1}{L^2}$ factor)

What next? *! 5-year post-doc starting April !*

(And other positions for other work packages – see Clare Watt's poster)

Follow up on variability and #1 above:

- When we incorporate mixed boundary conditions, how sensitive is radial diffusion to moving outer boundary?
- How sensitive is radial diffusion when loss and injection vary over time?

For these slides, including references, see my website

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References

- Bentley et al. (2024). *Phys. Plasmas* (this work) DOI: 10.1063/5.0217268. *(data, plotting tools available)*
- Lee et al. (2024). *JGR: Space Physics* (boundary experiments) 10.1029/2023JA032286.
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- Thompson et al. (2020). *JGR: Space Physics.* (numerical model; variability experiments) DOI: 10.1029/2019JA027254
- Watt et al. (2022). *Frontiers in Astronomy and Space Sciences* (variability pitch-angle diffusion experiments) DOI: 10.3389/fspas.2022.1004634

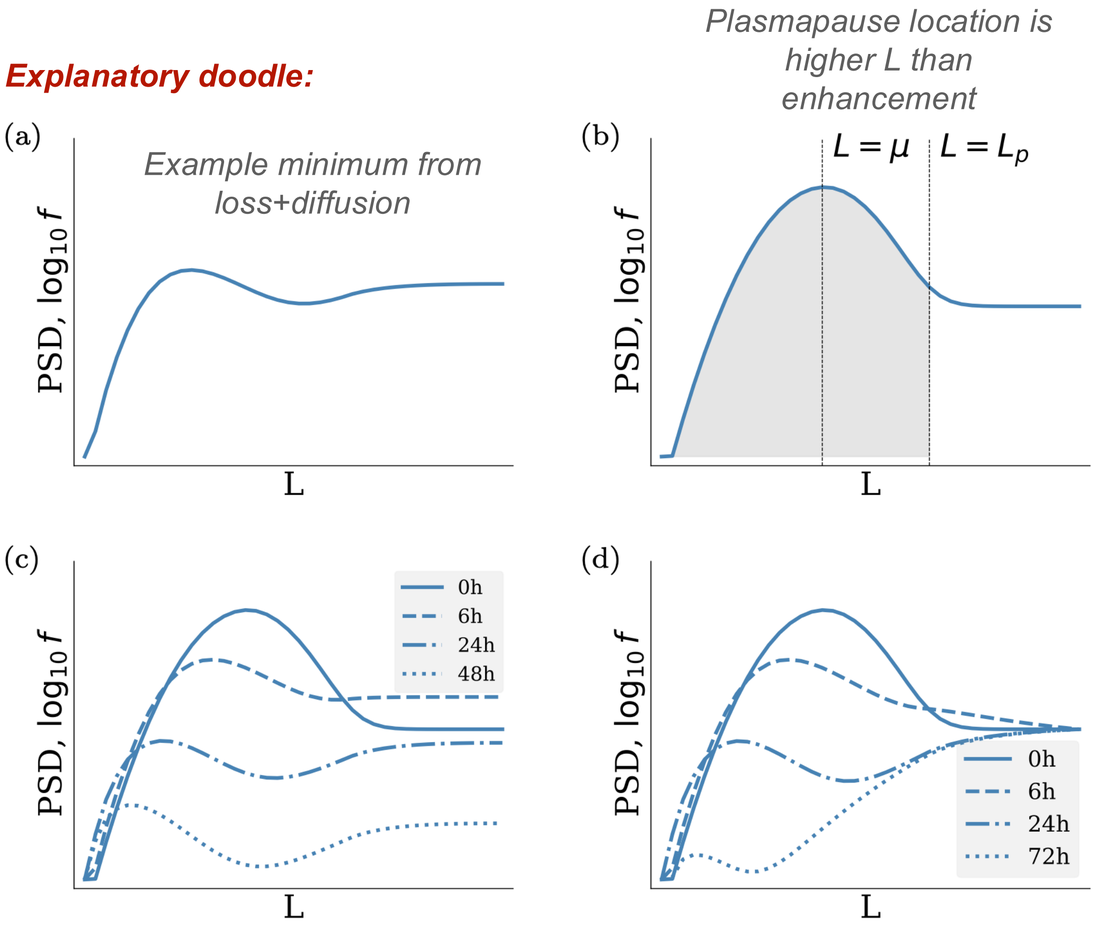
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Loss and the plasmapause

- If we add loss, then there is at least one new parameter to benchmark: the edge of that loss, the plasmapause.

- The location of the plasmapause compared to the enhancement can result in monotonicity never being reached: t_m would need to be adapted in this case.

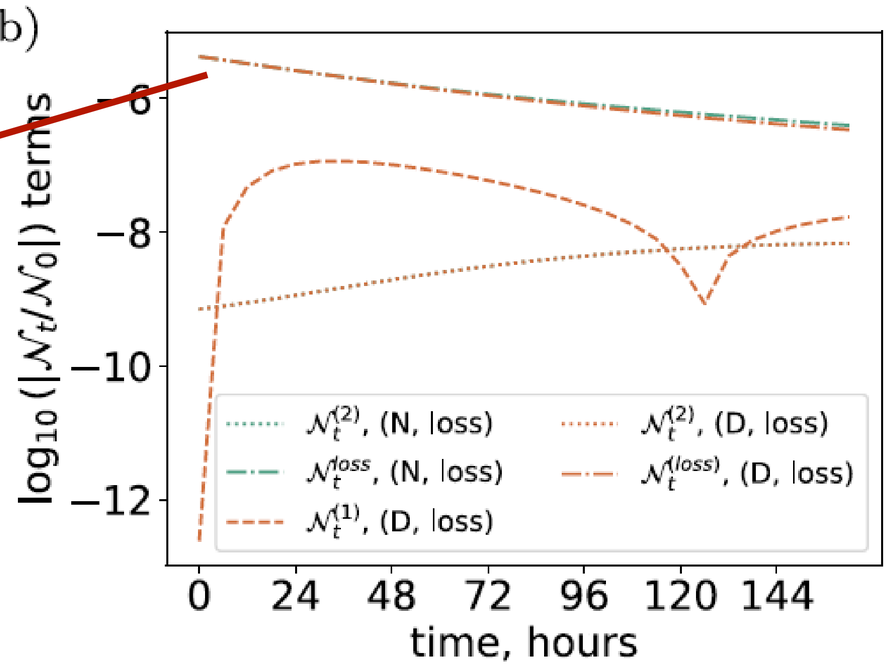
Explanatory doodle:



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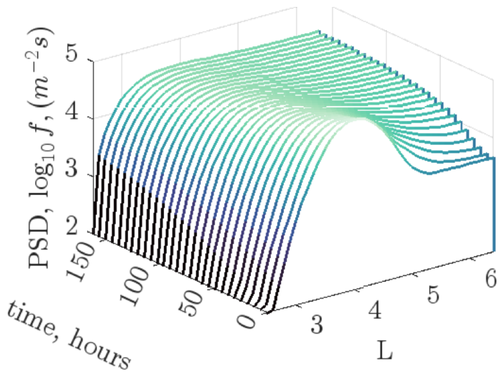
These effects are dominated by loss.

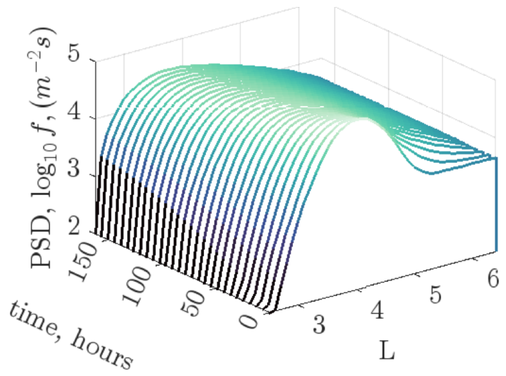
Calculating all components of $\mathcal{N}_t$, the biggest component is loss; loss contributes the most to the changing particle density.



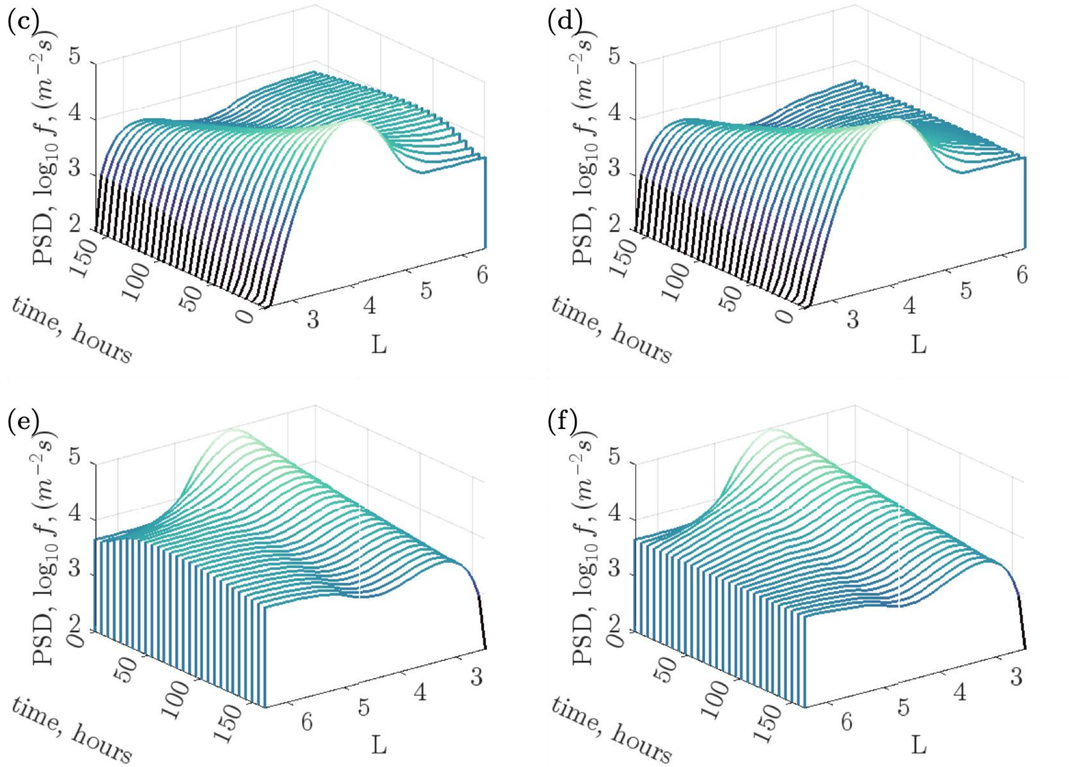
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These effects are dominated by loss.





Starting with a different outer boundary condition and no loss results in a different evolution.



Same simulations, with loss: The evolution appears much less boundary-condition dependent.

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Methodology

Numerical Experiments Thompson et al., 2020

$$D_{LL} \propto L^8 10^{aL+bKp^2+cKp}$$ Ozeke et al., 2014

$$D_{LL} \propto L^n, n = 8$$

- Diffusion equation

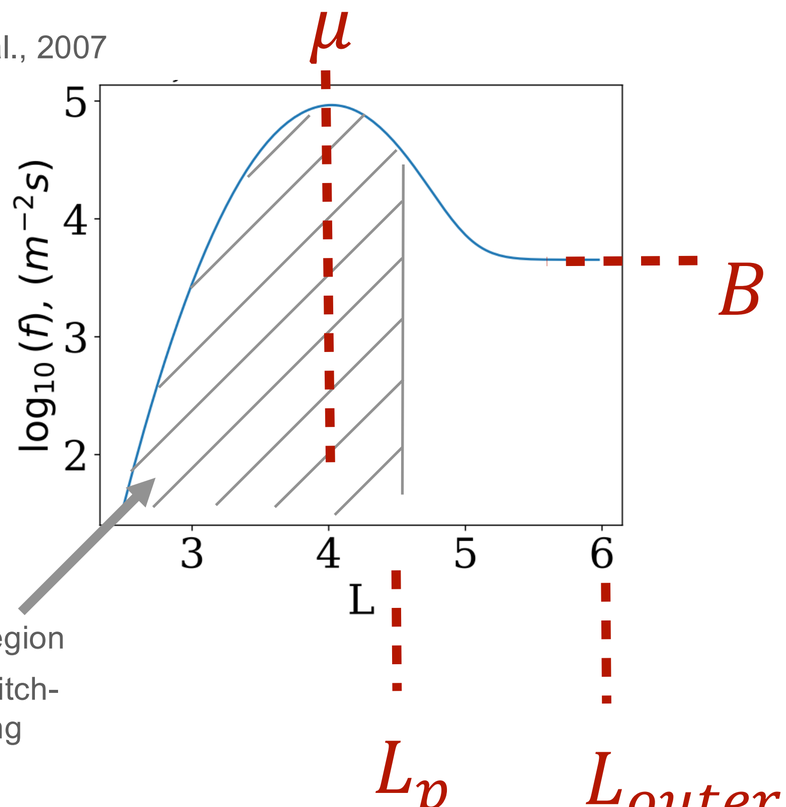
$$\frac{\partial f}{\partial t} = L^2 \left(\frac{D_{LL}}{L^2} \frac{\partial f}{\partial L} \right) - \mathcal{L} f$$

$$\mathcal{L} = \begin{cases} \frac{1}{\tau}, & \text{if } L \leq L_p \\ 0, & \text{otherwise} \end{cases}$$

Loss via pitch angle scattering
Electron timescale τ from Shprits et al., 2007

$L \sim$ "Distance" of drift orbit, $D_{LL} \sim$ Diffusion coefficient (effects of electromagnetic perturbations)

D_{LL} determines the amount of radial diffusion, and depends on L



- Initial phase space density (PSD) distributions f: background particles and an enhancement

Loss $\frac{1}{\tau} f$ in this region to approximate pitch-angle scattering

Bentley et al. 2024, Physics of Plasmas

Numerical Experiment setup

Thompson et al., 2020

- Diffusion equation

  (We run with, and without loss)

$$\frac{\partial f}{\partial t} = L^2 \left(\frac{D_{LL}}{L^2} \frac{\partial f}{\partial L} \right) - \mathcal{L} f$$

$L \sim$ "Distance" of drift orbit, $D_{LL} \sim$ Diffusion coefficient (effects of electromagnetic perturbations)

$$\mathcal{L} = \begin{cases} \frac{1}{\tau}, & \text{if } L \leq L_p \\ 0, & \text{otherwise} \end{cases}$$

Loss via pitch angle scattering
Electron timescale τ from Shprits et al., 2007

- Diffusion coefficients

$$(1) \quad D_{LL} = D_{LL}^B + D_{LL}^E$$

$$(2) \quad D_{LL} = D_0 L^n, n = 6$$

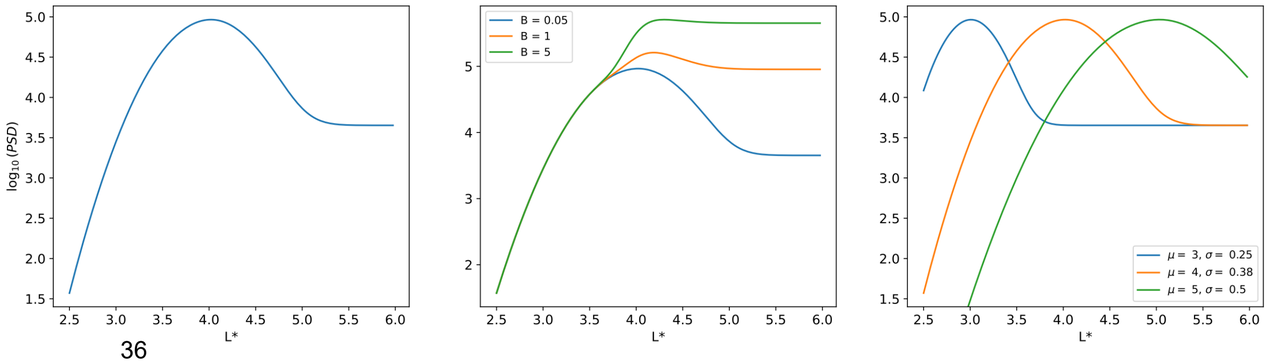
$$D_{LL}^E = 2.16 \times 10^{-8} L^6 10^{0.217L + 0.461Kp}$$

$$D_{LL}^B = 6.62 \times 10^{-13} L^8 10^{-0.0327L - 0.108K^2 p + 0.499Kp}$$

Diffusion coefficient parameterisation from Ozeke et al., 2014

- Initial phase space density (PSD) distributions: background particles and an enhancement

$$f = A \exp\left(-\frac{(L-\mu)^2}{2\sigma^2} \right) + \frac{1}{2} AB \left[erf(\gamma(L-\mu)) + 1 \right]$$



Bentley et al. 2024, Physics of Plasmas