Modeling the Terrestrial Ionosphere

Part I: motivations, basic considerations, and example applications

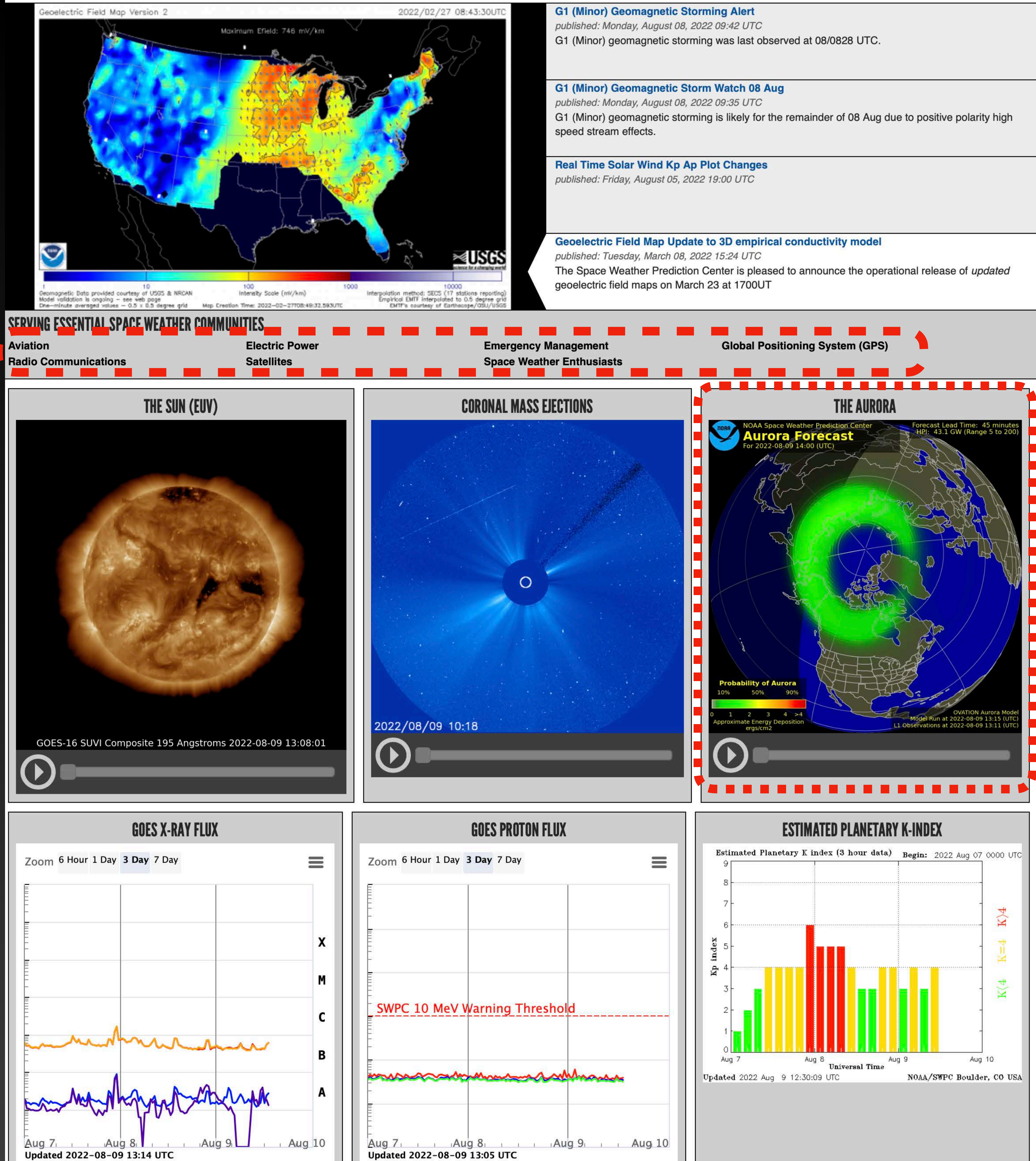
M. Zettergren 08/10/2022

Why?

...do we need modeling tools...

- Allow us to build fundamental physical understanding of the ionospheric systems including *how different parts (subsystems?) interact* — even in complicated "configurations".
- *Provide predictive capabilities* that can be operationally or scientifically useful
- Facilitate hypothetical and theoretical investigations into *nature of different elemental physics*.
- Provide context for interpretation of sparse data, e.g. what candidate processes could potentially lead to what is observed in dataset A or B.

https://www.swpc.noaa.gov

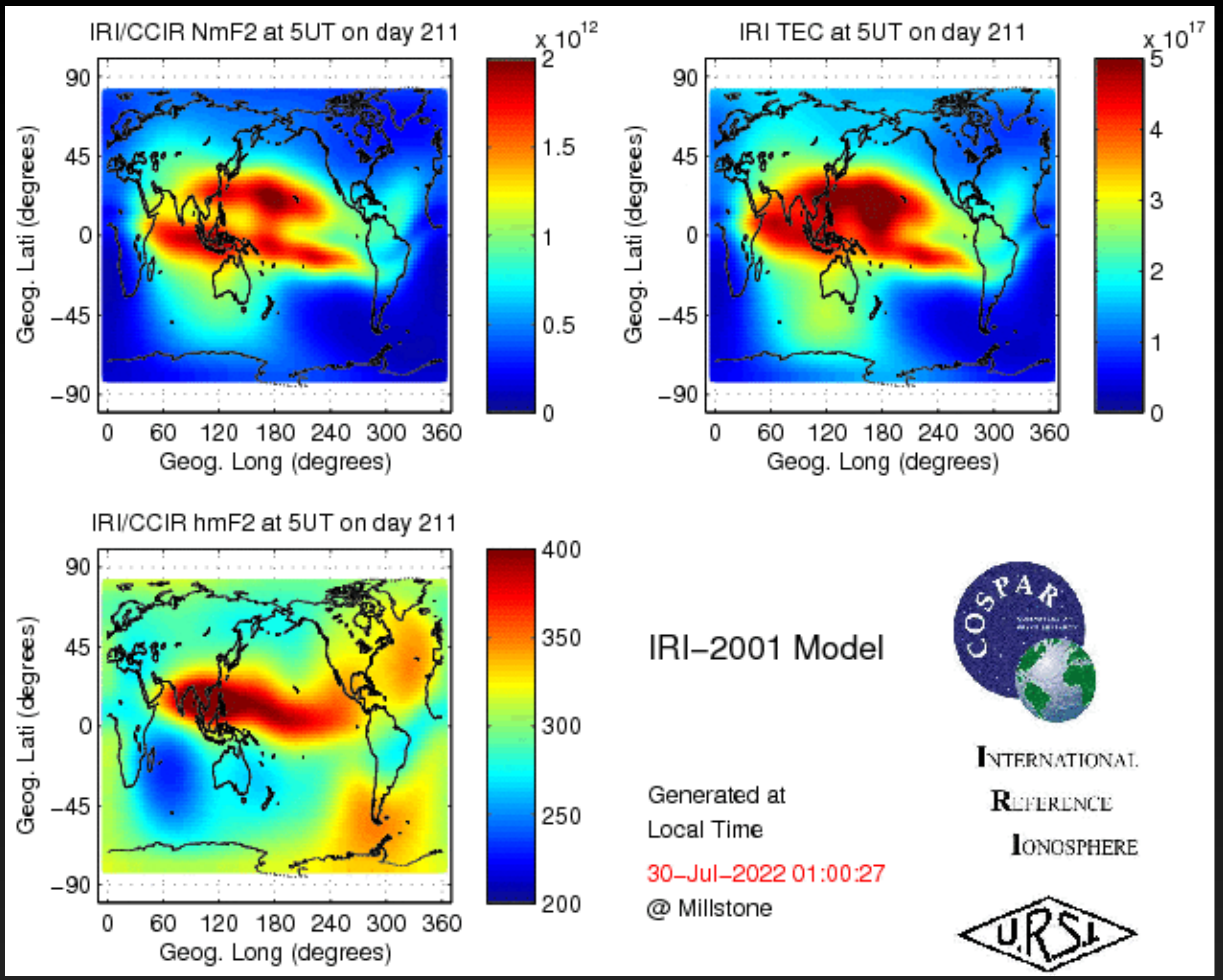


Basic Model Types

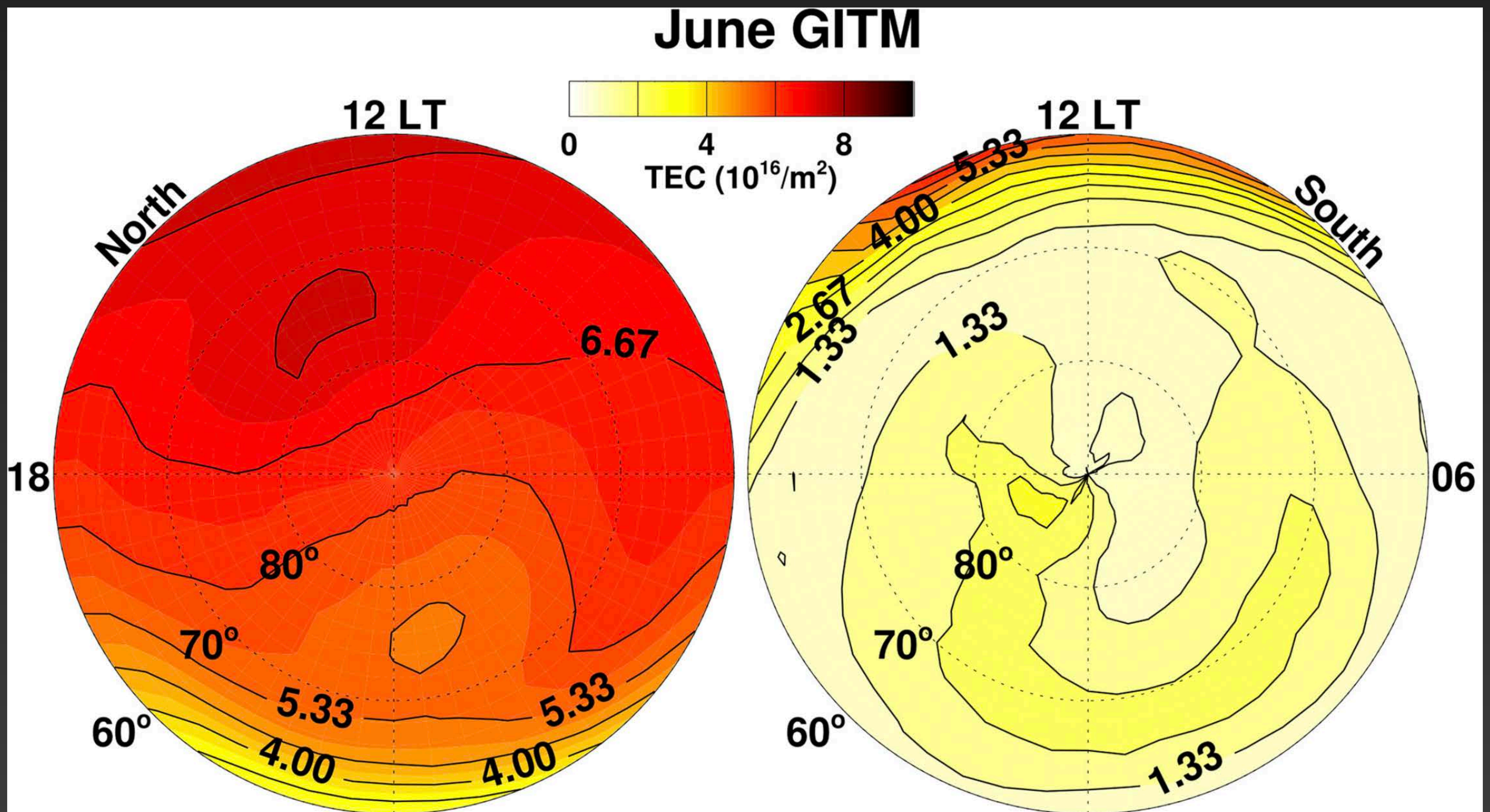
Empirical v. Physics-based approaches

- *Empirical models* are based on large datasets and characterize (generally) average behavior of the ionosphere or thermosphere.
- *Physics-based models* solve a set of equations based on some mathematical model or set of physical principles

https://irimodel.org



https://doi.org/10.1002/2017JA024411



Widely Used Empirical Models

Community Coordinated Modeling Center is an important resource

https://ccmc.gsfc.nasa.gov

- International Reference Ionosphere: IRI, https://irimodel.org, https://ccmc.gsfc.nasa.gov/modelweb/models/iri2016_vitmo.php
  - Mid- and low-latitude ionospheric climatology and background state
  - ~100-500 km
- Mass Spectrometer and Incoherent Scatter Atmosphere model: MSIS, https://kauai.ccmc.gsfc.nasa.gov/instantrun/msis
  - Thermosphere climatology and background states
  - Ground to exobase
- Horizontal Wind Model, HWM14, https://kauai.ccmc.gsfc.nasa.gov/instantrun/hwm
  - Neutral atmospheric winds, geographic horizontal components
  - Ground to exobase
- Weimer convection model - ionospheric potential, https://ccmc.gsfc.nasa.gov/cgi-bin/run_weimer.cgi
- Ovation Prime precipitation model - energetic electron precipitation, https://ccmc.gsfc.nasa.gov/requests/IT/user_registration_stat.php?model=OvationPrime

Example of basic procedures for empirical models

Voluminous data source

Binning and averaging according to space/time

Fitting to some set of basis functions yields expansion coeficients

Evaluation of basis at some new "coordinates" to "model" ionosphere

Widely Used Physics-Based Models

CCMC and GitHub are useful!

- Numerous bespoke codes that are used for specific problems/studies
- *There is no "master model" that can address all aspect of ionospheric science*!
- Global ionosphere-thermosphere model
  - GITM - https://github.com/aaronjridley/GITM
  - TIEGCM - https://www.hao.ucar.edu/modeling/tgcm/
  - WAM-IPE - https://www.swpc.noaa.gov/products/wam-ipe
- Local Scale ionospheric models
  - GEMINI - https://github.com/gemini3d/

Example of basic procedures for physics-based models

1. Mathematical model of system
2. Discretization, meshing, and assumptions
3. Numerical solutions for equations
4. Visualization of results

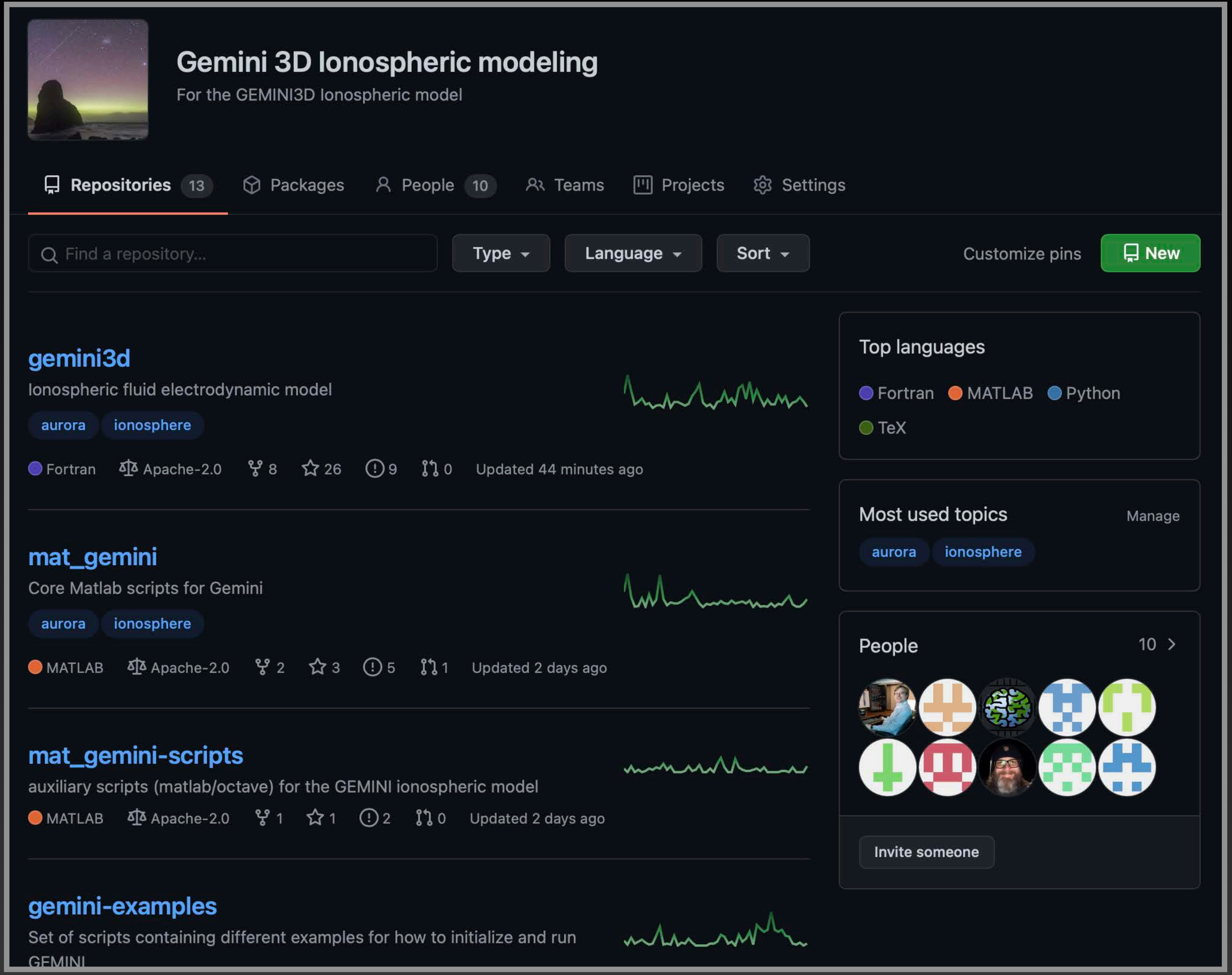
Example Uses of Ionospheric Models

Strongly biased toward my own research and experiences, of course :)

These illustrate modeling used:
- for theory
- to interpret data
- for mission design

These represent my research anyone involved in ionospheric model design will have similar slate of examples!

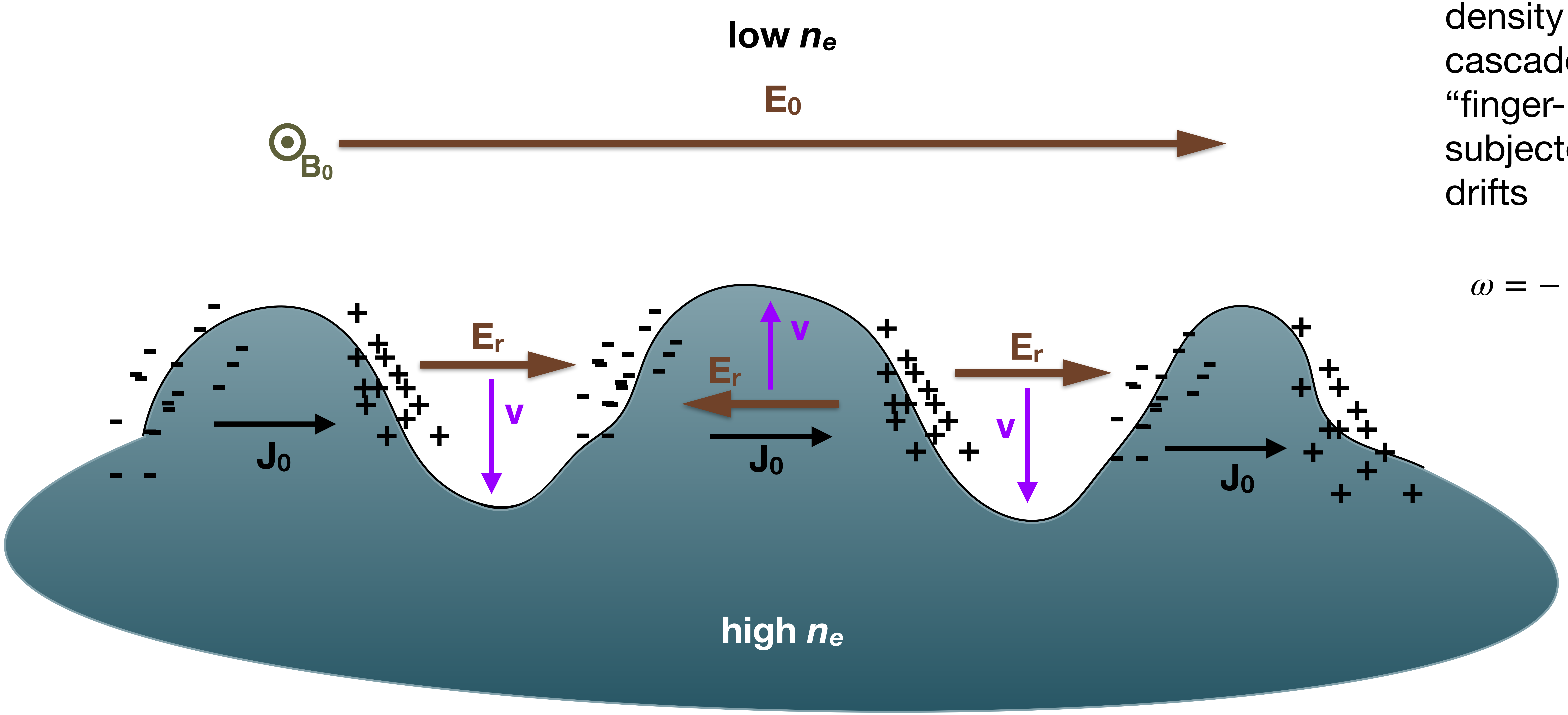
Our physics-based, open-source ionospheric model: GEMINI



Examples Part I: “Modeling for Theory”

Drift Instabilities Linear and Nonlinear Instability

gradient drift instability (GDI)



Strong F-region ionospheric density gradients can cascade into smaller-scale “finger-like” structures when subjected to background drifts

$$\omega = -\frac{1}{2}i\tilde{\nu} \pm \frac{1}{2}i\sqrt{\tilde{\nu}^2 + 4\tilde{\nu}\frac{E_0}{\ell B}};$$

$$\tilde{\nu} \equiv \frac{\Sigma_P}{C_M}$$

What Physical Processes Matter?

Scales based on basic dimensional analyses, E.g.

$$\frac{J_{displacement}}{J_{conduct}} \approx \left(\frac{\sigma}{\epsilon_0 \omega}\right)^{-1}$$

Pedersen drifts (scale independent)

Inertial effects (~1-4 km)

Potential mapping (~100-1000 m)

Diffusive drifts (~100-300 m)

Diamagnetic drifts (~50-300 m)

Scale sizes perp-to-B for physics to start to matter (e.g. Farley, 1959; Kintner and Seyler, 1985)

Time variability effects on polarization charge

$$\frac{J_{pol}}{J_{conduct}} \approx \frac{\omega}{\tilde{\nu}} = 1 \quad \text{when} \quad \tau \approx \frac{2\pi}{\tilde{\nu}} \approx 15 \text{ s}$$

Shearing effects on polarization current

$$\frac{J_{pol}}{J_{conduct}} \approx \frac{kv}{\tilde{\nu}} = 1 \quad \text{when} \quad \lambda = \frac{2\pi v}{\tilde{\nu}} \approx 3.5 \text{ km}$$

Pressure effects (diamagnetic/diffusive)

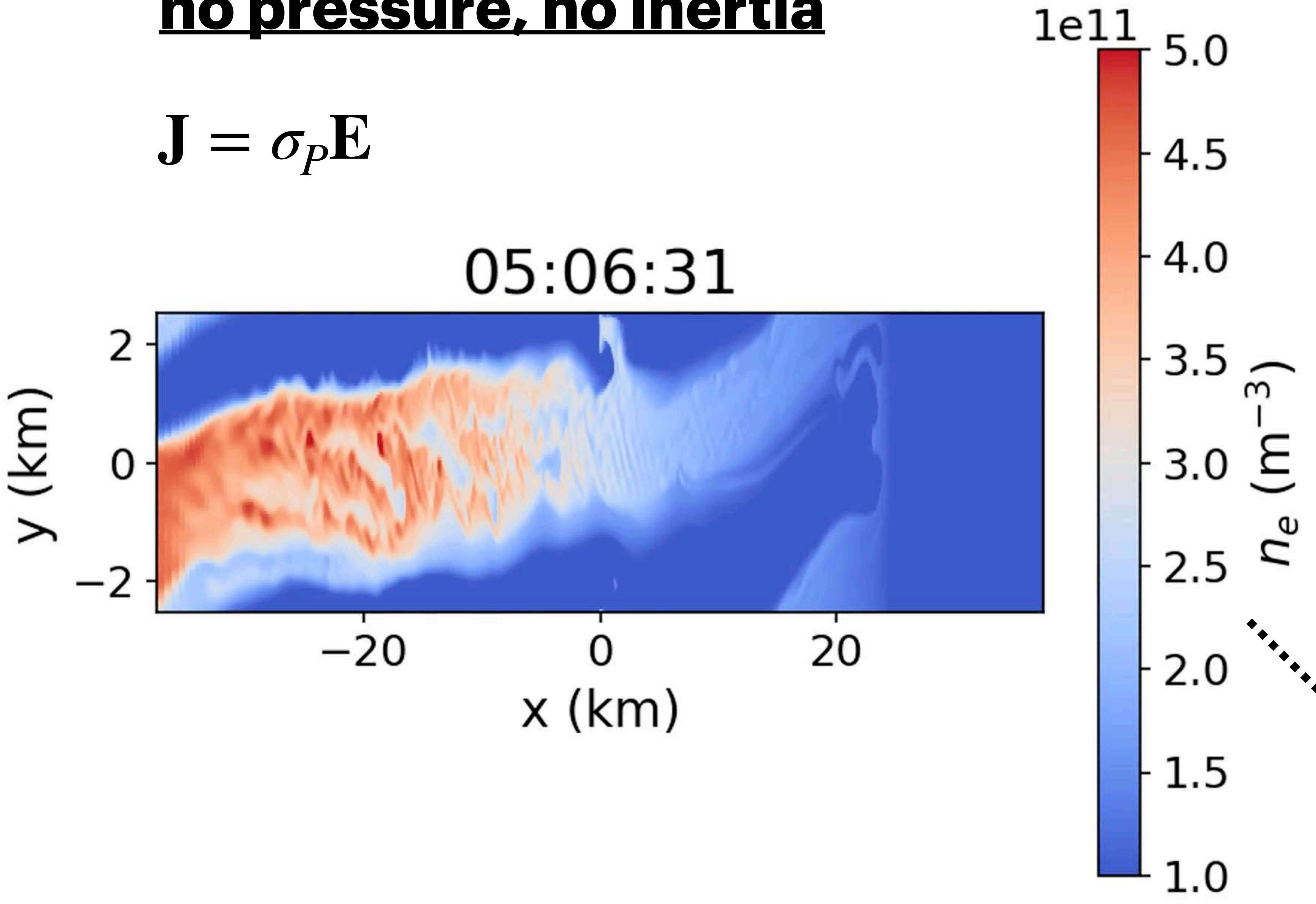
$$\frac{J_{pressure}}{J_{conduct}} \approx k\frac{k_B}{q}\frac{T}{E} = 1 \quad \text{when} \quad \lambda = 2\pi\frac{k_B}{q}\frac{T}{E} \approx 100 \text{ m}$$

Electric field mapping

$$\frac{\lambda_{\parallel}}{\lambda_{\perp}} \approx \sqrt{\frac{\sigma_{\parallel}}{\sigma_{\perp}}} = 1 \quad (\text{alt. dep.})$$

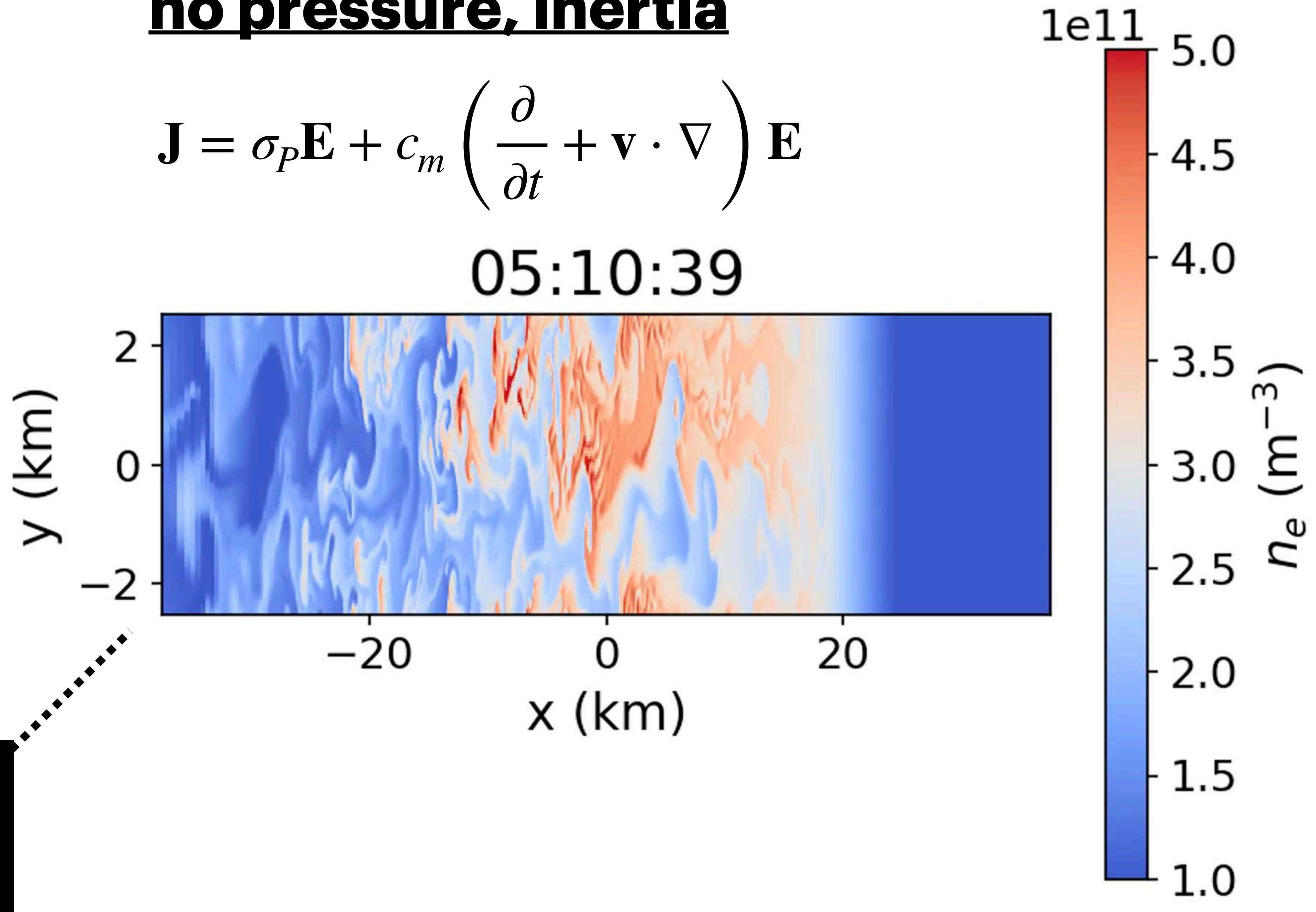
no pressure, no inertia

$$\mathbf{J} = \sigma_P \mathbf{E}$$



no pressure, inertia

$$\mathbf{J} = \sigma_P \mathbf{E} + c_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{E}$$



$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0$$

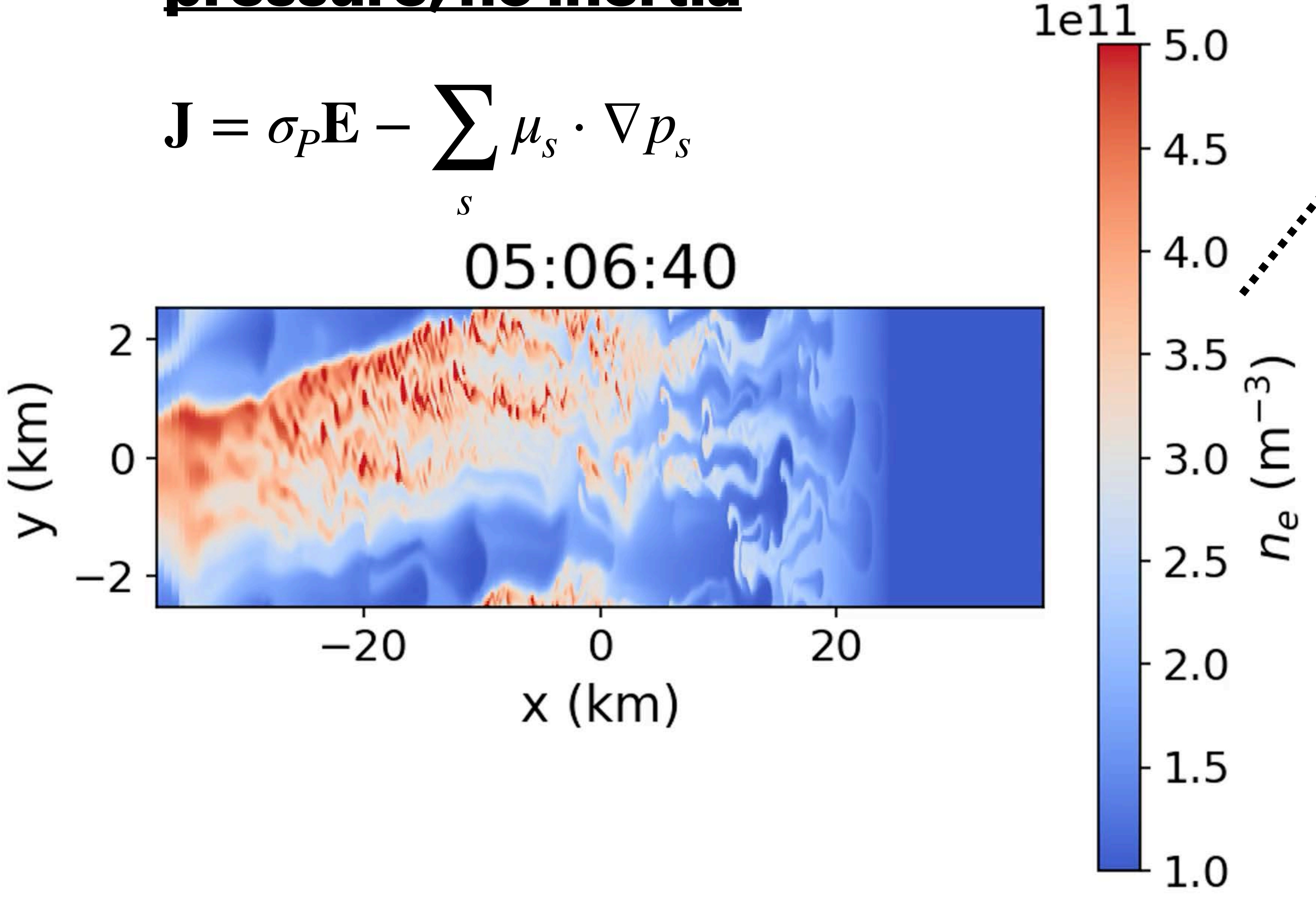
$$\nabla \cdot \mathbf{J} = 0$$

$$\mathbf{v} \approx \frac{\mathbf{E} \times \mathbf{B}}{B^2}$$

$$\mathbf{E} = -\nabla \Phi$$

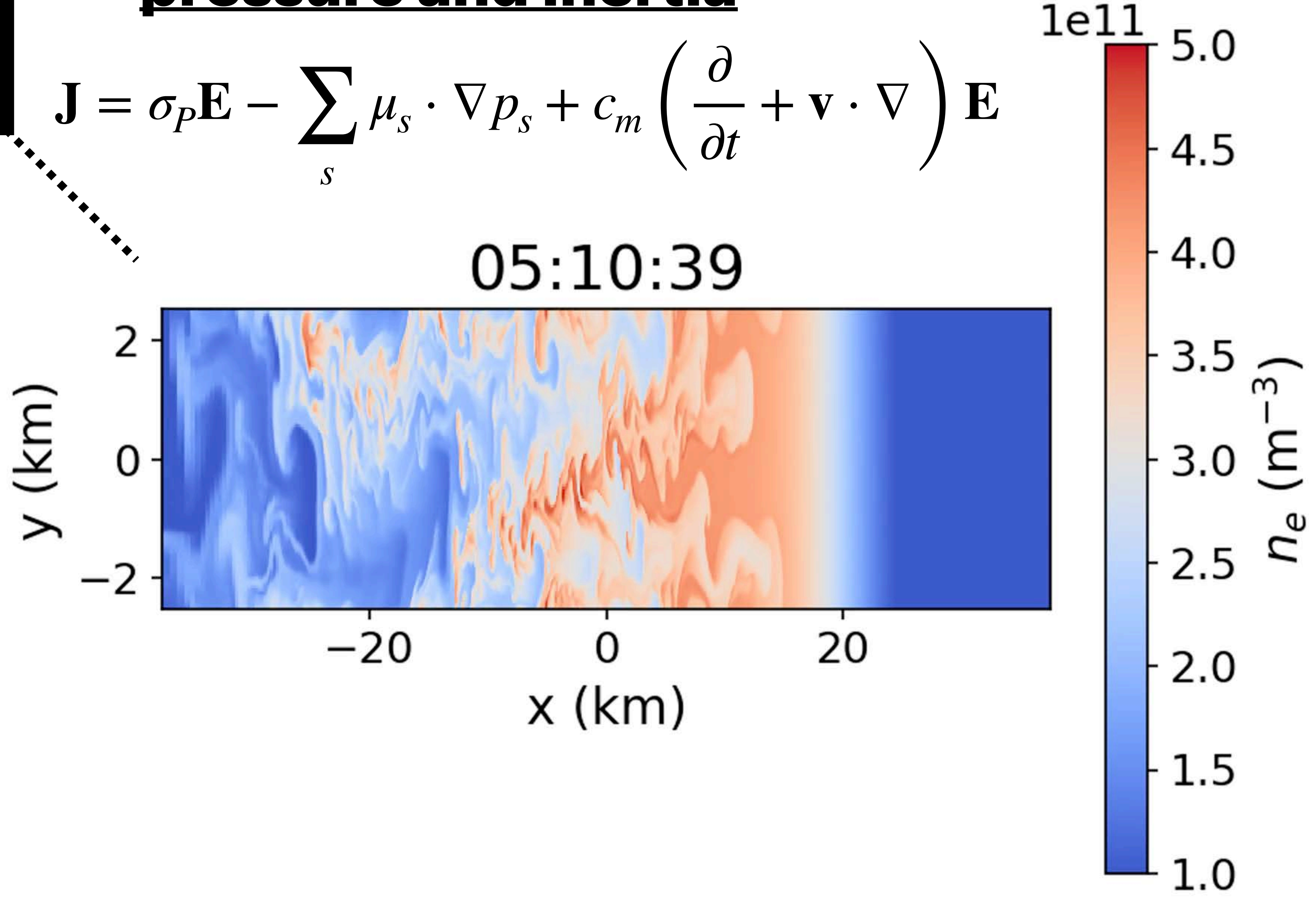
pressure, no inertia

$$\mathbf{J} = \sigma_P \mathbf{E} - \sum_s \mu_s \cdot \nabla p_s$$



pressure and inertia

$$\mathbf{J} = \sigma_P \mathbf{E} - \sum_s \mu_s \cdot \nabla p_s + c_m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{E}$$



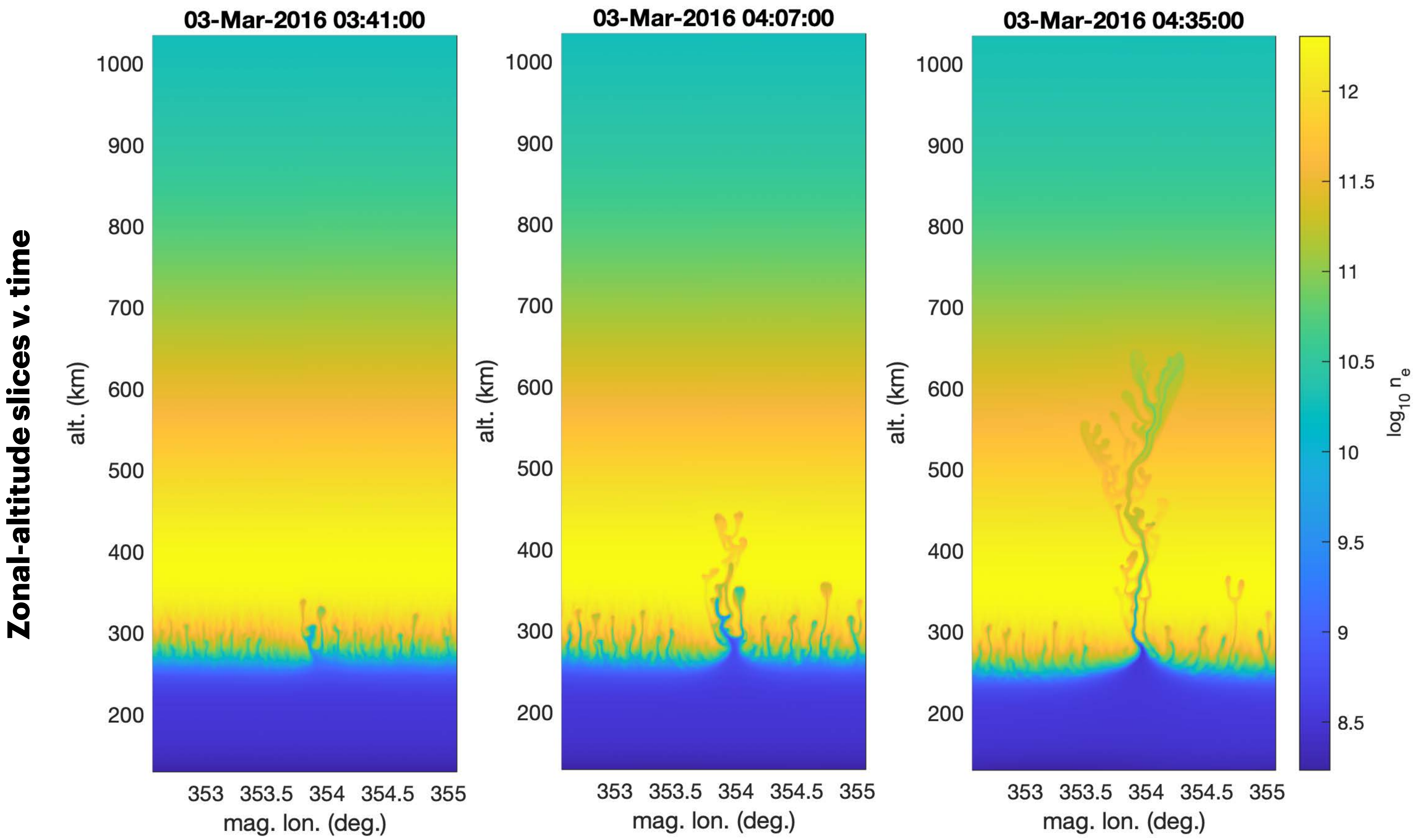
Rayleigh-Taylor Instability: Plasma Bubbles

Non-local Rayleigh-Taylor growth rate from Sultan (1996)

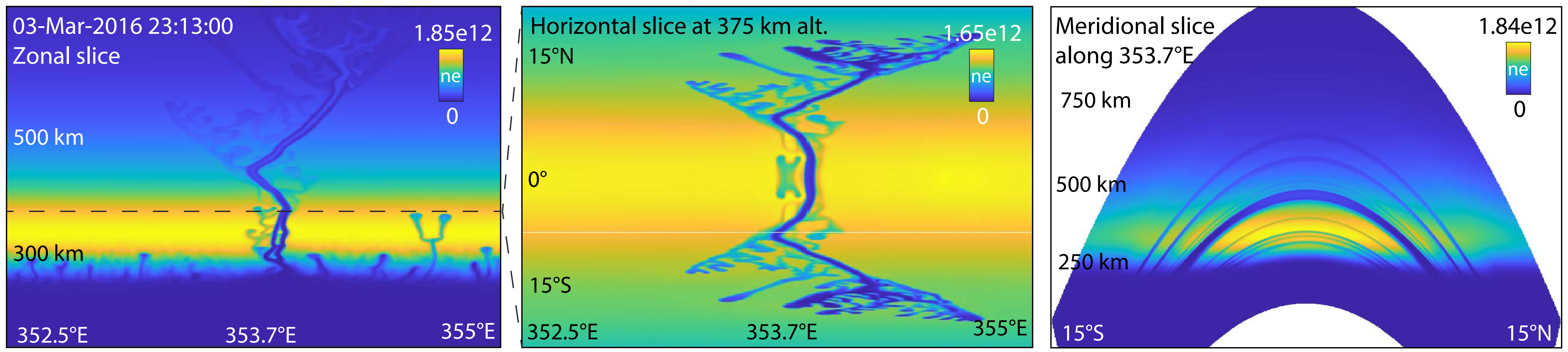
$$\gamma_{RT} = \frac{\tilde{\Sigma}^F_{P,0}}{\tilde{\Sigma}^E_{P,0} + \tilde{\Sigma}^F_{P,0}} \left(V_p - U^P_L - \frac{g_e}{\nu^F_{eff}} \right) K^F - R_T$$

Modeling Plasma Bubbles with GEMINI

- As a basic demo, GEMINI was run at ~1km resolution with noise-like seeding, no AGWs, and a jump-like variation in conductance (neutral atmosphere) across the middle of the simulation to mimic "stationary" forcing.
- Bifurcation, branching, and merging of bubble structures is far more apparent at finer scales- this is known but should be more carefully in the context of wave forcing which contains a spectrum of scales.



3D snapshot of bubble structure(s) late in simulation



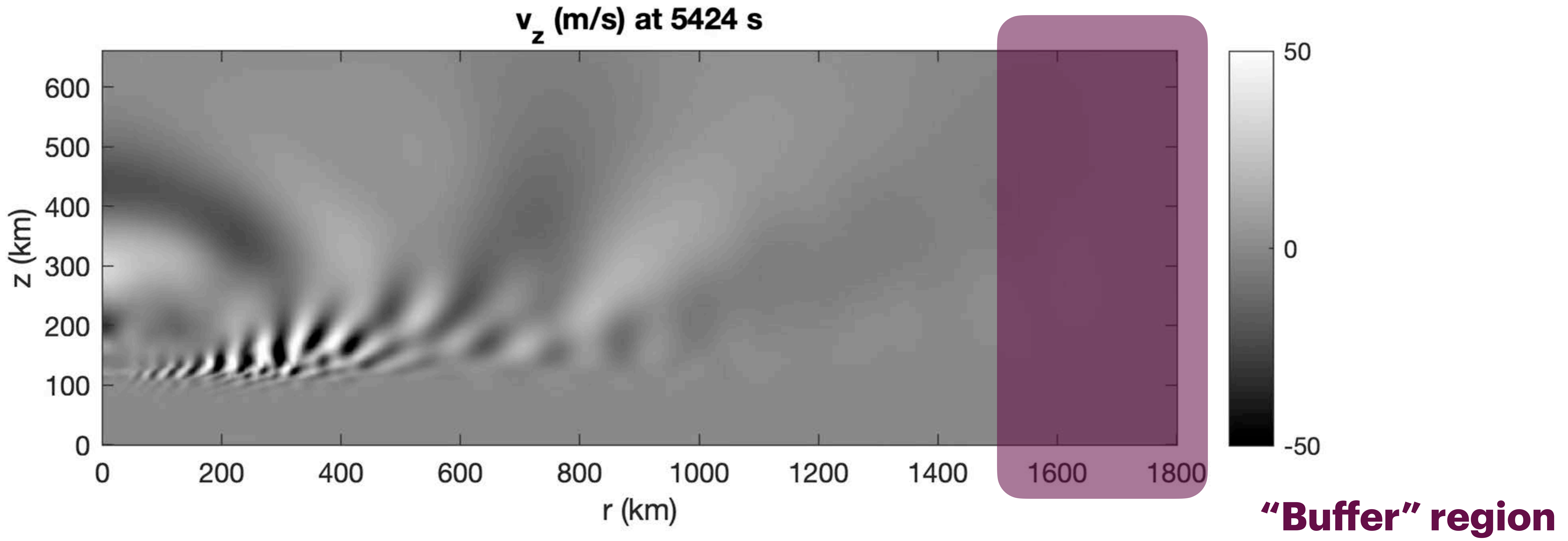
Hypothetical Study of Plasma Bubbles from Atmospheric Forcing

$$\rho A \sim \frac{\delta}{\delta t}\left(\rho \mathbf{v}\right) \cdot \hat{\mathbf{e}}_z = \rho A_0 e^{-\frac{(r-r_0)^2}{2\sigma_r^2}-\frac{(z-z_0)^2}{2\sigma_z^2}-\frac{(t-t_0)^2}{2\sigma_t^2}}$$

Horizontal width: $\sigma_r = 5$ km
Vertical width: $\sigma_z = 3$ km
Time "width": $\sigma_t = 60$ s

Vertical location: $z_0 = 12$ km
Time "location": $t_0 = 300$ s
Ref. Amplitude: $A_0 = 0.075$ m/s^2

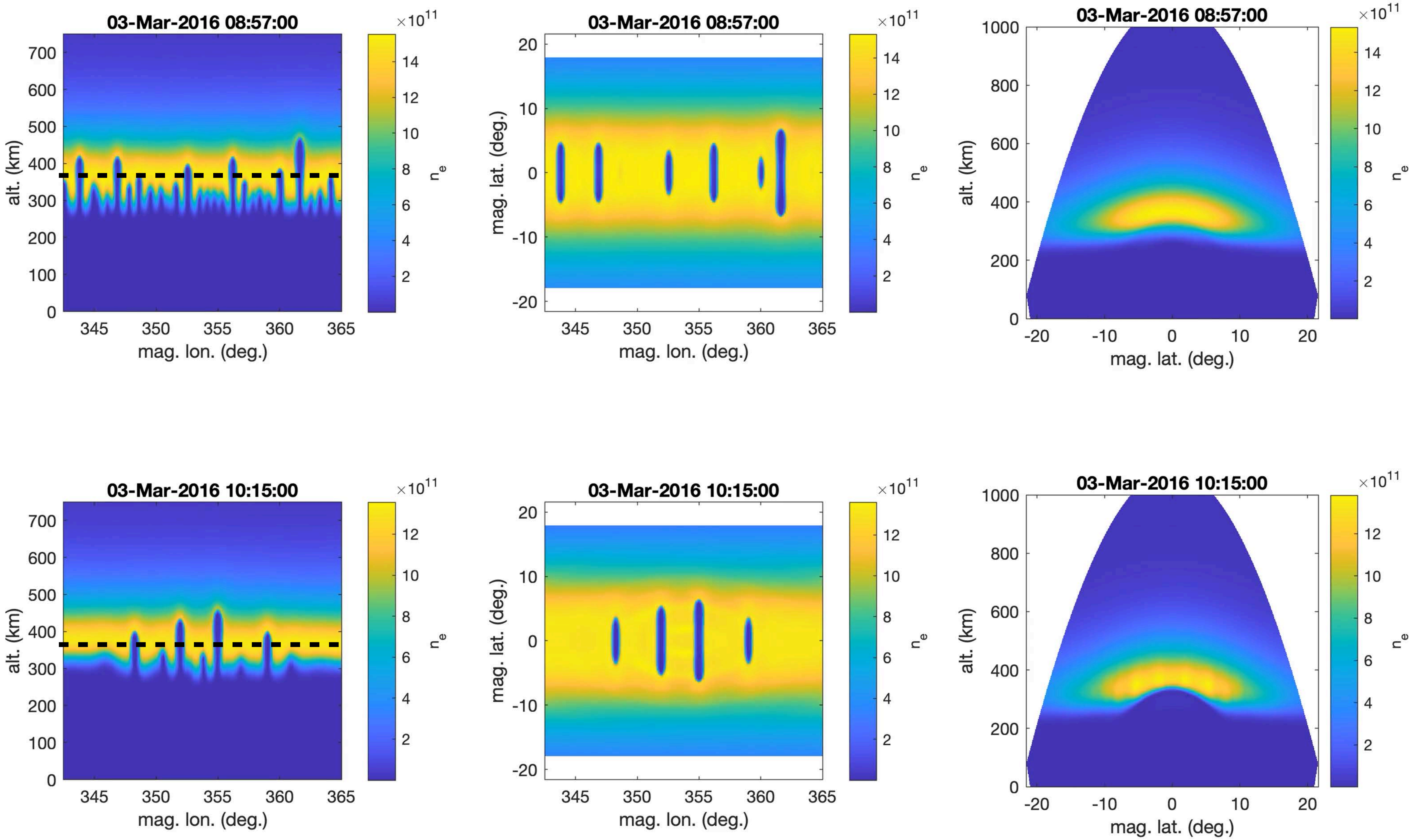
Body force applied near tropopause in MAGIC momentum equation. "Broadband" source used — represents convective uplift.



Plasma Bubble Seeding by Atmospheric Waves

- Comparisons of GEMINI simulations of unstable nighttime equatorial plasma seeded by:
  - Broadband Noise
  - Convectively generated atmospheric gravity waves
- Noise-like perturbations result in fast growth of bottom side instabilities; resolution here is likely insufficient to get details of bubbles correct.
- Waves are a source of band-limited fluctuations and manifest in seeding at longer wavelengths and nearer to convective source.
- *Implies that seeding sources can be in some way related to bubble structures.*

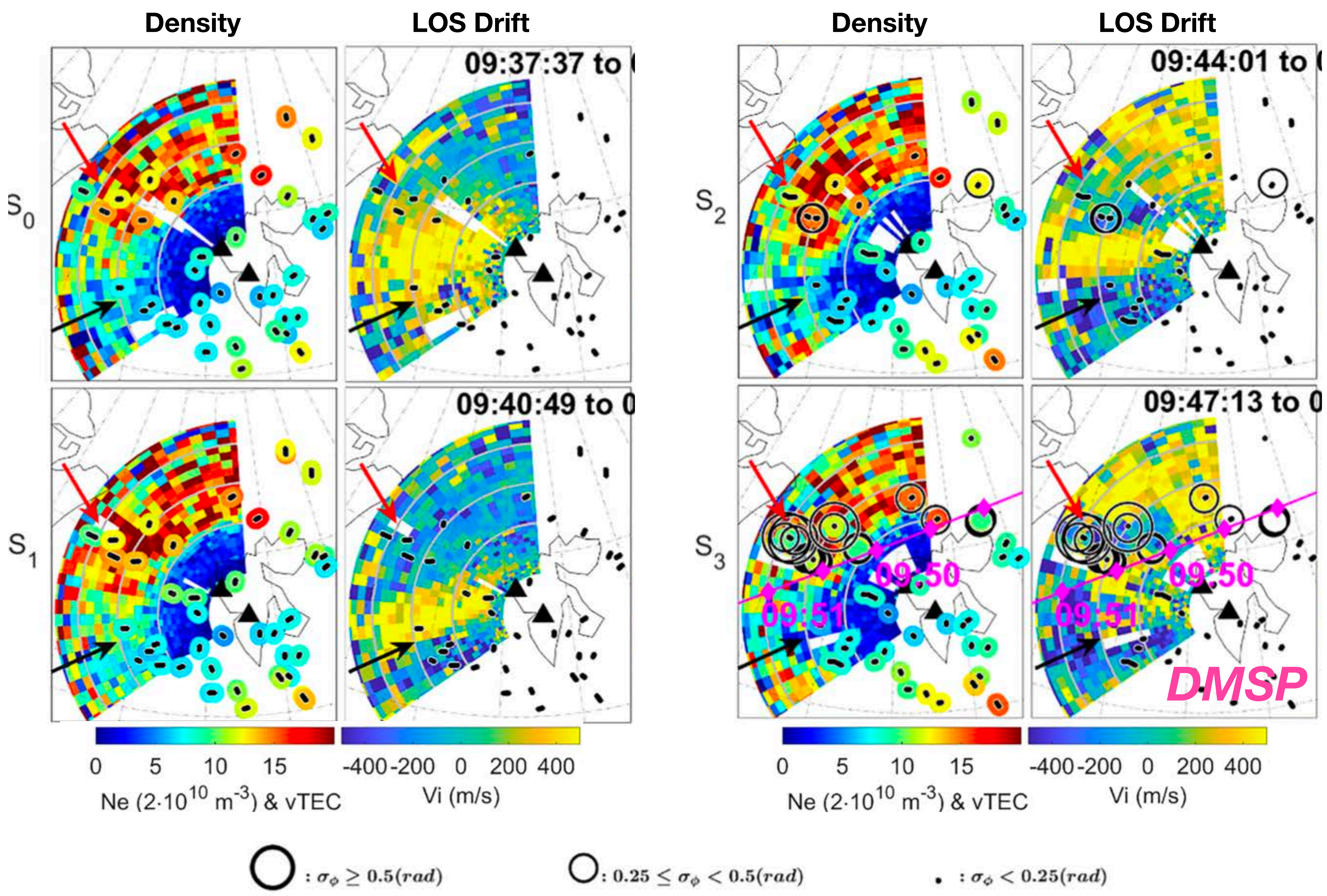
Noise-seeded simulation



Double amplitude, equatorial location simulation

Examples Part II: Modeling to help interpret data

Ionospheric Cusps: Dynamics of Narrow Flow Channels

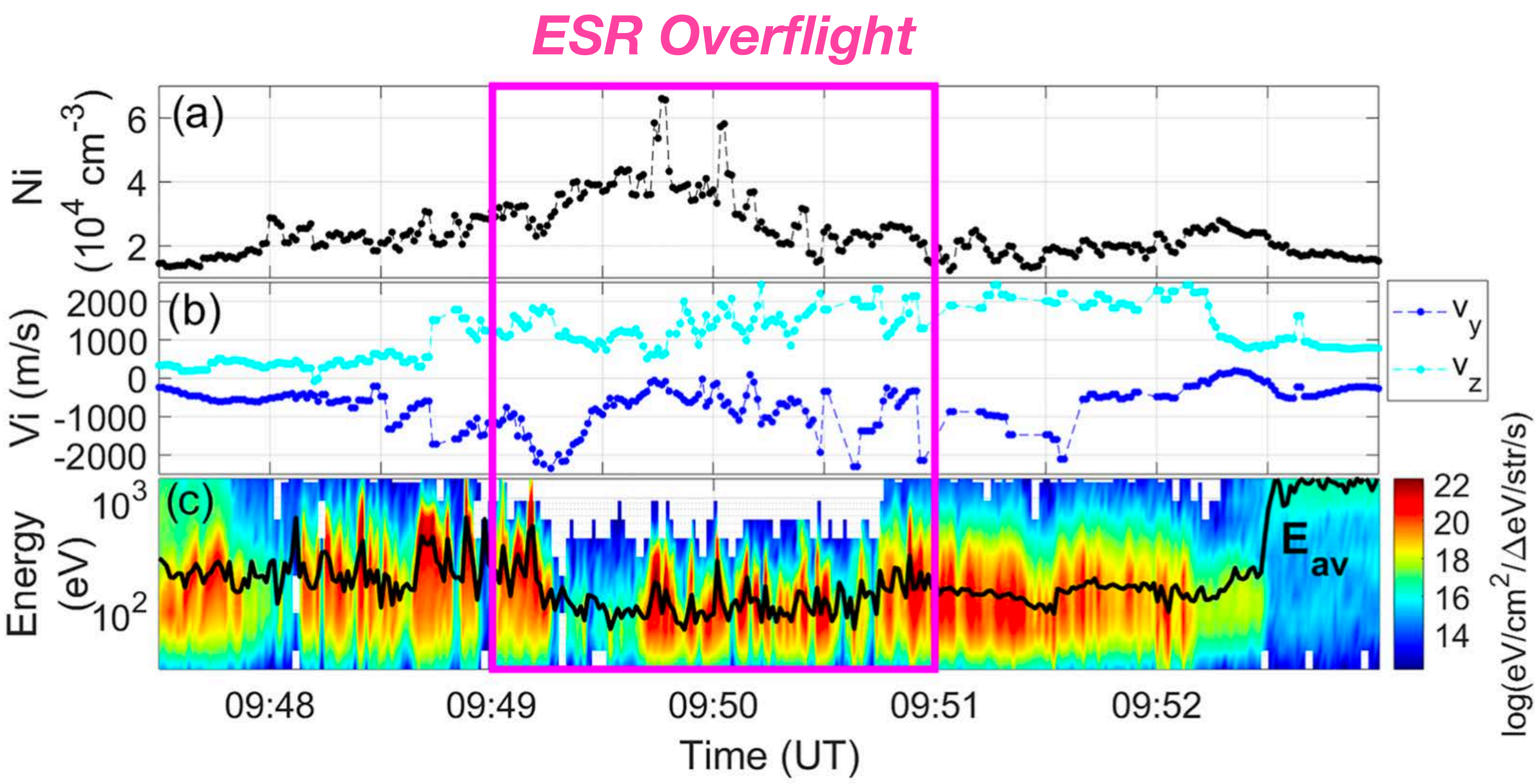


Spicher et al (2020)

Four successive ESR azimuthal scans covering 15 mins. show:

- *narrow flow channels*
- *northward movement of channels and*
- *associated scintillation in or on the edge of flow channels (L-band)*

Ionospheric Cusps: DMSP Observations



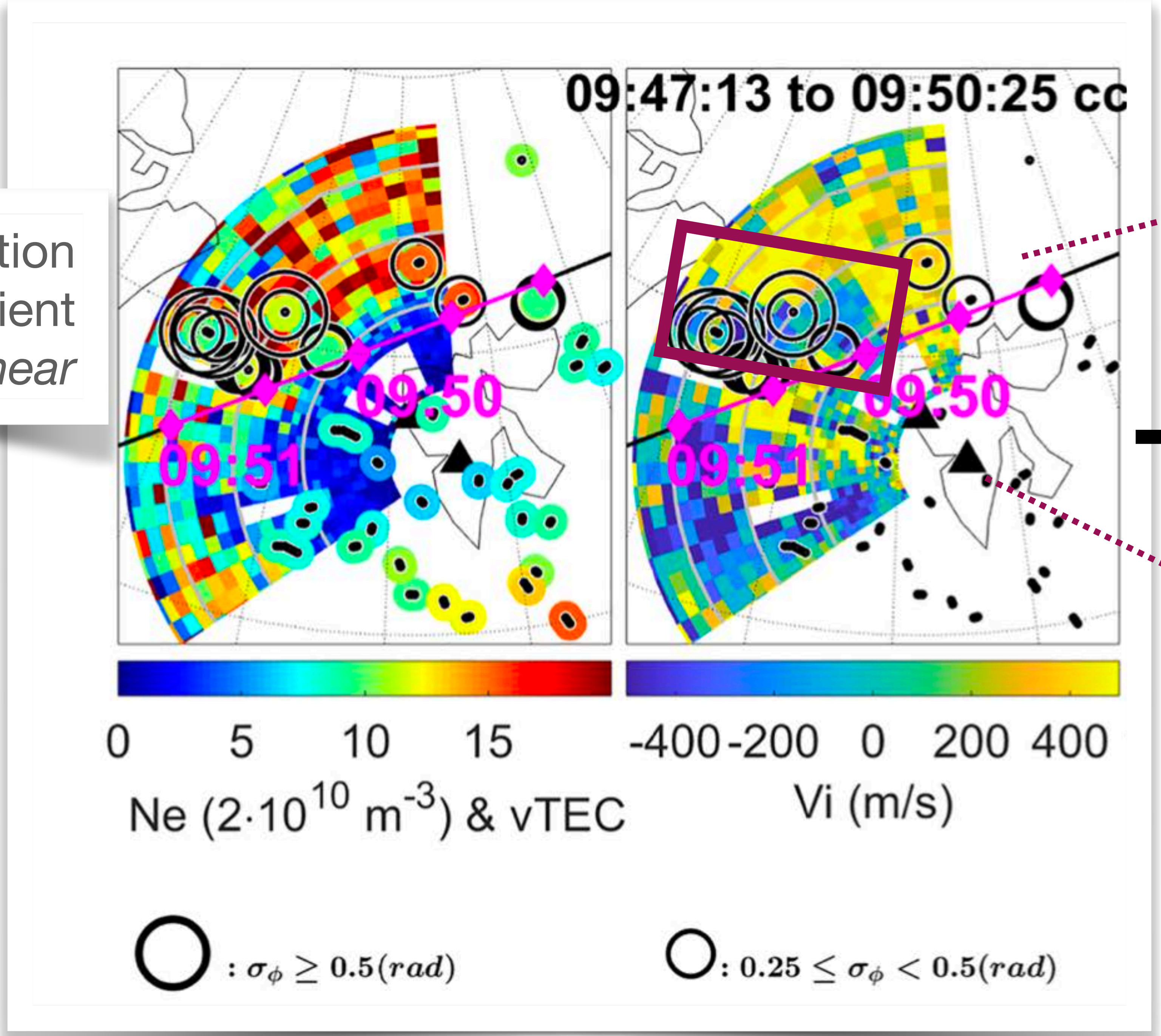
Spicher et al (2020)

DMSP thermal plasma data shows:

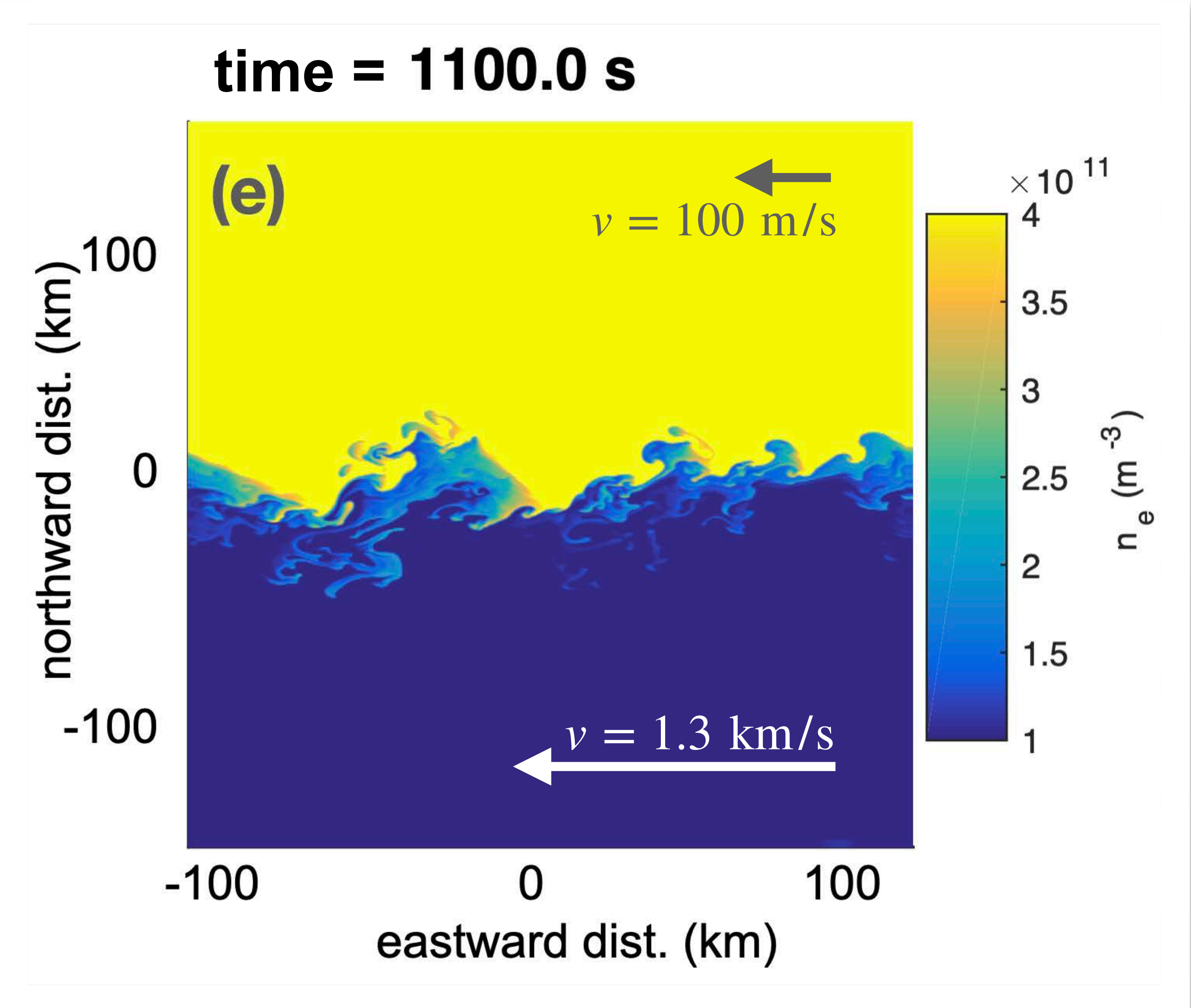
- *strong variations in cross track velocity during overpass.*
- *Also coincident are instances of soft electron precipitation*

Ionospheric Cusp: GEMINI Modeling

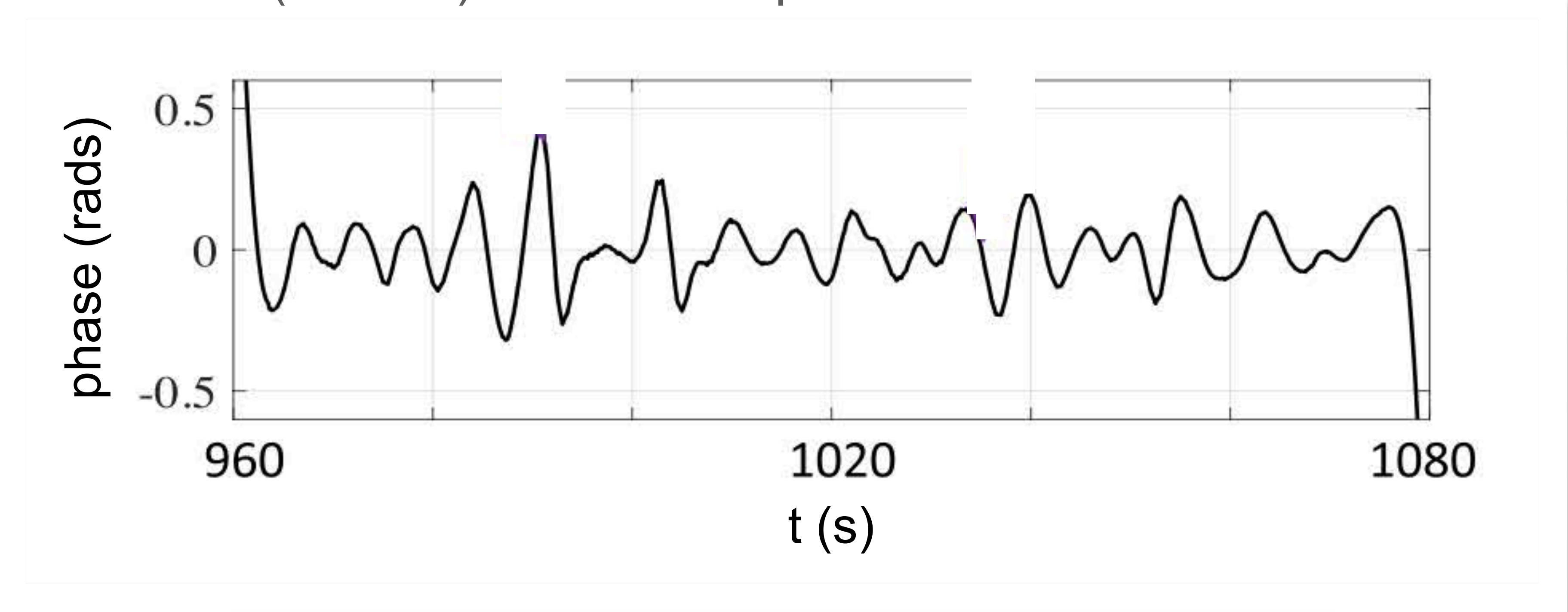
Strong scintillation near density gradient and *plasma flow shear*



Simulation initialized with velocity and density consistent with ESR/DMSP; *energetic electrons not included*



Irregularities fed into radio propagation model (SIGMA) to simulate phase variations

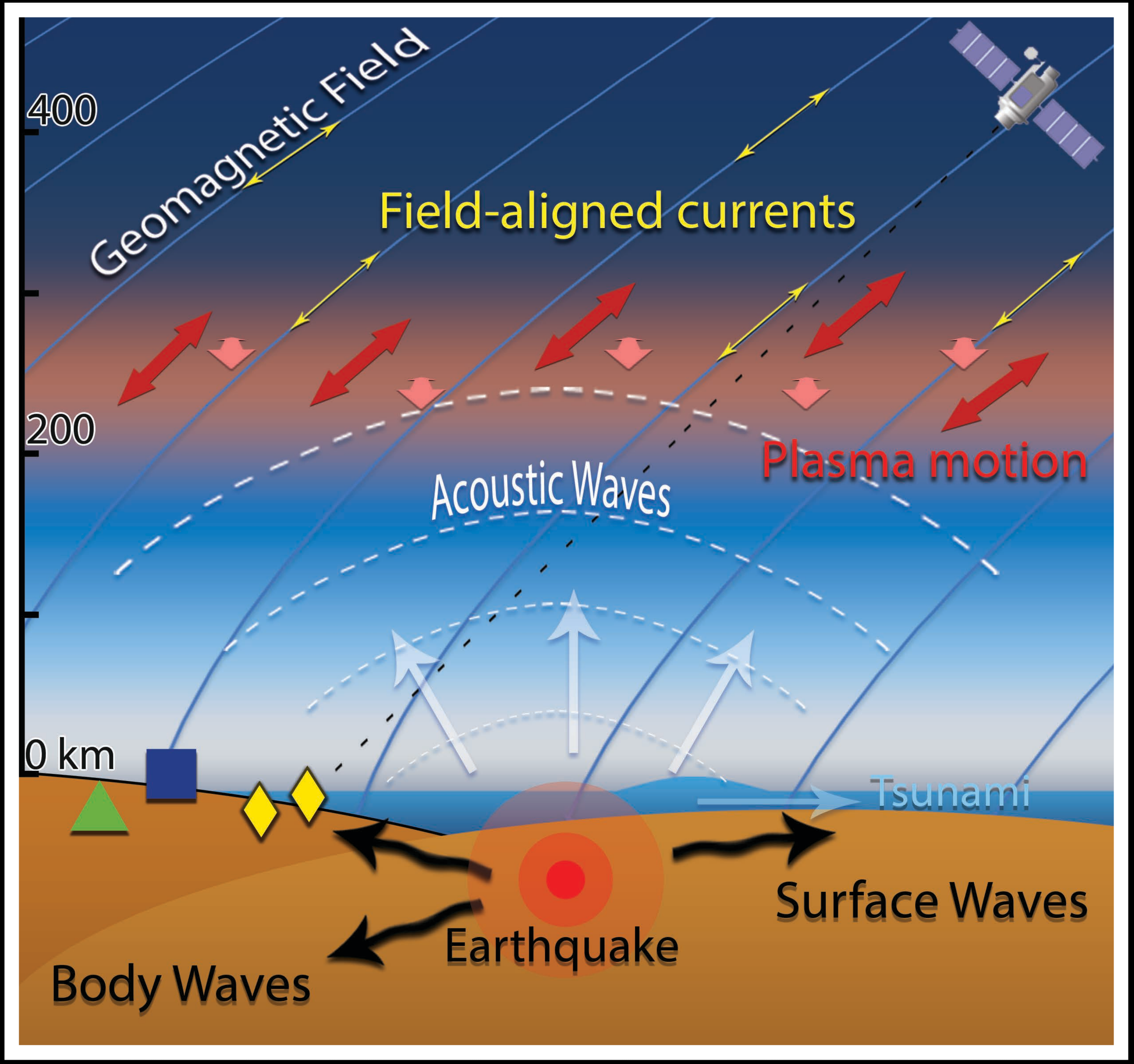


Spicher et al (2020)

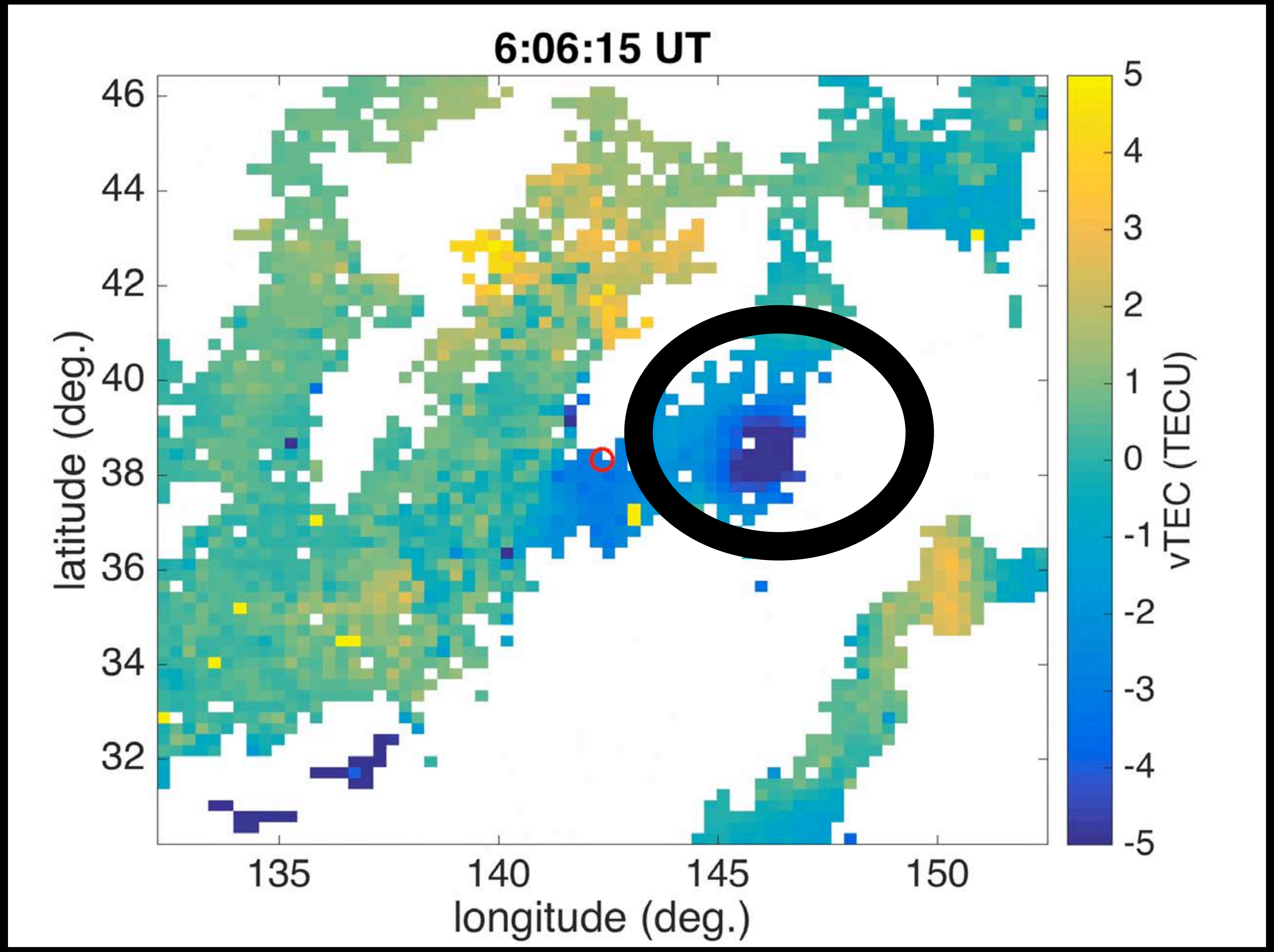
- Coincident **DMSP** and ESR and phase scintillation measurements used to explore consequences of flow structures at multiple scales
- These conditions can be used for parametric initialization of simulations in GEMINI — allows us to study notional cascade

Wave Processes Associated with Submarine Earthquakes

- **Ocean surface displacement leads to several important effects:**
  - Tsunami formation and propagation
  - Atmospheric acoustic and gravity wave (AGW) radiation and propagation
- **Large-amplitude atmospheric infrasound impacts in space:**
  - Ionospheric density and TEC perturbations
  - Dynamo currents and magnetic field perturbations
  - *We seek to develop, via simulation, a better understanding of regional structure TEC and magnetic field response*

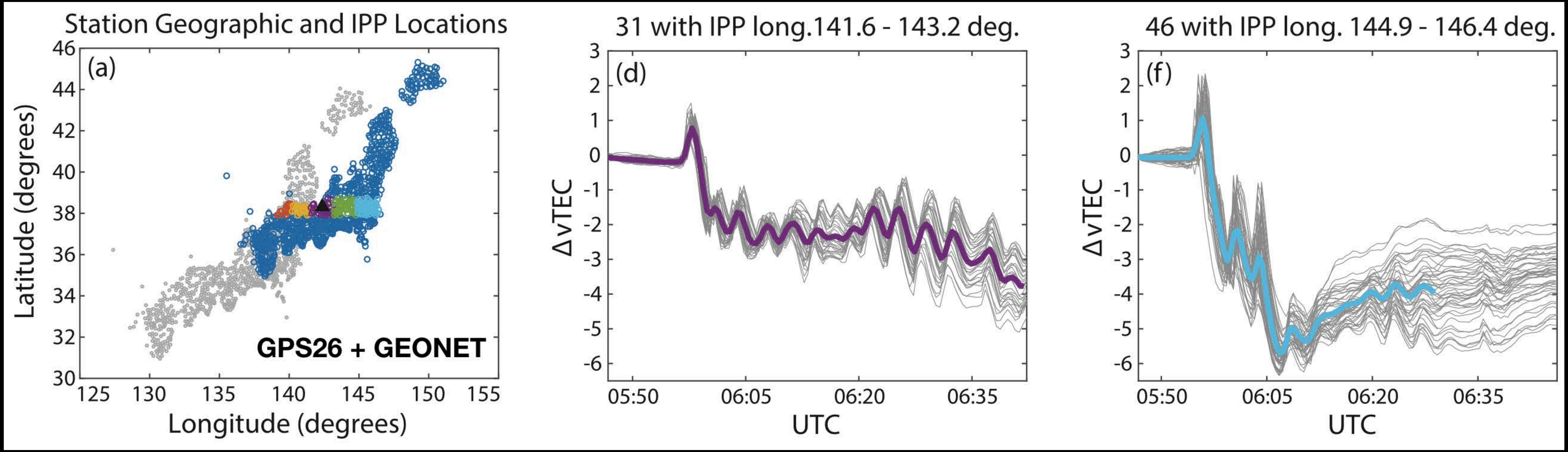


2011 Tohoku Mapped Vertical Total Electron Content Data

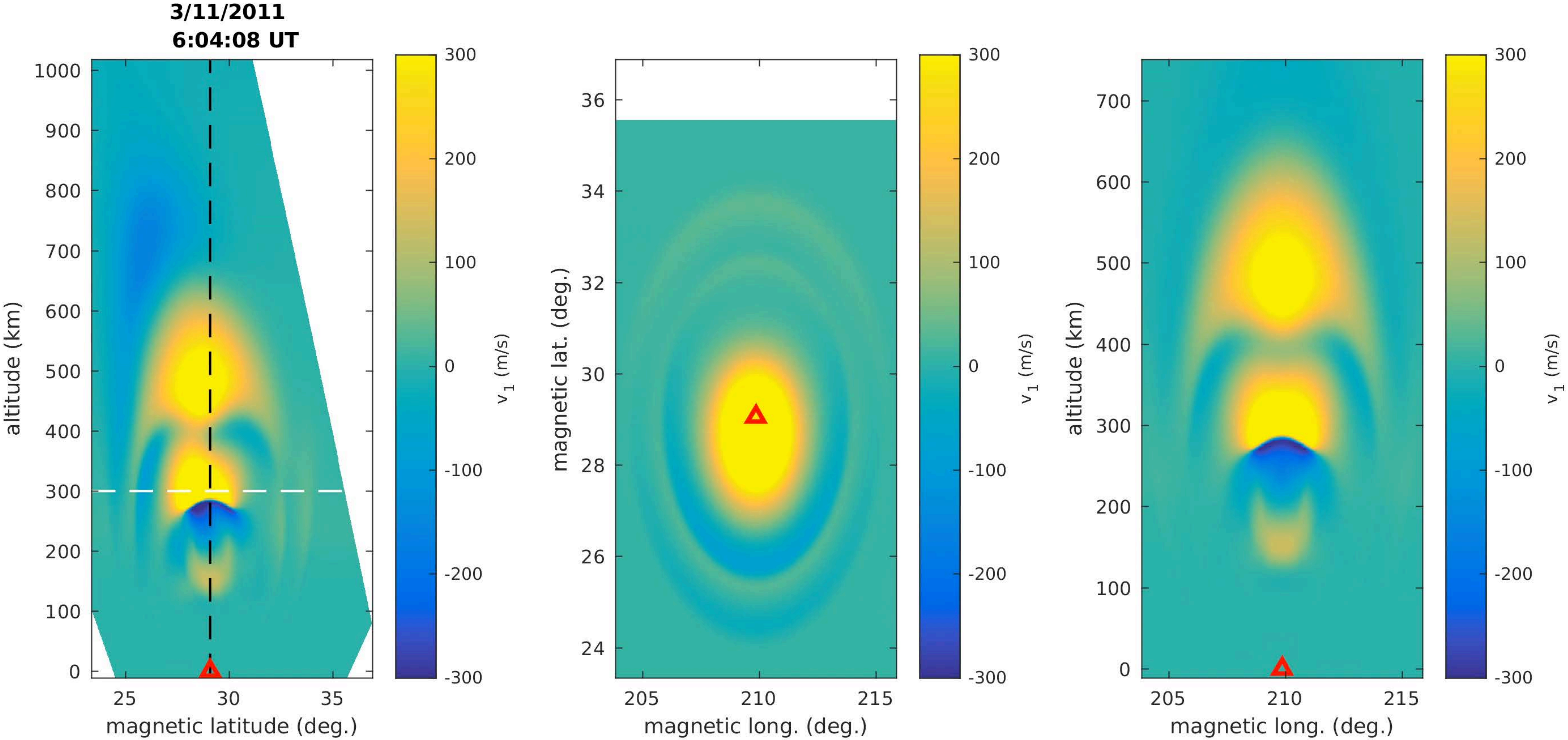


TEC reponses show clear longitudinal dependence (in addition to latitude structure)

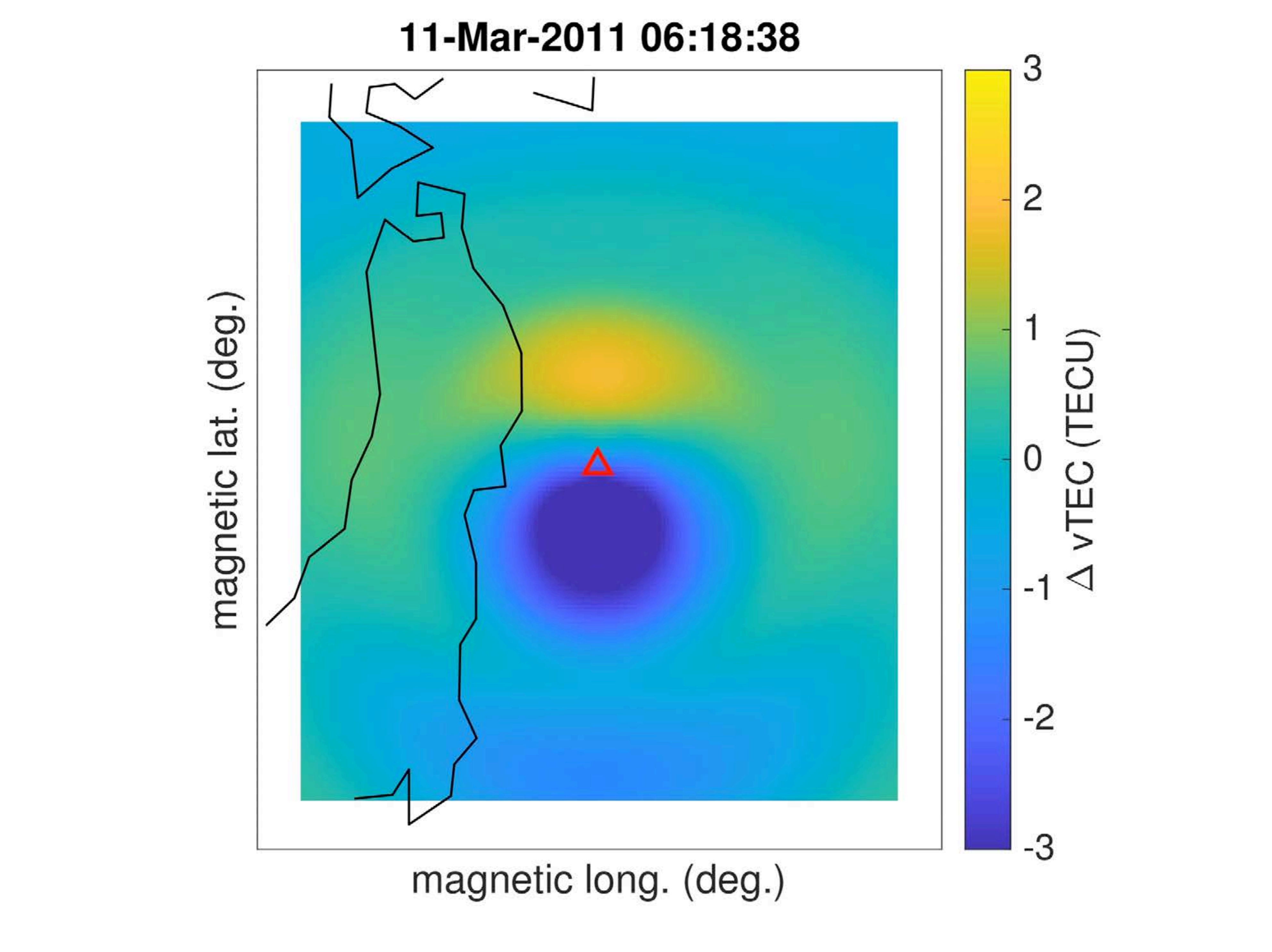
Both a TEC depletion and persistence of AWs is evident in the GPS data

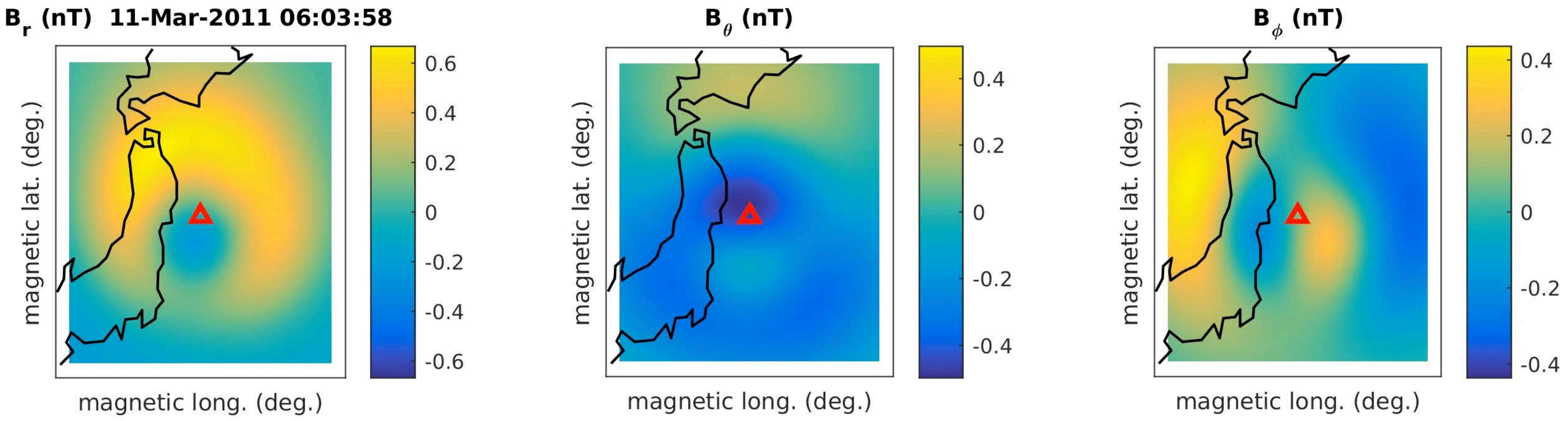


Geomagnetic Field-aligned Plasma Drift



Observable Signatures of 2011 Tohoku EQ





Examples Part III: Modeling for Mission Design

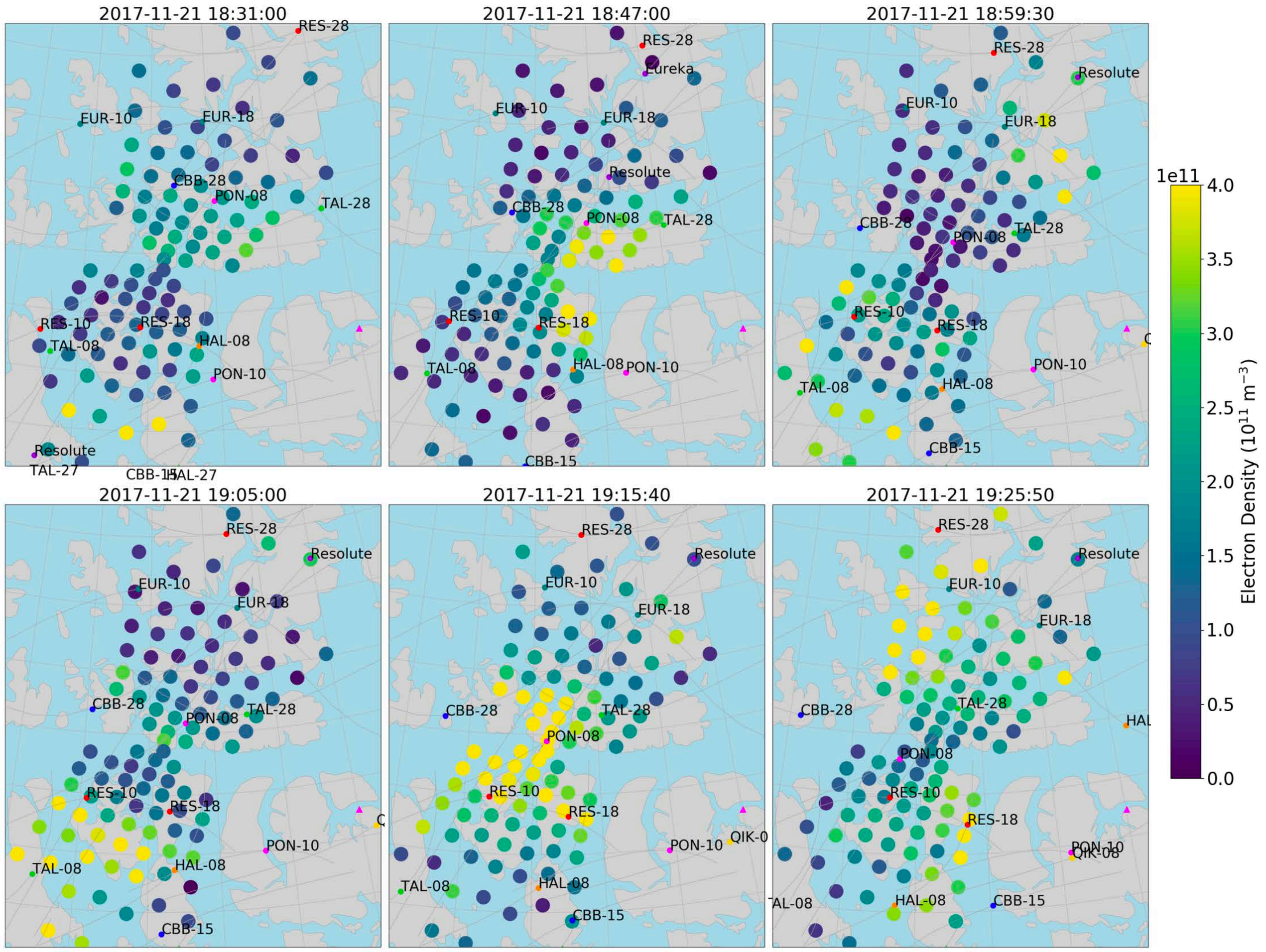
Polar Cap Patches: RISR Observations

Illustrating structure and time-evolution

RISR-N+C imaged a sequence of two patches passing through the FOV over the course of ~1 hour. Internal structuring of these patches is apparent in these data

Patch 1

Patch 2



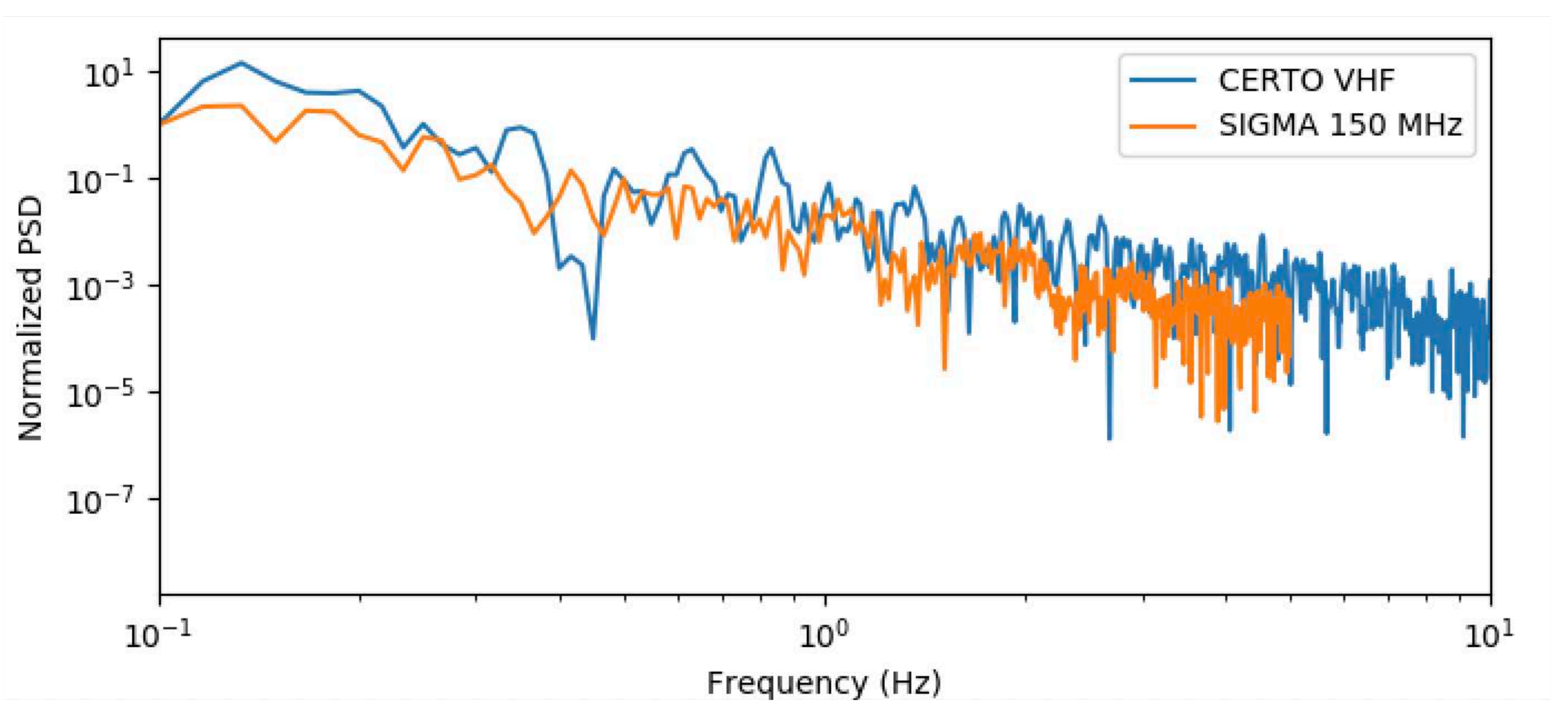
after Lamarche and Varney (2020 CEDAR)

Lamarche et al (2022)

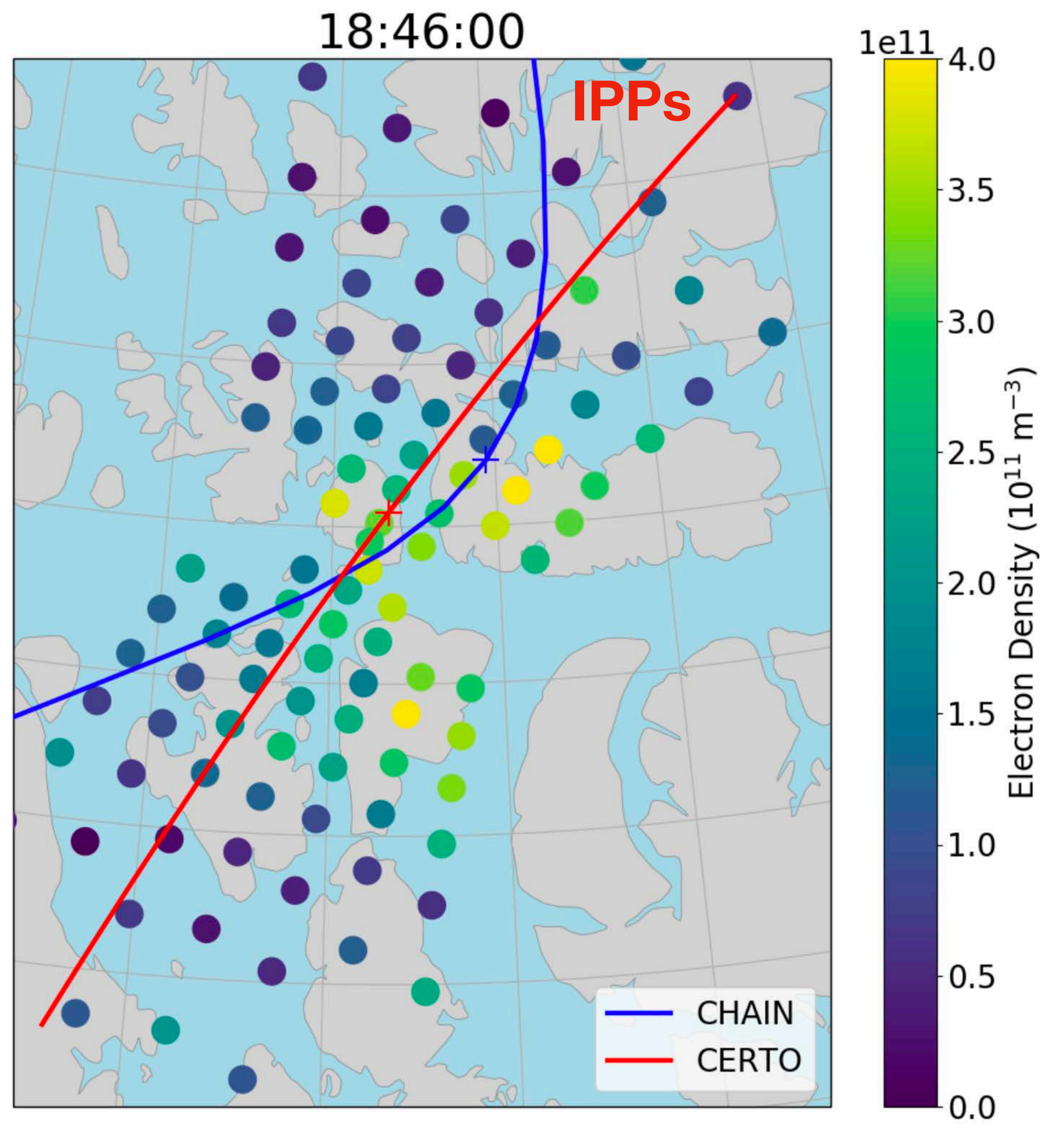
Polar Patches Modeling Scintillation

- Freq. dependent scintillation accompanying patch propagation thru RISR FOV - these are produced by structures near and below the Fresnel scale

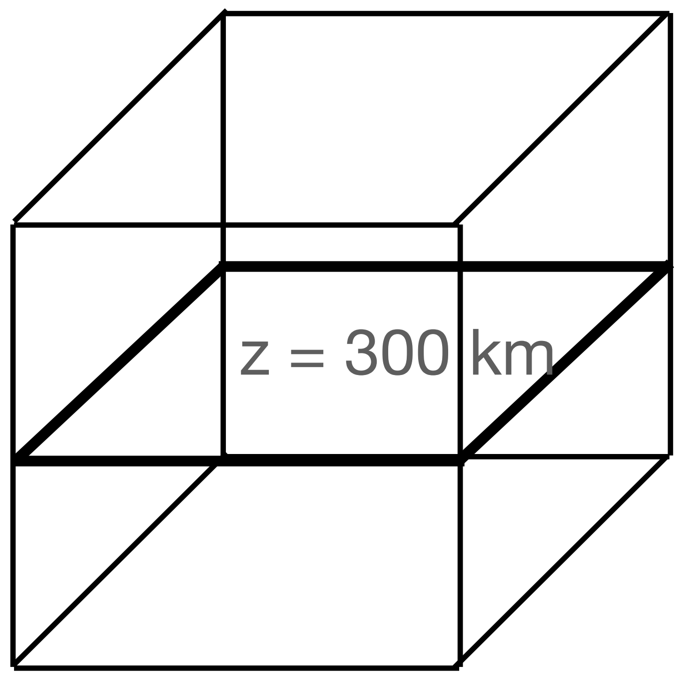
- Modeled v. observed spectrum of VHF

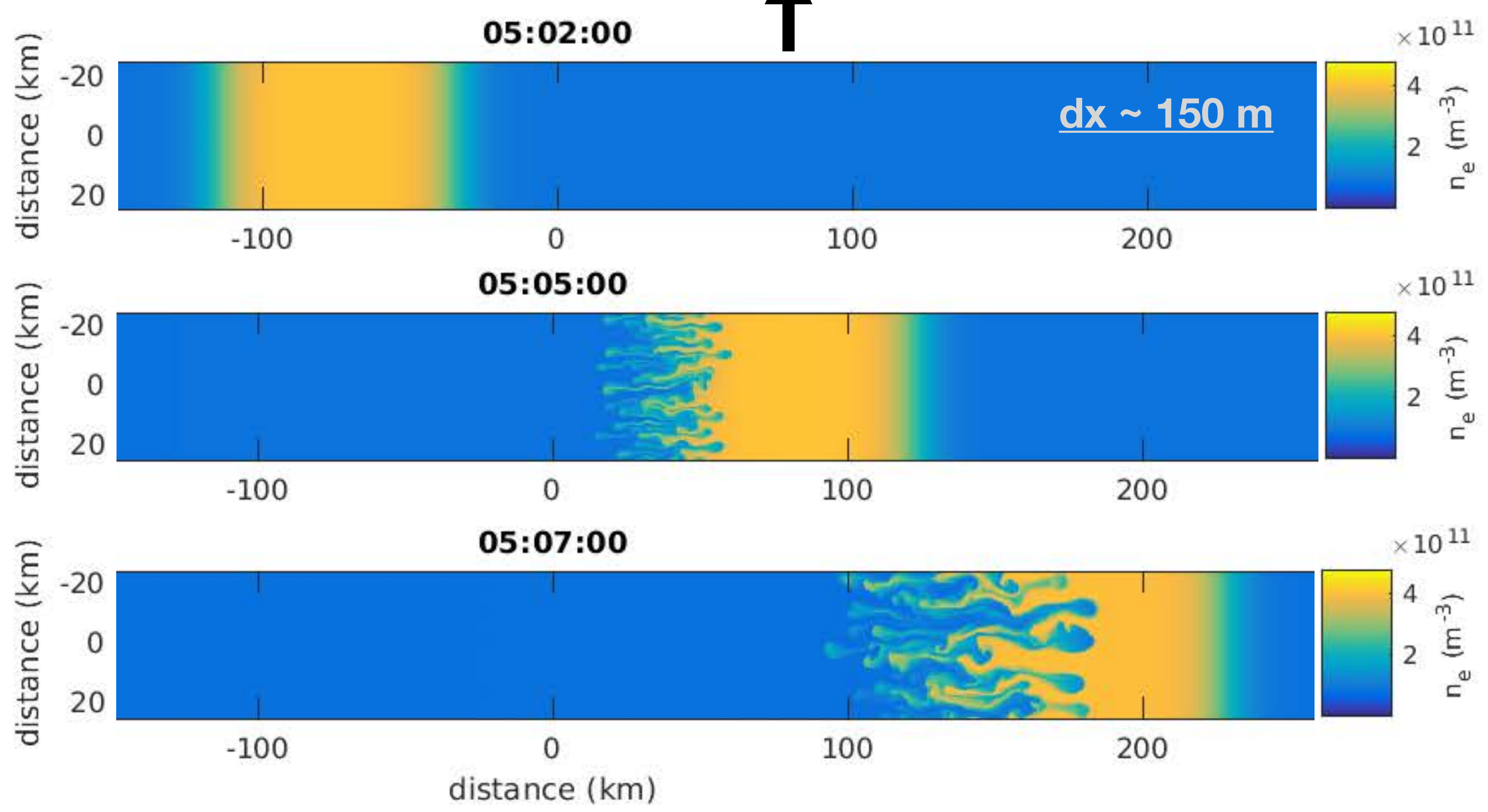


Results using irregularities as input to a radio propagation model (SIGMA) *somewhat* resemble the data

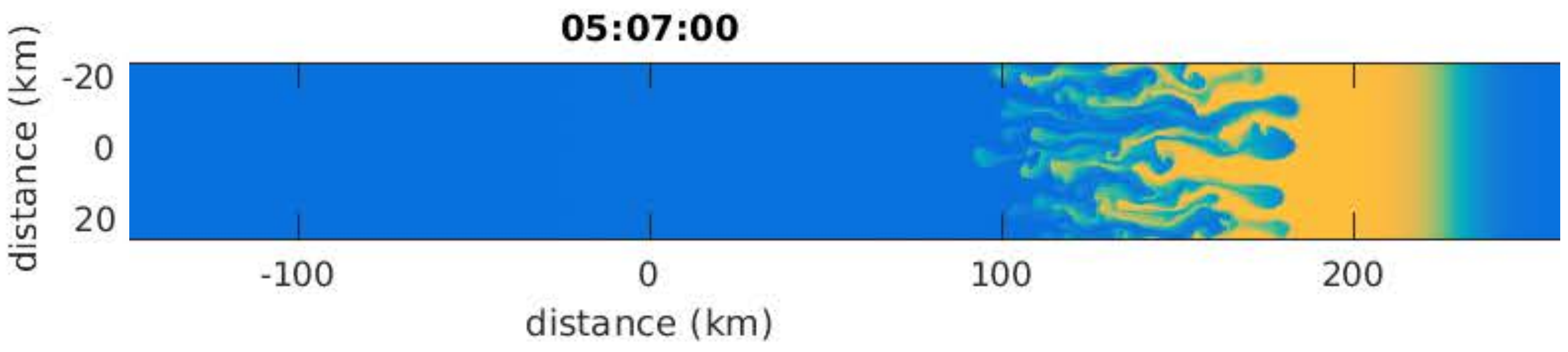


Simulation initialized with velocity and density consistent with ESR/DMSP





Multi-spacecraft Mission to Study Polar Cap Patches



By flying a virtual spacecraft through the model we can understand the types of structures that would be observed during different epochs of evolution and for different orbits

Case 1: vertical alignment

Case 2: horizontal alignment

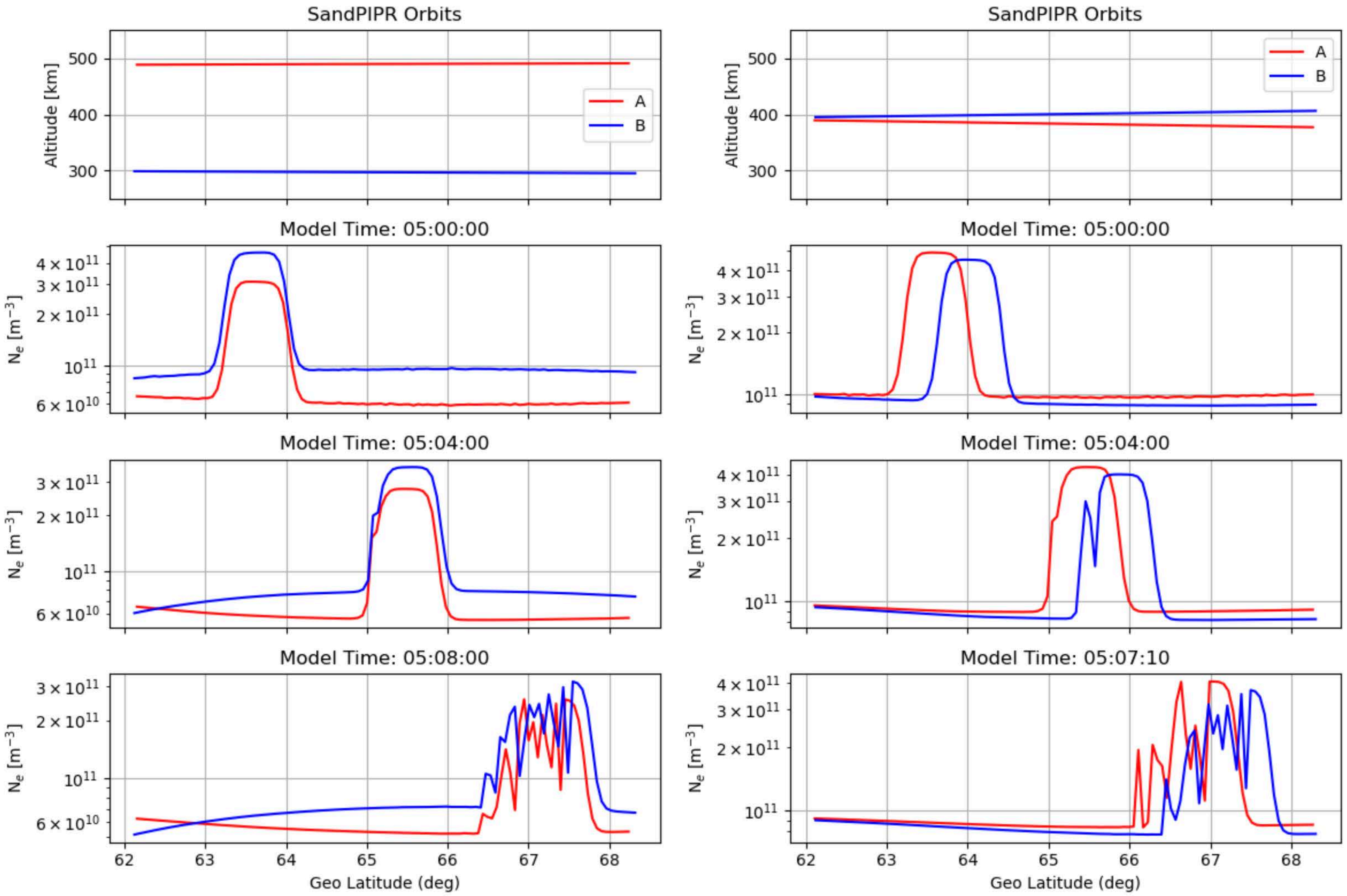
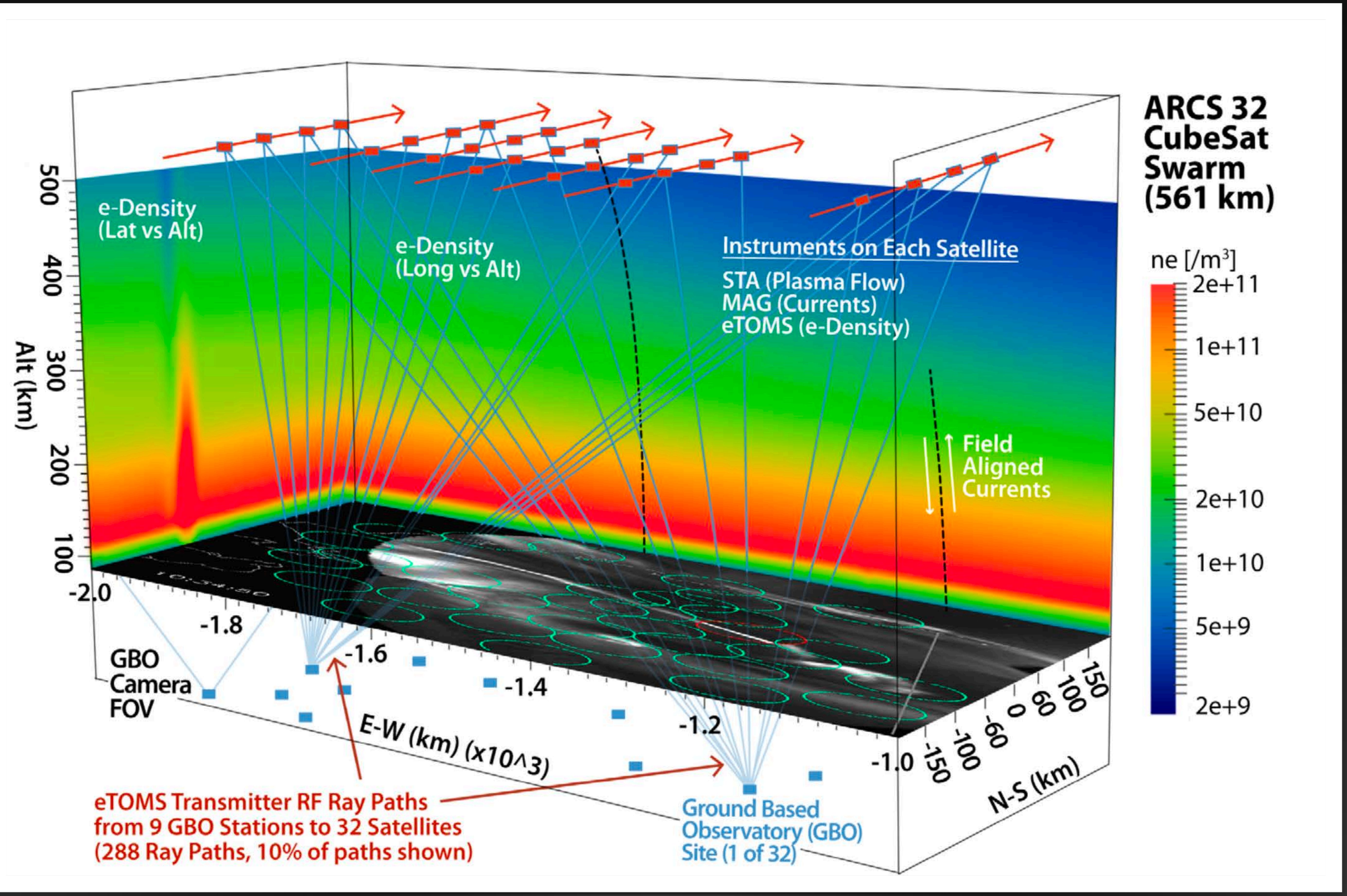
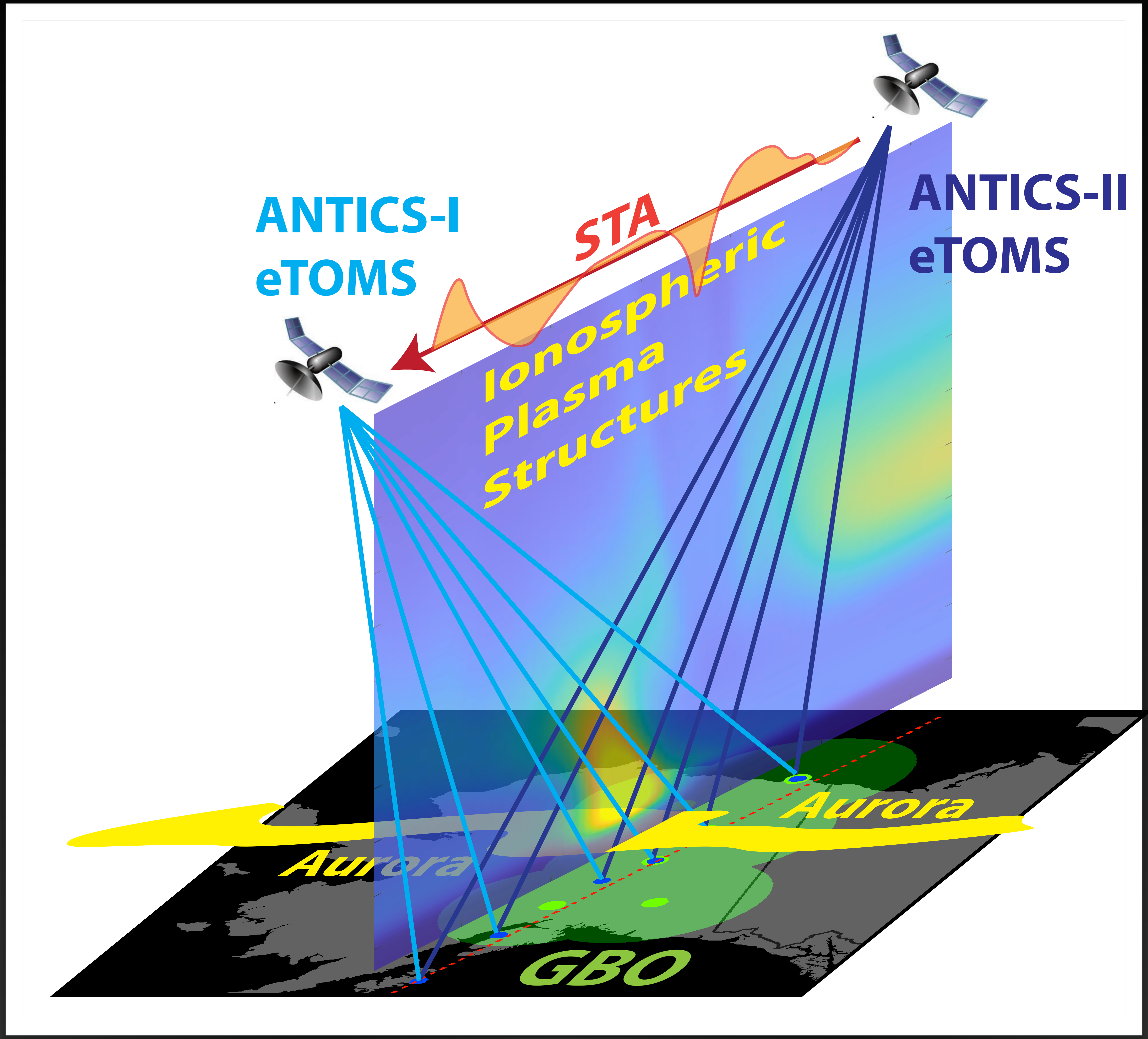


Figure courtesy J. Klenzing

~1 min lag between spacecraft

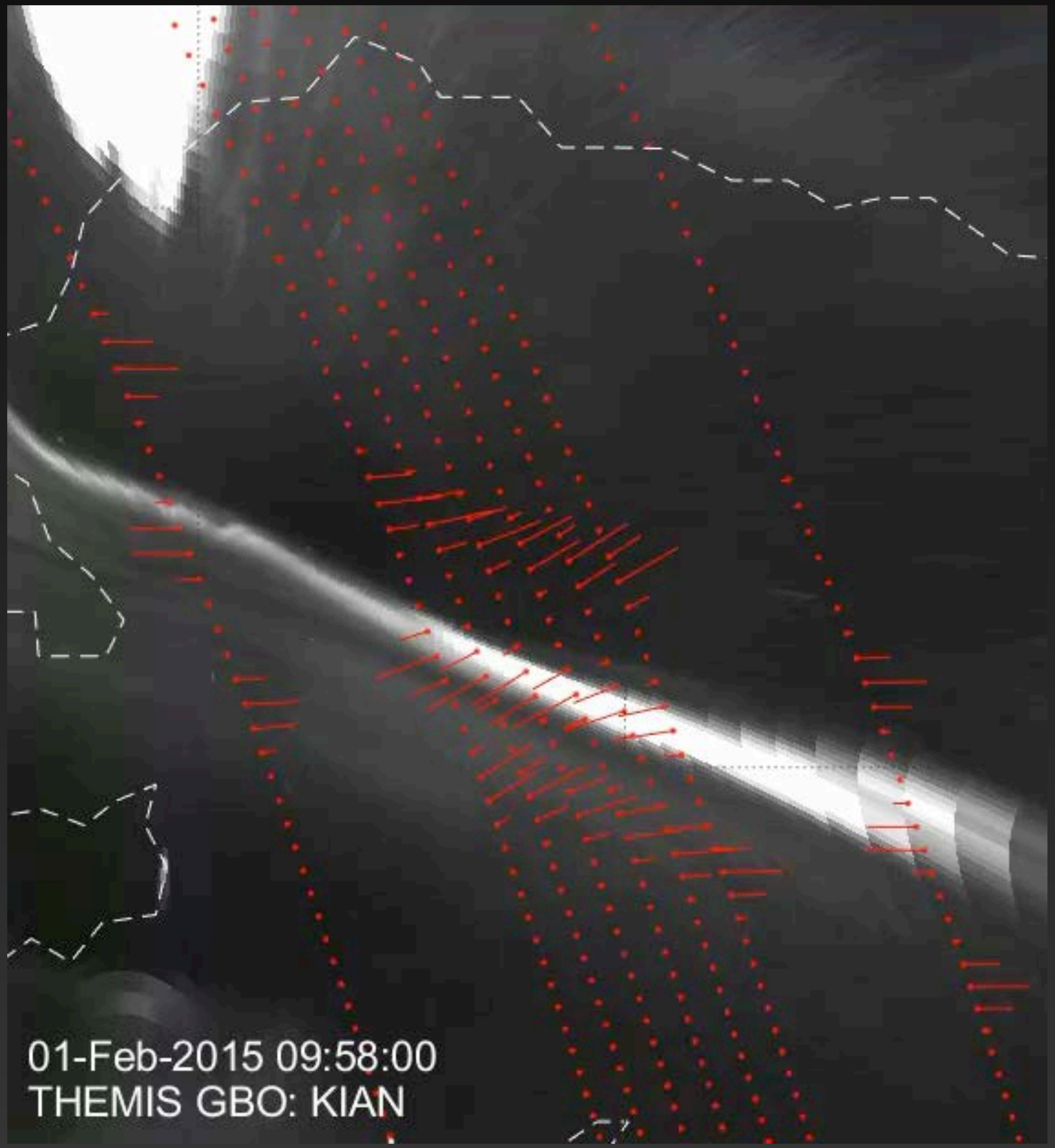
Auroral Mission Design
ARCS and ANTICS

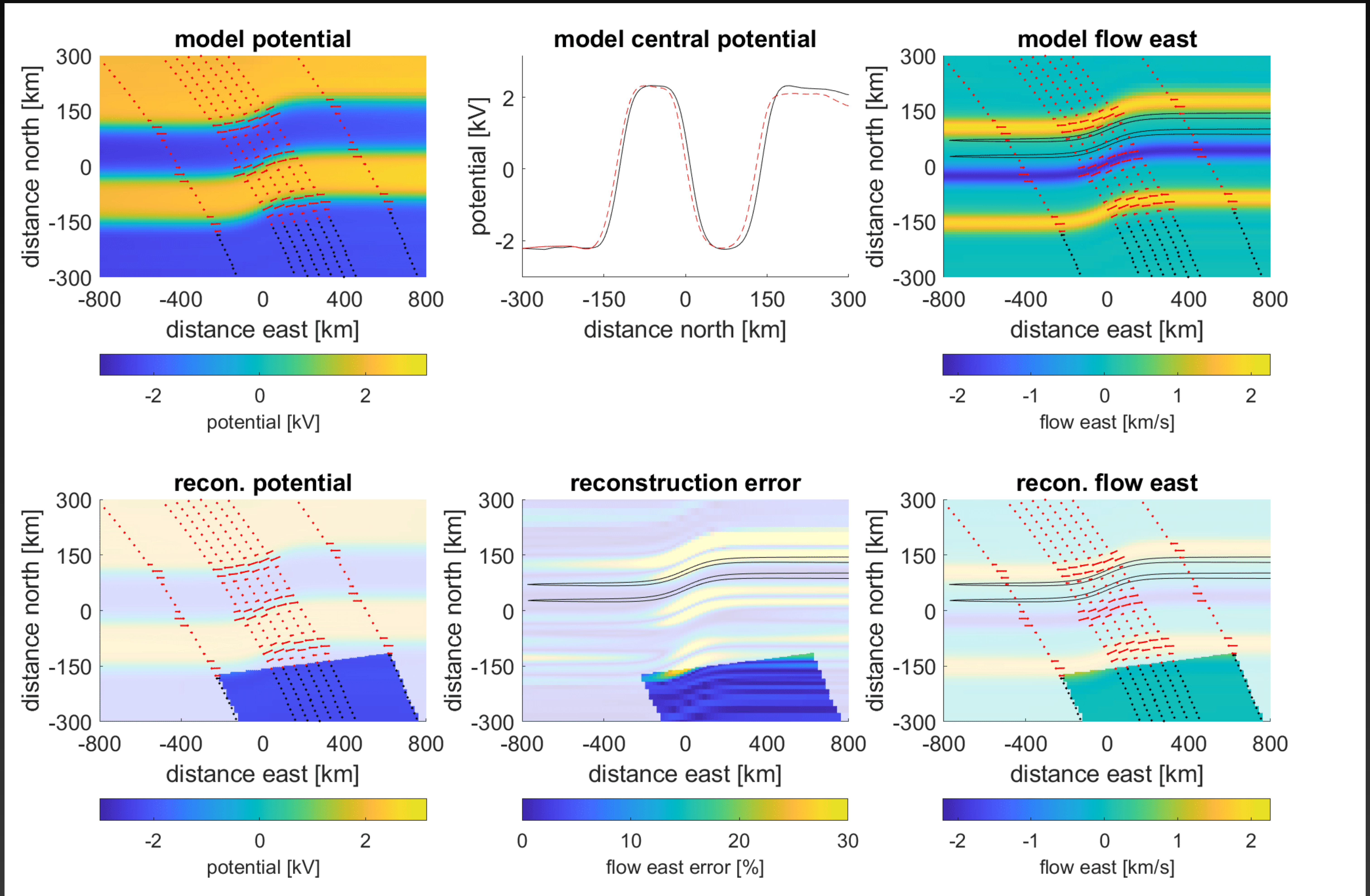




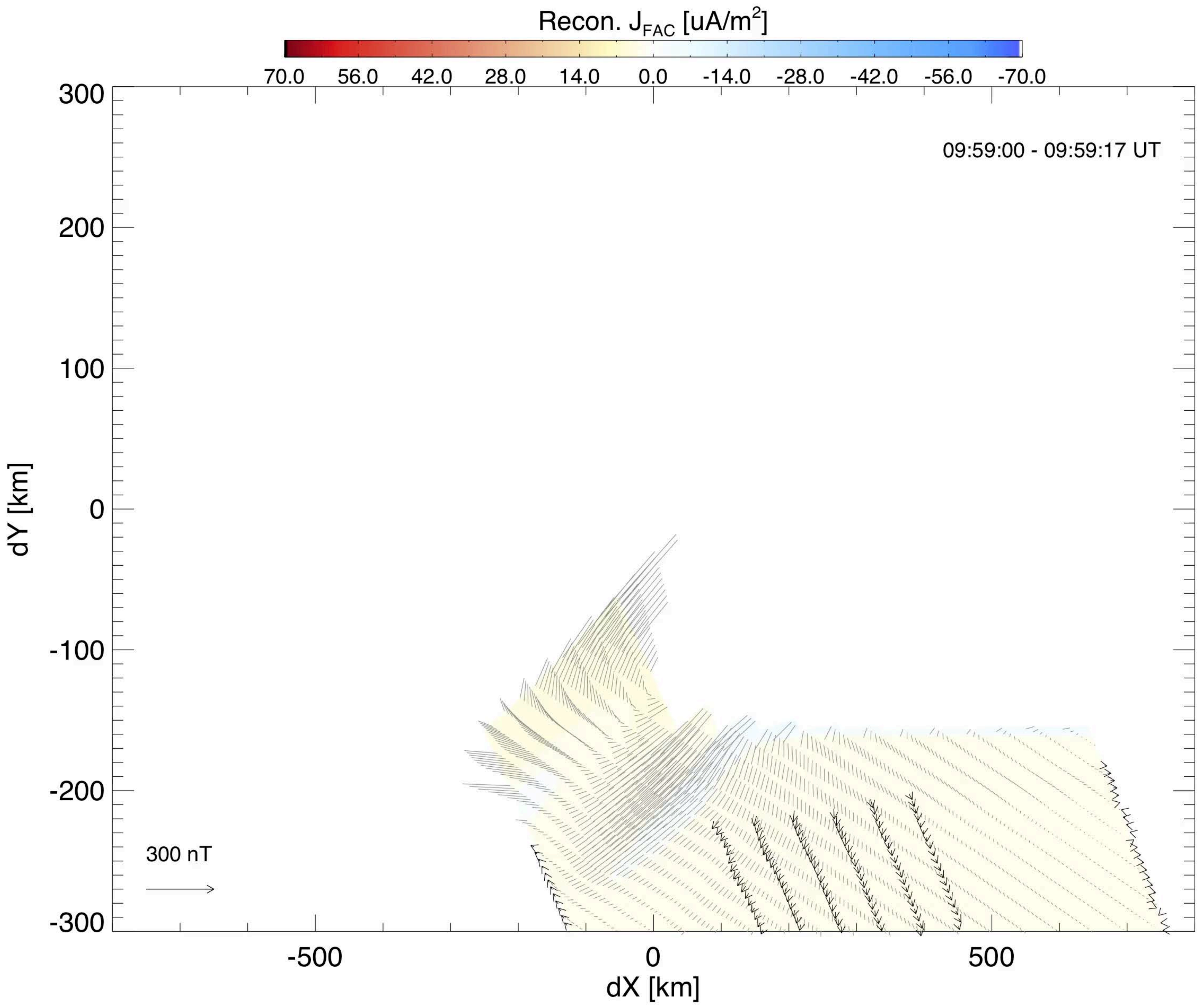
Testing ARCS Using Synthetic Data

Verifying orbital configuration —> science closure





Field-aligned Current Density Reconstruction From Synthetic Data



Modeling the Terrestrial Ionosphere

Part II: fundamental physics, numerical implementation, and future needs

M. Zettergren 08/10/2022

The ionosphere is a plasma — ionized gas — ; to model it we requires descriptions of:

(a) motions (e.g. momentum and energy), and
(b) electromagnetic fields

Each of these requires decisions to be made about physics formulations used in modeling

Plasma Physical Paradigms

Kinetic descriptions

Fluid descriptions

Exact description (Klimontovich)

Time evolution of distribution of particles (Boltzmann)

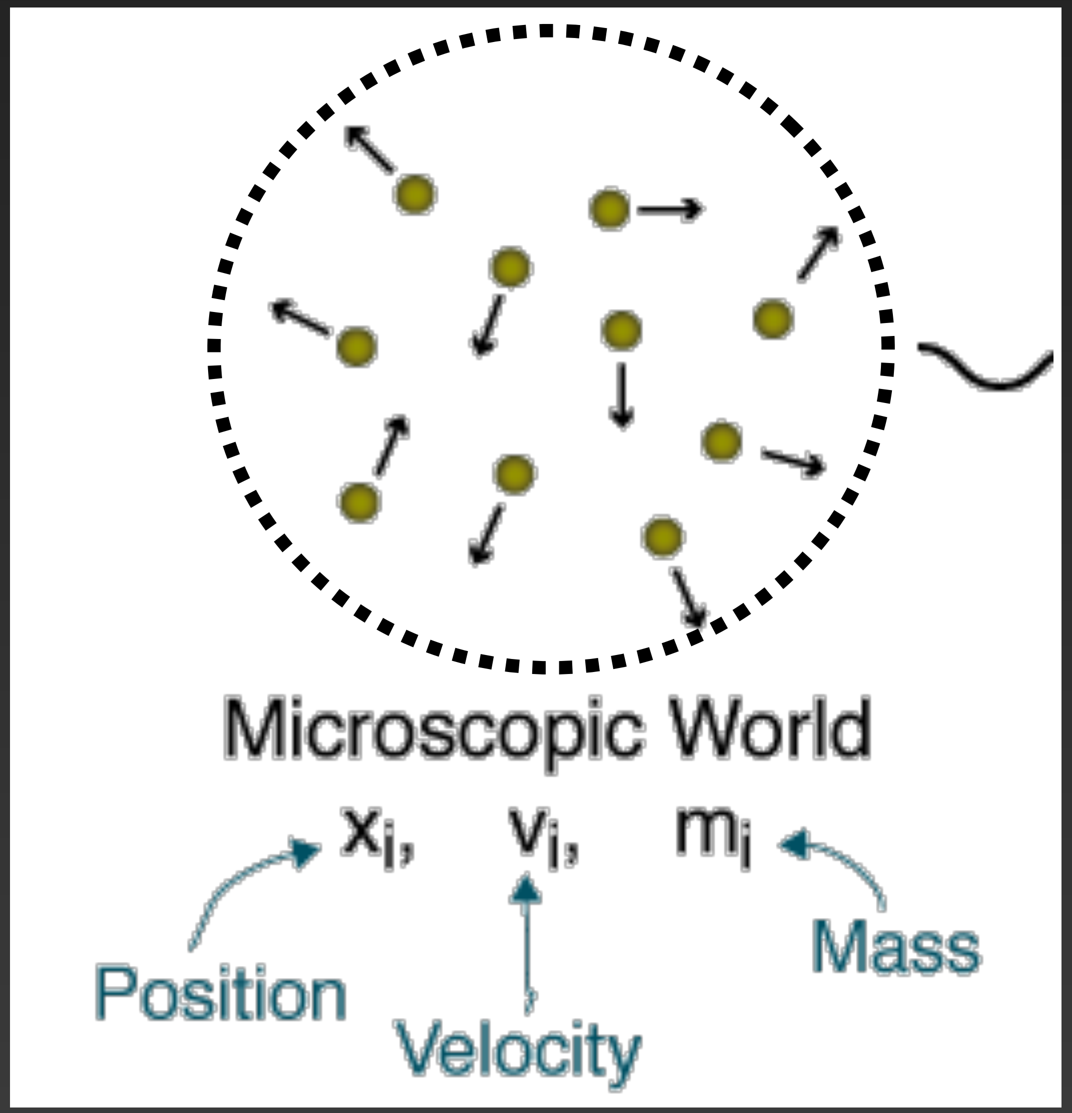
Evolution of macroscopic params. (fluid moments)

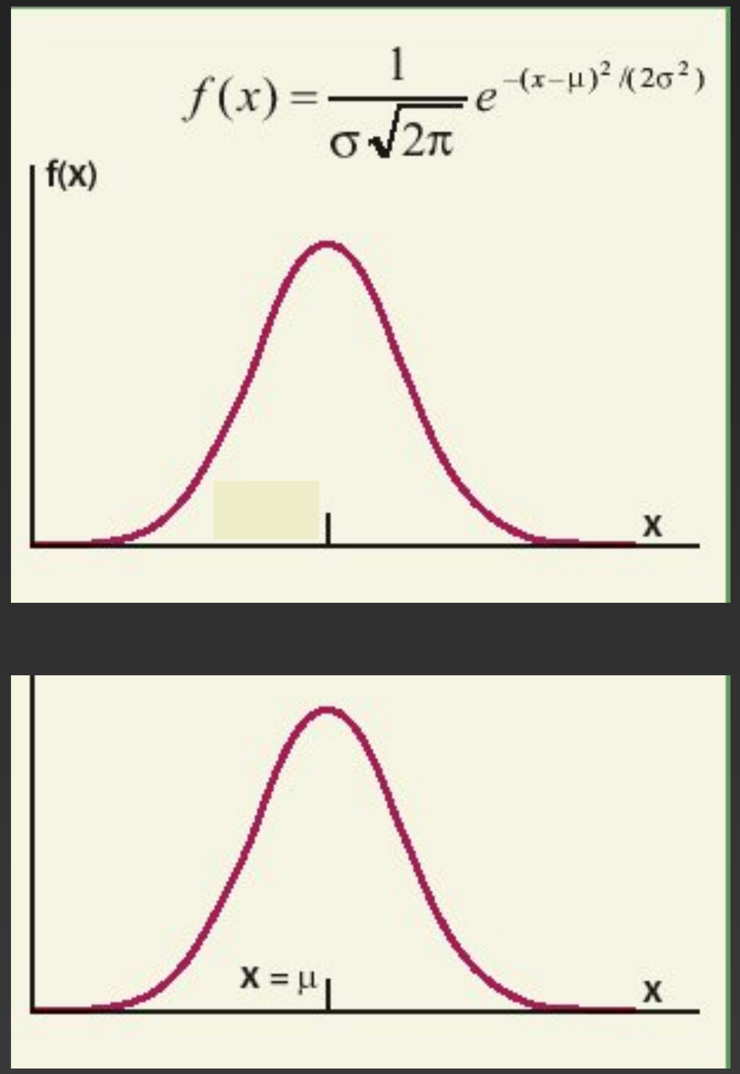
Evolution of total fluid/fields (MHD)

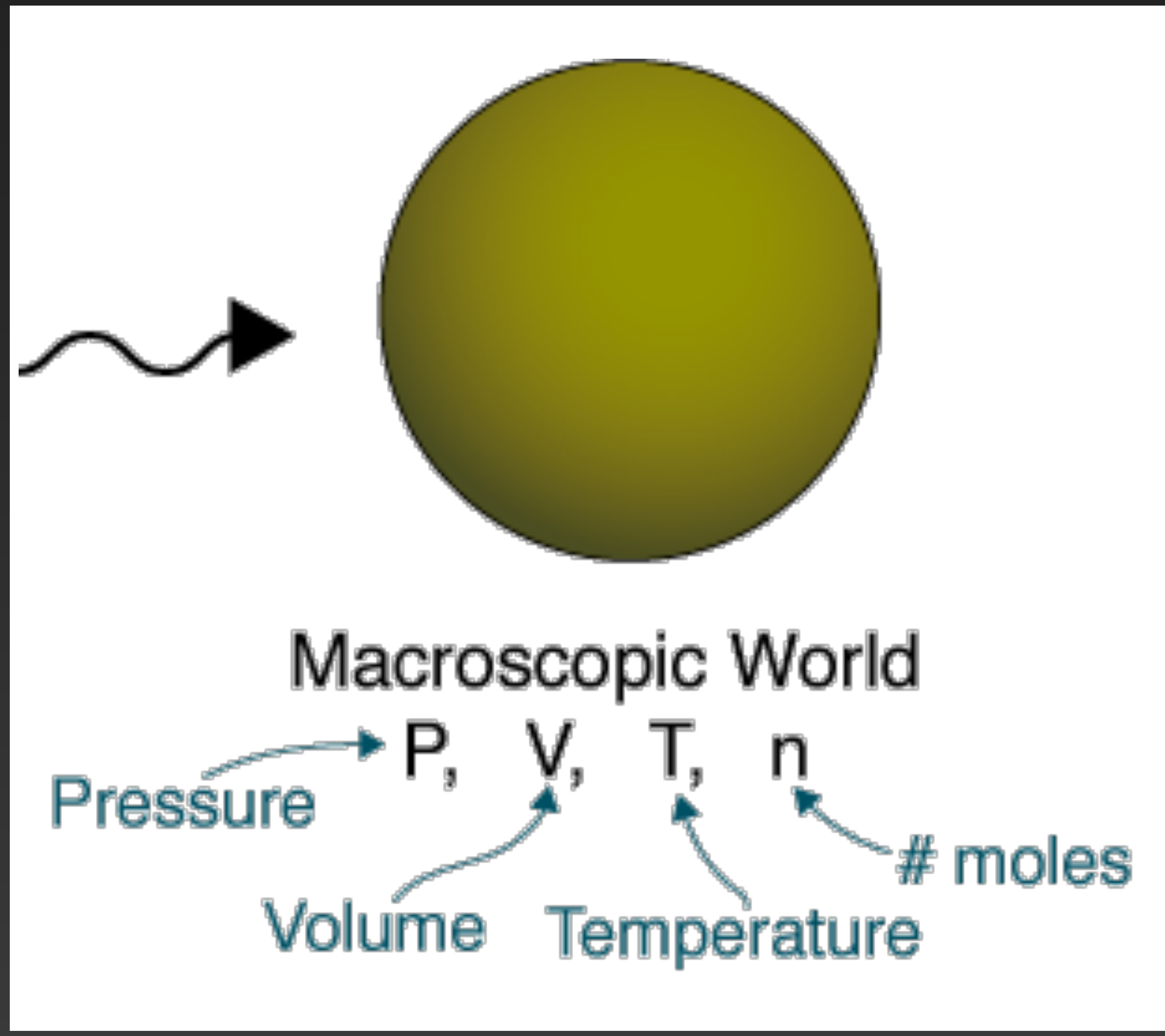
Ensemble averaging

distribution averaging

Averaging over fluids







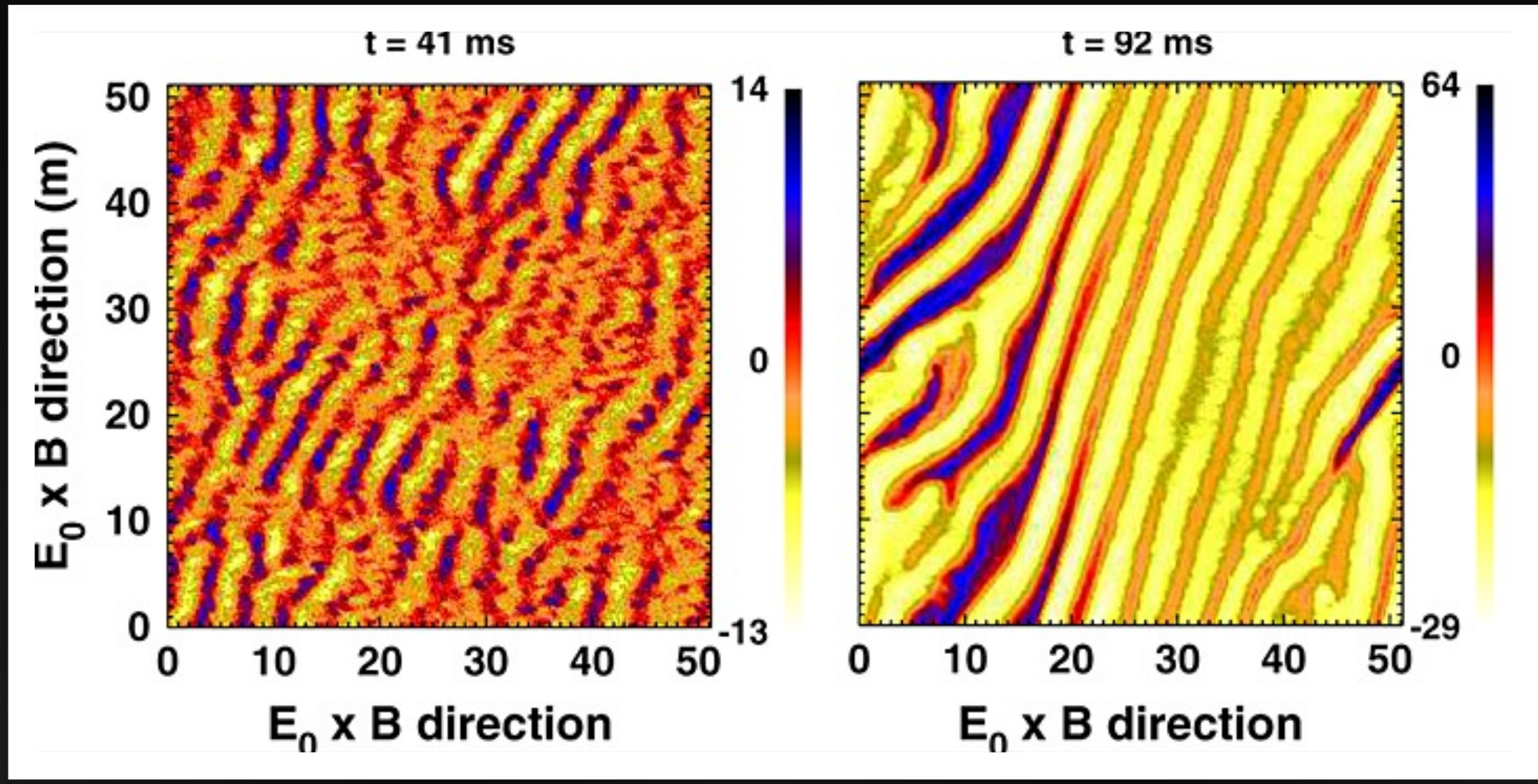
“Exact Descriptions” (sort of)

the particle-in-cell approach

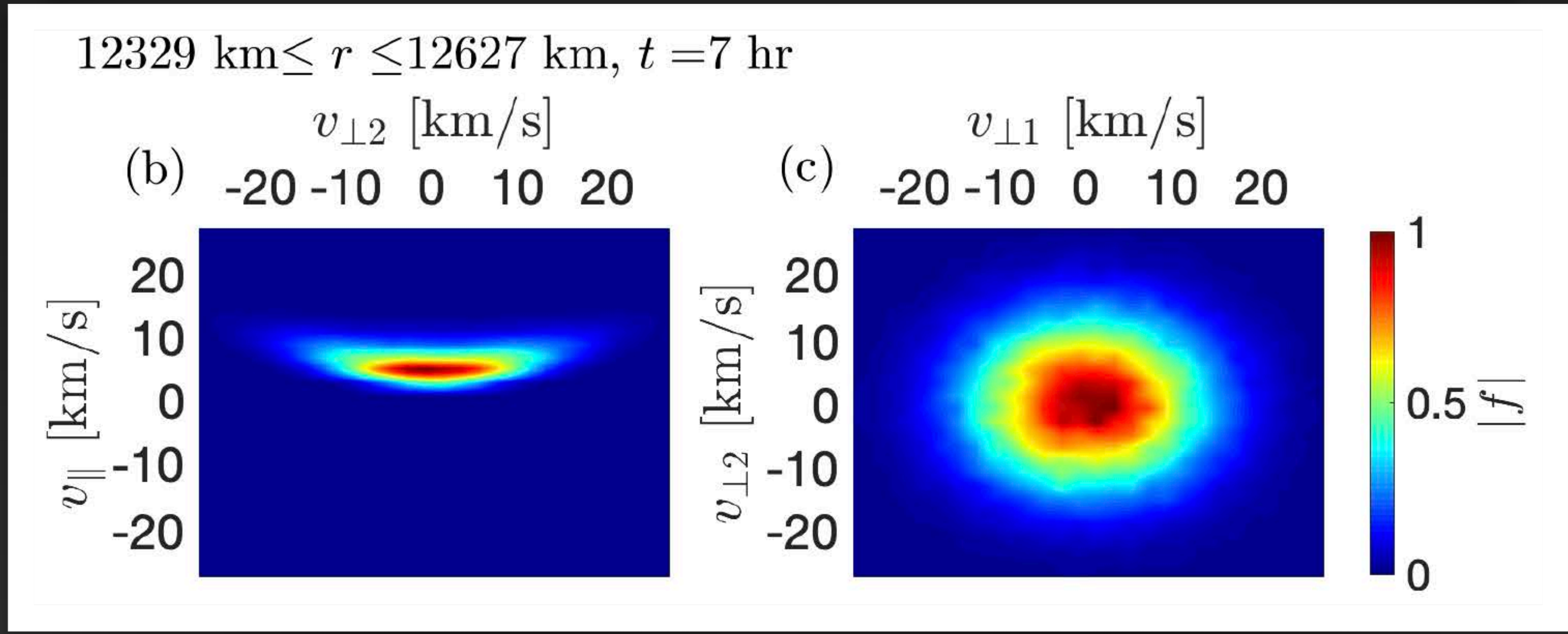
- Literally solving Newton’s Law for every “particle” and some expression of Maxwell’s equations, e.g for each particle:

$$m\frac{d\mathbf{v}_k}{dt} = q\left(\mathbf{E} + \mathbf{v}_k \times \mathbf{B}\right) \qquad \text{(Binning/gridding)} \qquad \nabla^2\Phi = -\frac{\rho_c}{\epsilon_0}$$

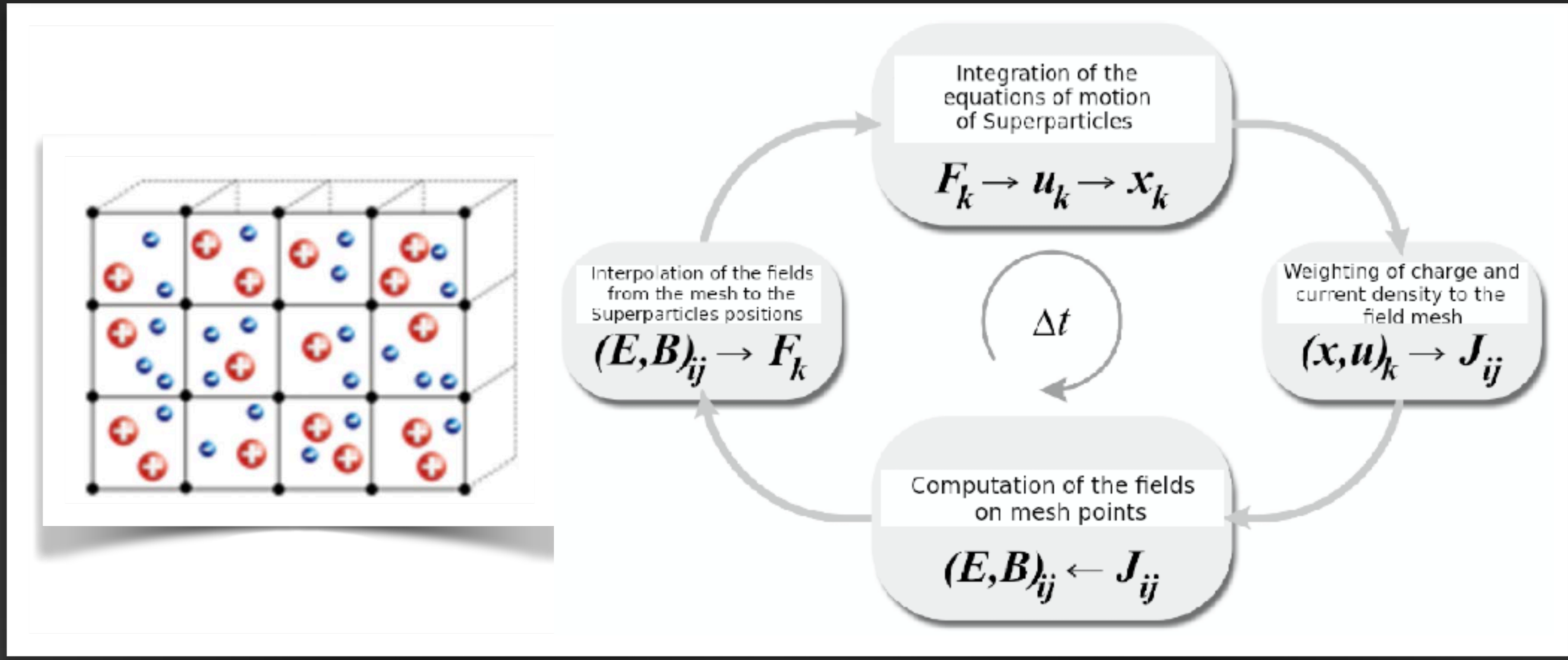
- Used for very small-scale or low dimensional kinetic simulations; incredible detail but very little space-time coverage (EPIC code https://doi.org/10.1002/jgra.50196)



Oppenheim and Dimant (2013)



R. Albarran (2022)



PIC methods can be inefficient or unworkable for very large numbers of particles

Tracking evolution of a distribution of particles

Phase fluid approaches

- Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = \frac{\delta f}{\delta t}$$

Advection (motion) in configuration space

Advection in velocity space

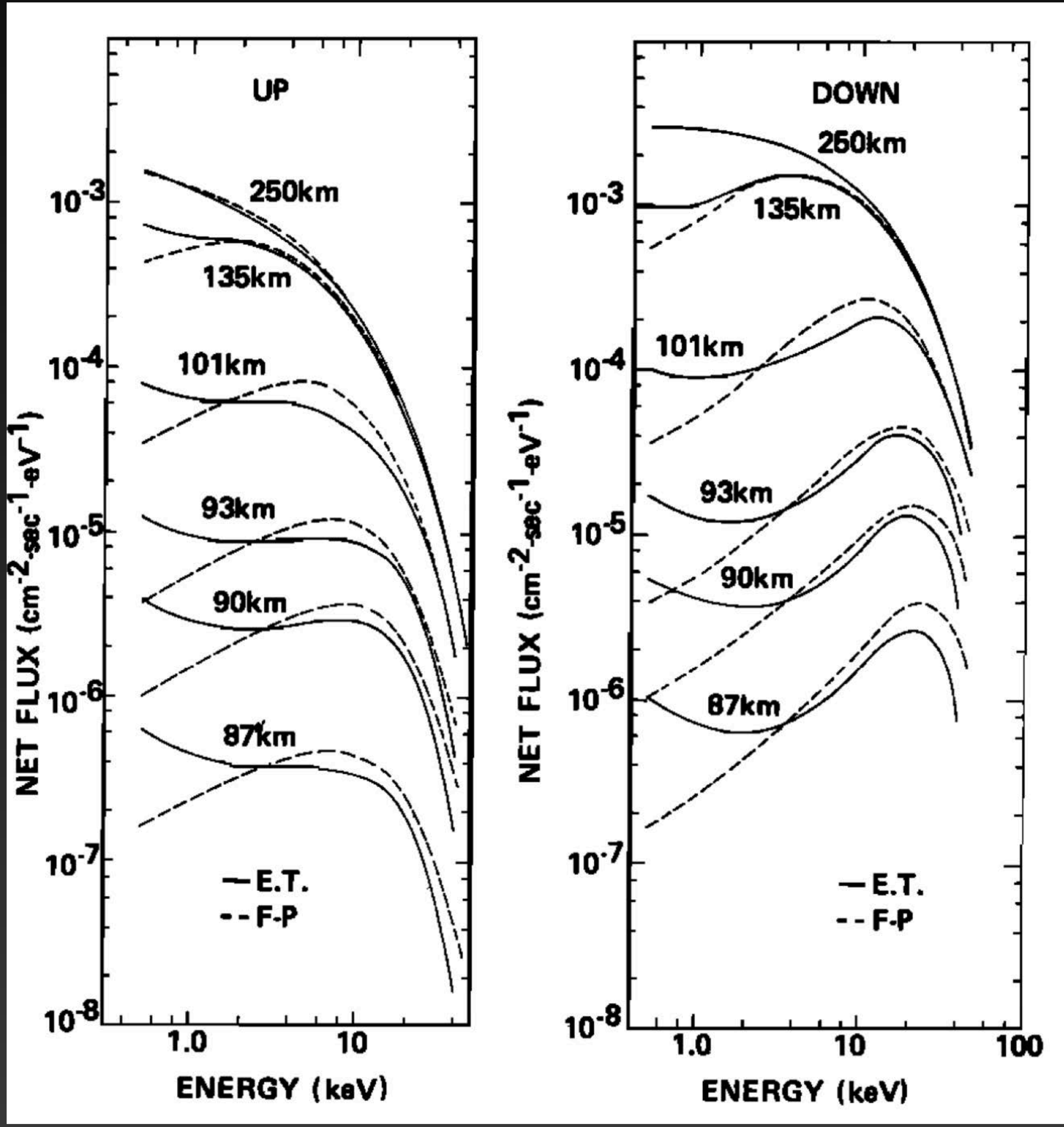
Change in distribution with collisions

$$\mathbf{a} = \sum_i \frac{\mathbf{F}_i}{m}$$

$$f(\mathbf{x}, \mathbf{v}, t)d^3v \rightarrow n(\mathbf{x}, t)$$

Number density in velocity volume element

- Collision operators: Lorentz gas model, Fokker-Plank
- Used for modeling processes that are far from equilibrium or are very sensitive to energetics, e.g. energetic auroral electron scattering in the atmosphere (GLOW model https://github.com/space-physics/glowaurora)
- *Even though we have only one equation to solve it is effectively 7-dimensional!*



Strickland et al., (1976)

What physical description is appropriate?

Motions

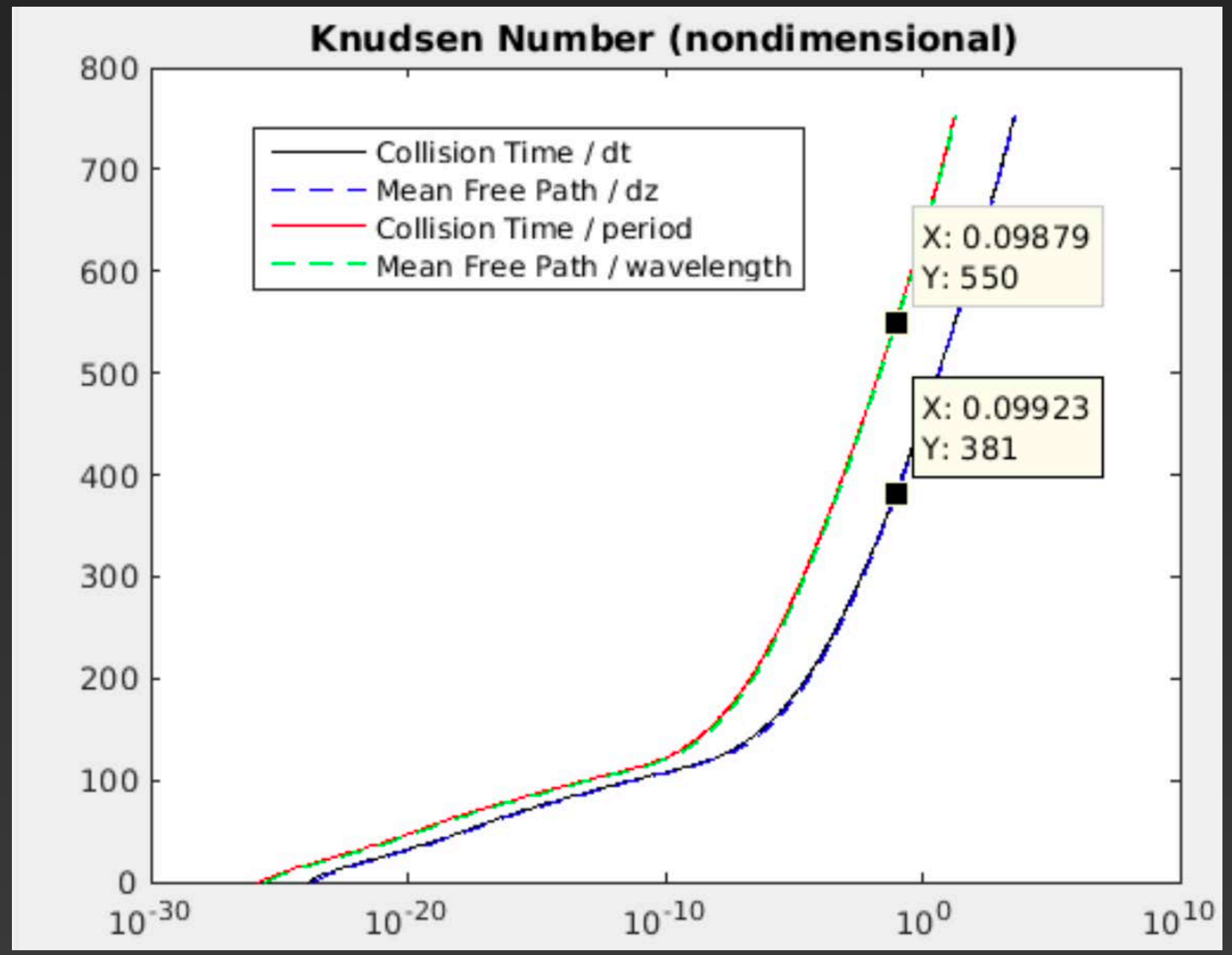
- One decision to make is kinetic vs. fluid - which is largely a decision of spatial and time scales of interest BUT also depends on free energy sources and boundary conditions as well.
- Knudsen number describes a nominal kinetic-to-fluid transition in terms of scale sizes of interest.
- In a plasma things are complicated at bit; essentially anything that cannot be accurately described by moments (i.e. near thermal equilibrium) is probably not "fluid"
- Other important scales in plasma physics: ion gyroradius, Debye length, inertial scale lengths, etc.
- Nearness to thermal equilibrium is also important
  - how strongly driven is the plasma in terms of electromagnetic fields?
  - Are particle inputs energetic enough to trigger highly energy-dependent inelastic processes?

$$\mathrm{Kn} = \frac{\lambda_{mfp}}{\ell} \qquad \frac{\text{Mean free path}}{\text{Length scale}}$$

Kn ~ 1 often taken to be the nominal transition from fluid to kinetic system behavior, i.e. the exobase, where the length scale is taken to be a scale height.

For neutral particles (hard/soft sphere collisions) this occurs around 450-500 km altitude

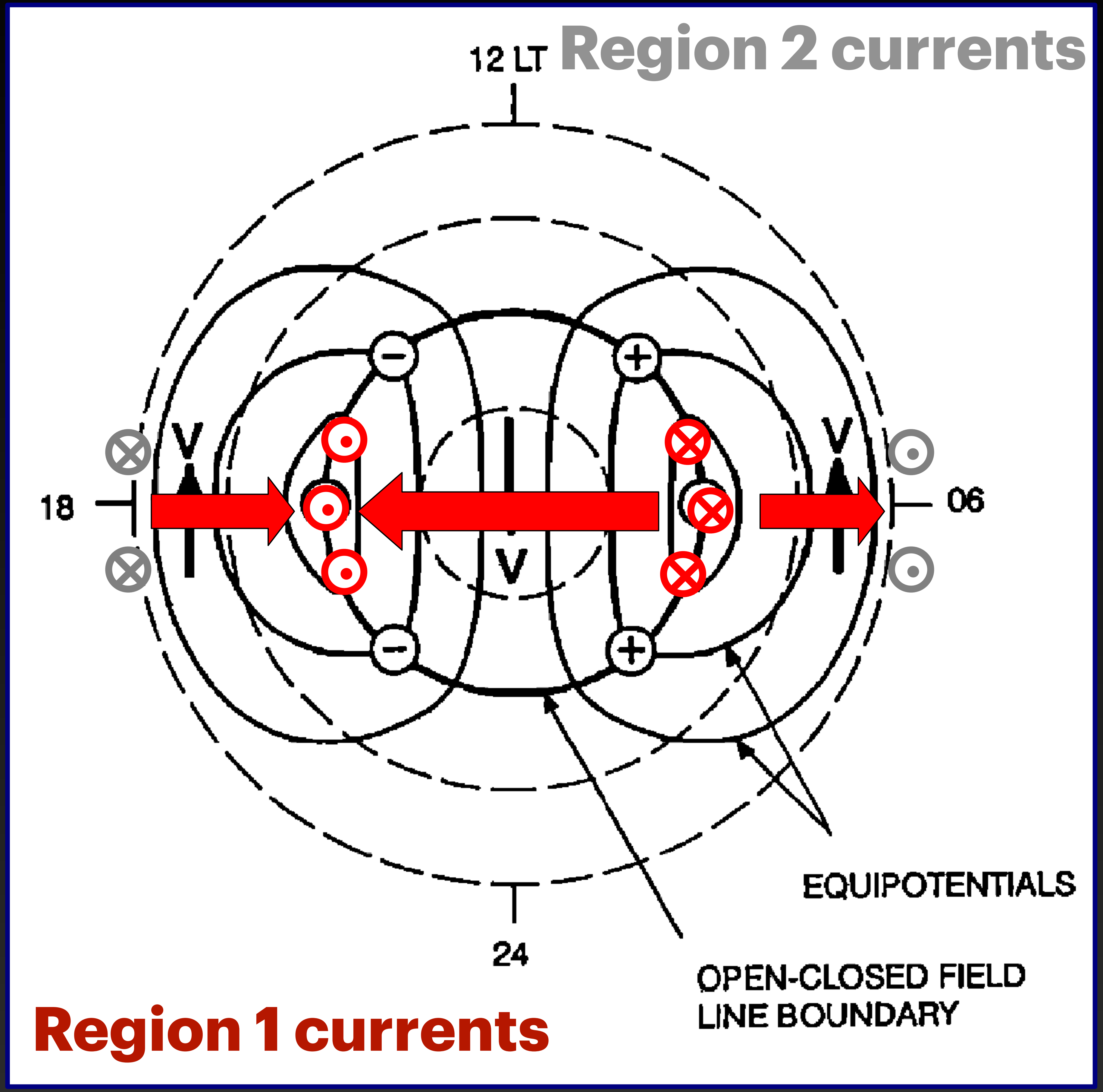
For charge particles (Coulomb collisions) the interactions are much longer-range and transition is ~2000 km altitude



What physical description is appropriate?

Electromagnetic

- Stationary charges: electrostatic. This is the most common formulation used in ionospheric simulation.
- Steady current - assuming the displacement current can be neglected fields and currents are related via Ampere's Law.
- *In the ionosphere this is basically always implemented in a quasi-static static sense. I.e. static solutions that are updated as the conductivity/charge density slowly changes.*
- Inductive ~ Rapidly varying ***J***,***B*** ~ important at small-scales *(e.g Strelsov and Lotko, 2008)*
- OR div(***J***) not zero; must use generalized Ampere's Law; e.g. done for radio propagation problems (magneto-ionic theory)



$$\mathbf{J} = \sigma \cdot \mathbf{E} \qquad \nabla \cdot \mathbf{J} = 0$$

$$\mathbf{E} = -\nabla\Phi$$

Ionospheric Physics

What processes other than transport and electromagnetic must be considered?

- EUV and soft X-ray sources of plasma
- Energetic electron precipitation
- Interactions (collisions) between different plasma constituents
- Chemical reactions that destroy or change identity of charged species
- Higher-order transport (e.g. thermal conduction, polarization drifts)
- Must solve equations for each type of charged particle due to need to account different chemical reactions!

Example mathematical ionospheric model (fluid)

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{v}_s) = m_s P_s - L_s \rho_s$$

Mass Flow; Photoionization + Chemical production + Impact Ionization; Chemical loss

$$\frac{\partial}{\partial t}(\rho_s \mathbf{v}_s) + \nabla \cdot (\rho_s \mathbf{v}_s \mathbf{v}_s) = -\nabla p_s + \rho_s \mathbf{g} + \frac{\rho_s}{m_s} q_s (\mathbf{E} + \mathbf{v}_s \times \mathbf{B}) + \sum_t \rho_s \nu_{st} (\mathbf{v}_t - \mathbf{v}_s)$$

Momentum Flow; Press + gravity + Lorentz forces; Frictional force (drag)

$$\frac{\partial}{\partial t}(\rho_s \epsilon_s) + \nabla \cdot (\rho_s \epsilon_s \mathbf{v}_s) = -p_s(\nabla \cdot \mathbf{v}_s) - \nabla \cdot \mathbf{h}_s - \frac{1}{(\gamma_s - 1)} \sum_t \frac{\rho_s k_B \nu_{st}}{m_s + m_t} \left[2(T_s - T_t) - \frac{2}{3} \frac{m_t}{k_B} (\mathbf{v}_s - \mathbf{v}_t)^2 \right]$$

Internal Energy Flow; Adiabatic Expansion; Thermal conduction; Heat Exchange; Frictional Heating

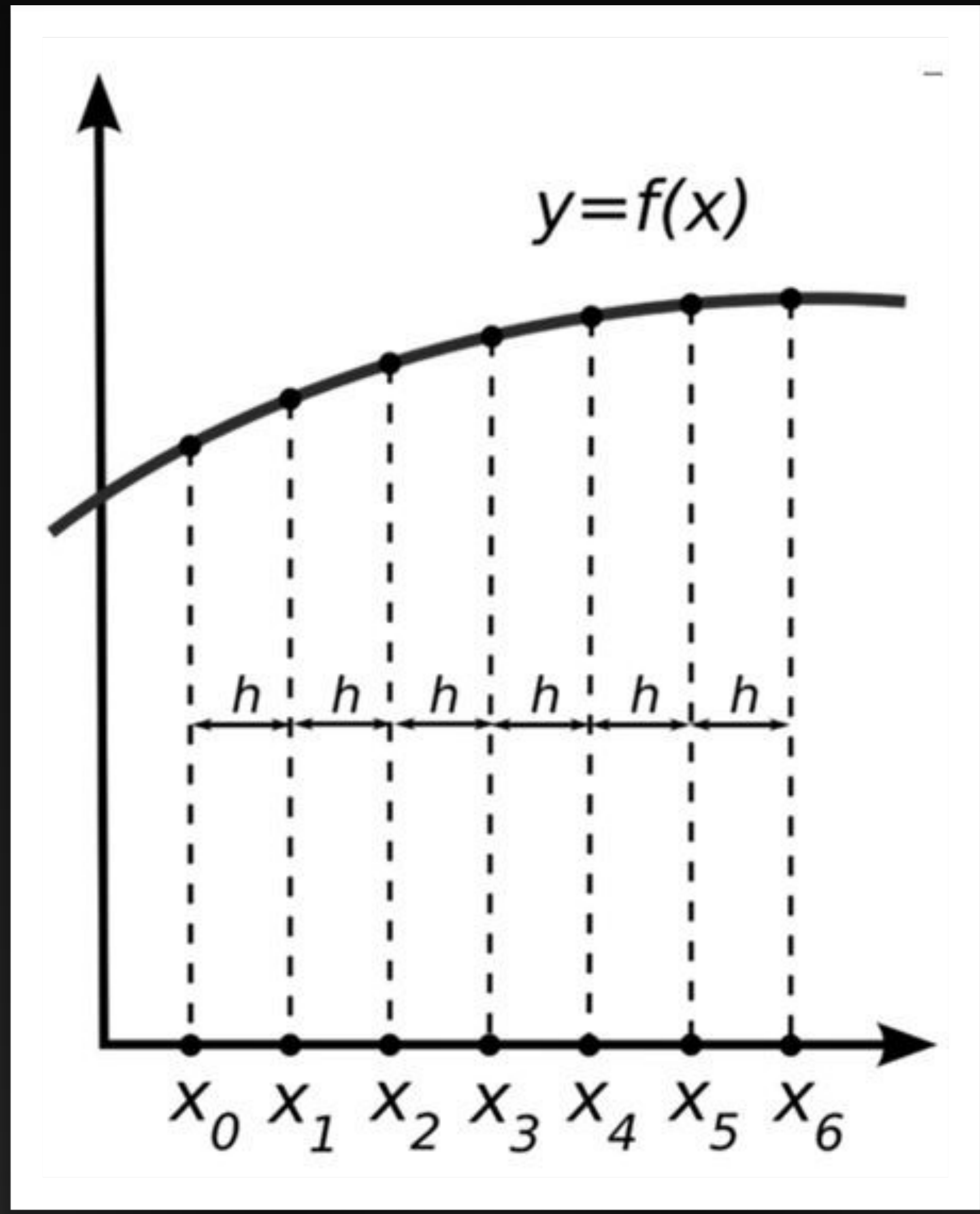
$$\nabla \cdot \mathbf{J} = 0 \qquad \mathbf{J} = \boldsymbol{\sigma} \cdot \mathbf{E} \qquad \mathbf{E} = -\nabla \Phi$$

Current Continuity; Ohm’s Law; Electrostatic

Numerical Approaches to Ionospheric Equations

Types and Basic Approaches

- Ionospheric Equations are *mixed-type*, viz. a combination of hyperbolic, parabolic, and elliptic terms.
  - Flow terms are hyperbolic (wave-like)
  - Heat conduction is parabolic (dissipation)
  - Electrostatic version of current continuity is elliptic (steady-state)
- Numerical solutions are achieved by *discretization* of state variable data onto meshes containing grid points (locations in space) or cells (small volumetric elements)
- Discretization permits approximate of derivatives via algebraic equations, viz. *finite differences*.
- Storage via regular arrays in a computer language.



$$f(t) \rightarrow f(t_n) \rightarrow f^n$$

$$f(x) \rightarrow f(x_i) \rightarrow f_i$$

Discrete "samples" in space and time separated by:

$$\Delta x, \Delta t$$

$$f(x, y, z, t) \rightarrow f(x_i, y_j, z_k, t_n) \rightarrow f^n_{i,j,k}$$

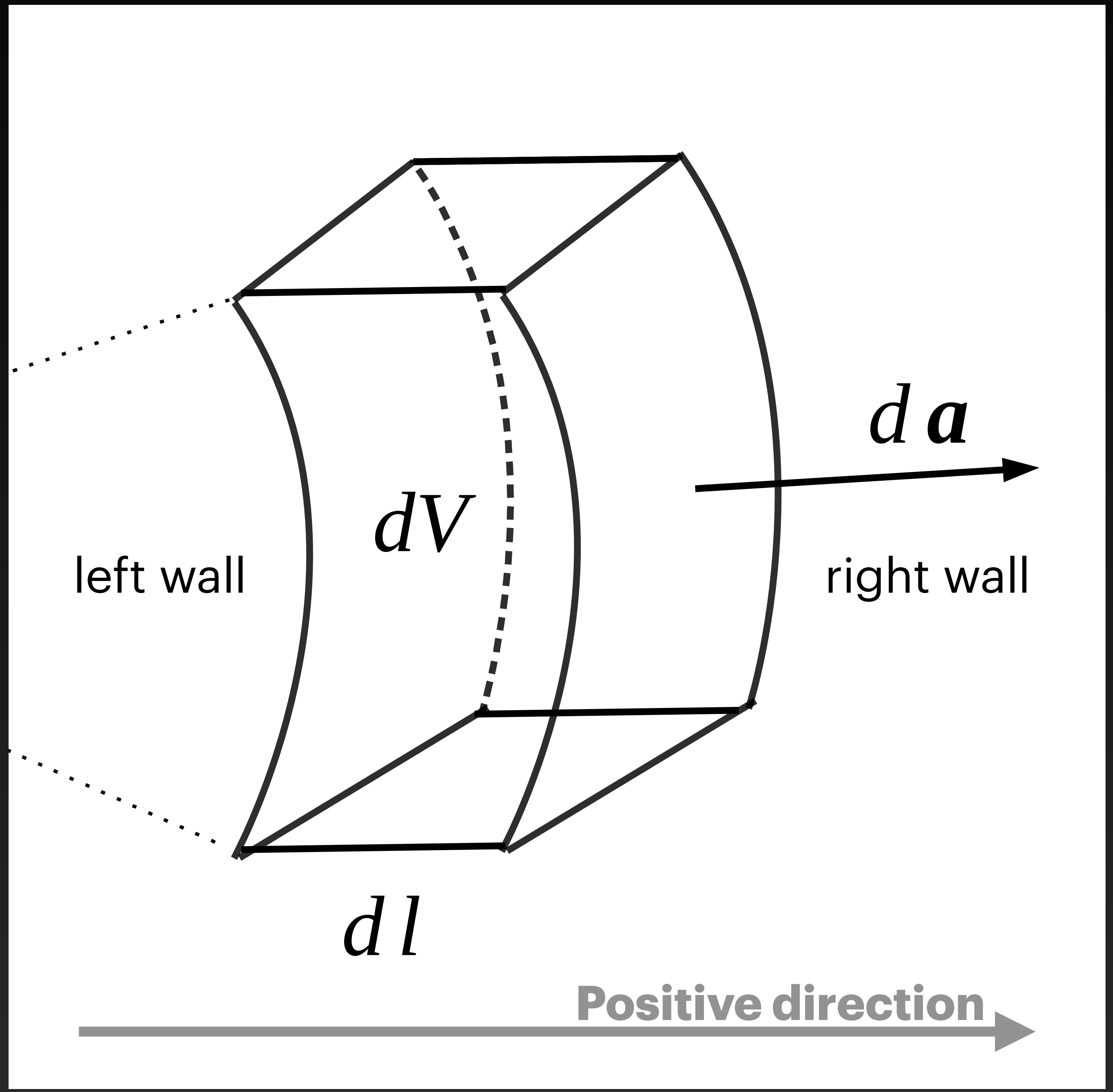
$$\frac{\partial f}{\partial t} = \frac{f(t + \Delta t) - f(t - \Delta t)}{2\Delta t} + \mathcal{O}(\Delta t^2)$$

$$\left[\frac{\partial f}{\partial x}\right]_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Finite Volumes

Another conceptualization of discretization

- In practice the implementation is quite similar to finite differences but conceptualized in an alternative way
- Good for describing flow (hyperbolic) terms which naturally lend themselves to integral forms (divergence theorem!)
- E.g. the LHS of the ionospheric transport equations listed previously are effectively solved in this manner
- Mean Value Theorem + evaluation of cell wall "flux" terms allows solution for, in this case, mass density.



$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\frac{d}{dt}\int \rho dV + \oint \rho \mathbf{v} \cdot d\mathbf{a} = 0$$

To the extent that discretized quantities represent cell averages and all transport is 1D we can develop a simple discretization

$$\frac{d}{dt}(\rho_i \Delta V) = \int_{right} [\rho v]_{i+1/2} da - \int_{left} [\rho v]_{i-1/2} da$$

Approaches to Solving Partial Differential Equations

- Generally speaking PDEs less straightforward to solve than ODEs
- Methods are generally organized by equation types, hyperbolic, parabolic, or elliptic.

	Canonical form	*Ionospheric form(s)*		
Hyperbolic	$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$	$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \mathbf{v}\right) = 0$	$\frac{\partial}{\partial t}\left(\rho \mathbf{v}\right) + \nabla \cdot \left(\rho \mathbf{v}\mathbf{v}\right) = 0$	(Mass/momentum flow)
Parabolic	$\frac{\partial f}{\partial t} - \alpha\frac{\partial^2 f}{\partial x^2} = 0$	$\frac{\partial T}{\partial t} - \nabla \cdot (\alpha \nabla T) = 0$		(Heat equation)
Elliptic	$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$	$\nabla \cdot (\boldsymbol{\sigma} \nabla \Phi) = 0$		(Current continuity)

- One could teach an entire course in solutions to these three problem types!
- Here we aim to present some very basic approaches but please do not consider these comprehensive or perhaps even advisable!

Elliptic Solutions

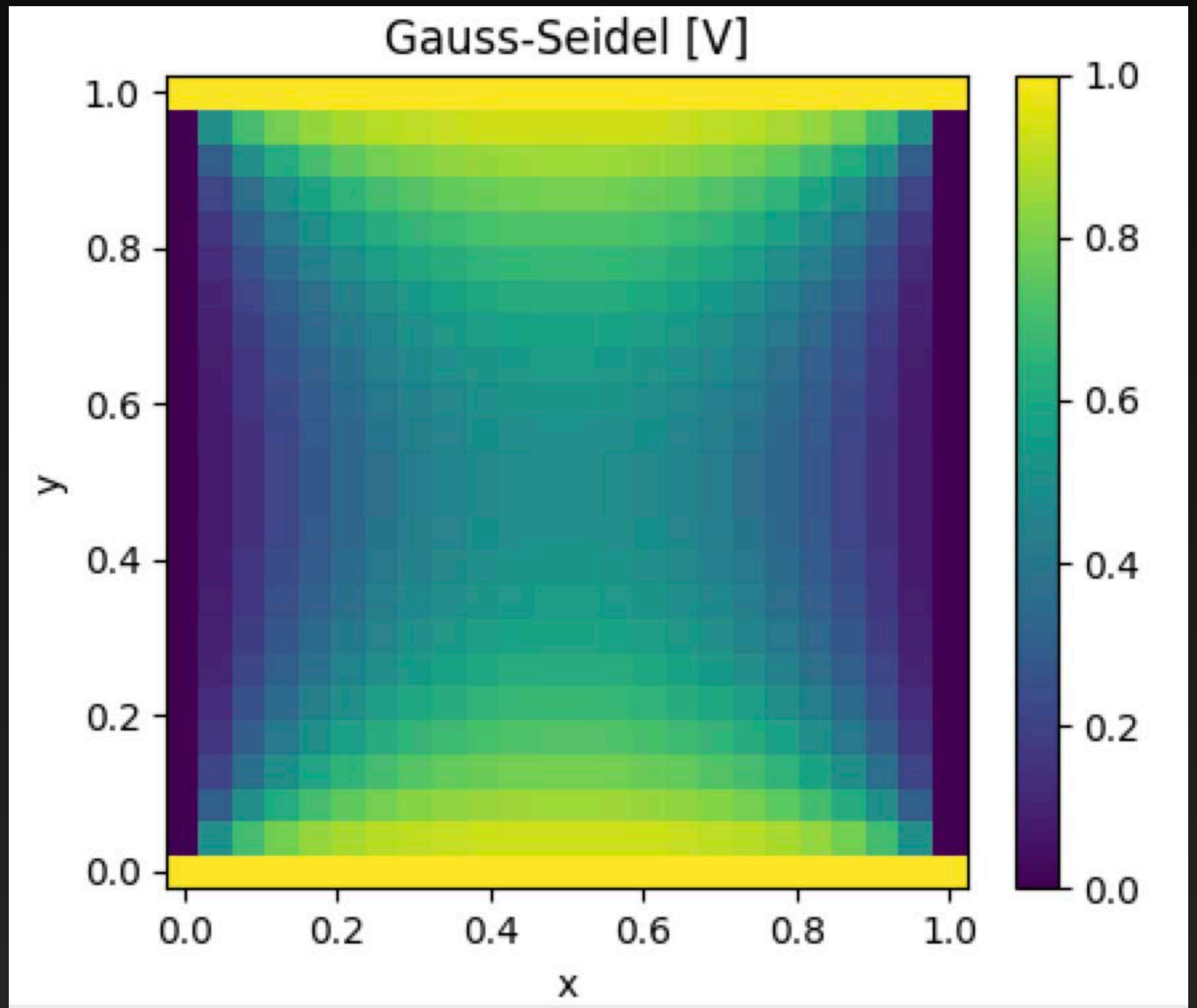
- Canonical equation is the Poisson equation. In 2D:

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0 \qquad \frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

- Standard approach is to generate a system of equations using centered spatial differences:

$$\frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{\Delta x^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{\Delta y^2} = 0$$

- Notice each equation has five unknowns; so this forms a banded system
- Number of unknowns is very large, N^2, where N is number of grid points in one dimension. This means the matrix has size N^2 x N^2.
- Even for 2D problems, special methods are needed to produce a solution.
  - Older (slower) methods are usually based on successive over-relaxation or Gauss-Seidel iterations. Sometimes these are still used but they are basically outdated at this point.
  - Newer methods implemented in the UMFPACK and MUMPS software packages are based on sparse LU factorization strategies, Intel has similar software (PARDISO).
- 3D problems with 10^6 or more grid points are extraordinarily difficult...



https://github.com/mattzett/numerical_electromagnetics/blob/main/electrostatics/2Dpotential.py

Parabolic Solutions

- Canonical form is the heat equation:

$$\frac{\partial f}{\partial t} - \alpha \frac{\partial^2 f}{\partial x^2} = 0$$

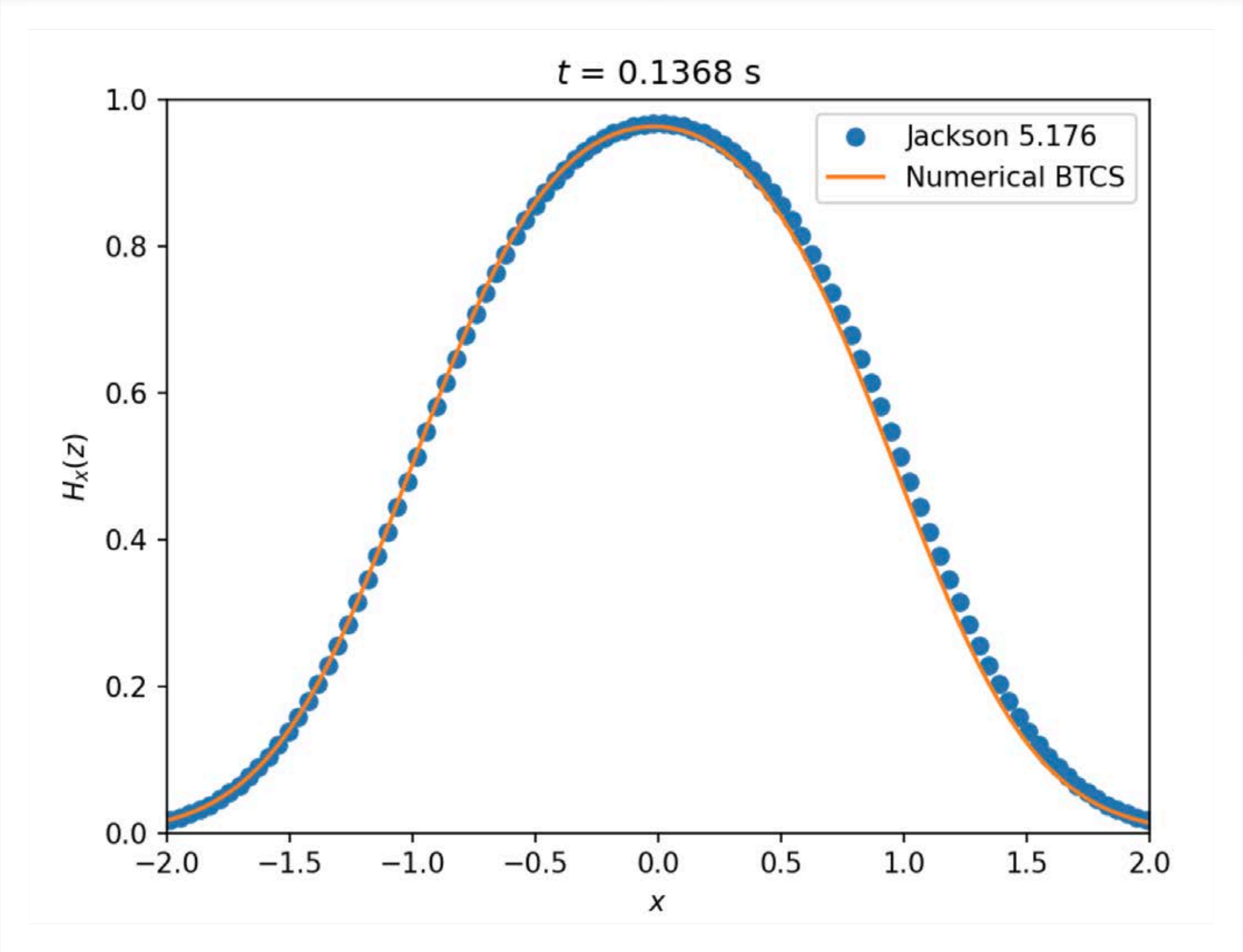
- If we difference first-order in time and second order is space: BTCS algorithm

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} - \alpha \frac{f_{i+1,j}^{n+1} - 2f_{i,j}^{n+1} + f_{i-1,j}^{n+1}}{\Delta x^2} = 0$$

- Solving to produce an algorith/update formula:

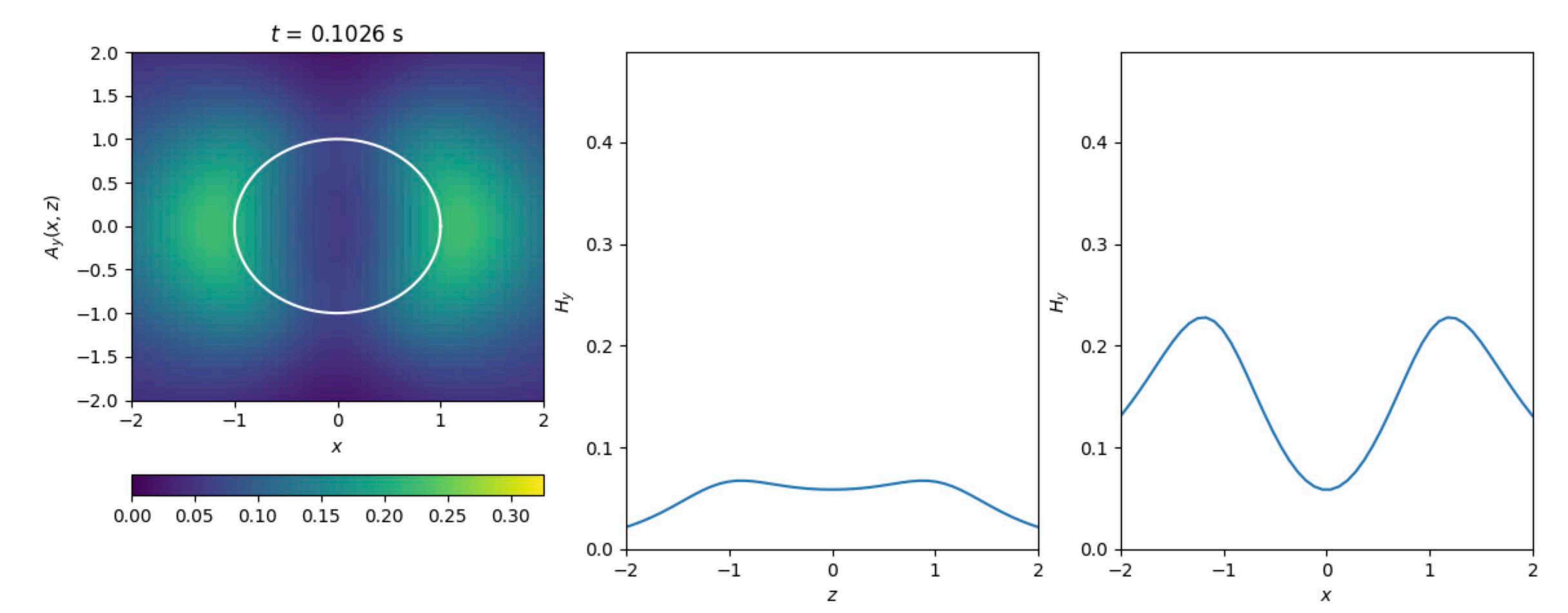
$$-\alpha \frac{\Delta t}{\Delta x^2} f_i^{n+1} + \left(1 + 2\alpha \frac{\Delta t}{\Delta x^2}\right) f_i^{n+1} - \alpha \frac{\Delta t}{\Delta x^2} f_{i-2}^{n+1} = f_i^n$$

- To update from time level n to n+1 we must solve a matrix system (tridiagonal in this case)



1D toy problem: https://github.com/mattzett/numerical_electromagnetics/blob/main/magnetic_diffusion/diffusion1D.py

2D toy problem: https://github.com/mattzett/numerical_electromagnetics/blob/main/magnetic_diffusion/diffusion2D.py



Hyperbolic Solutions

- Canonical equation is scalar advection equation (wave equation):

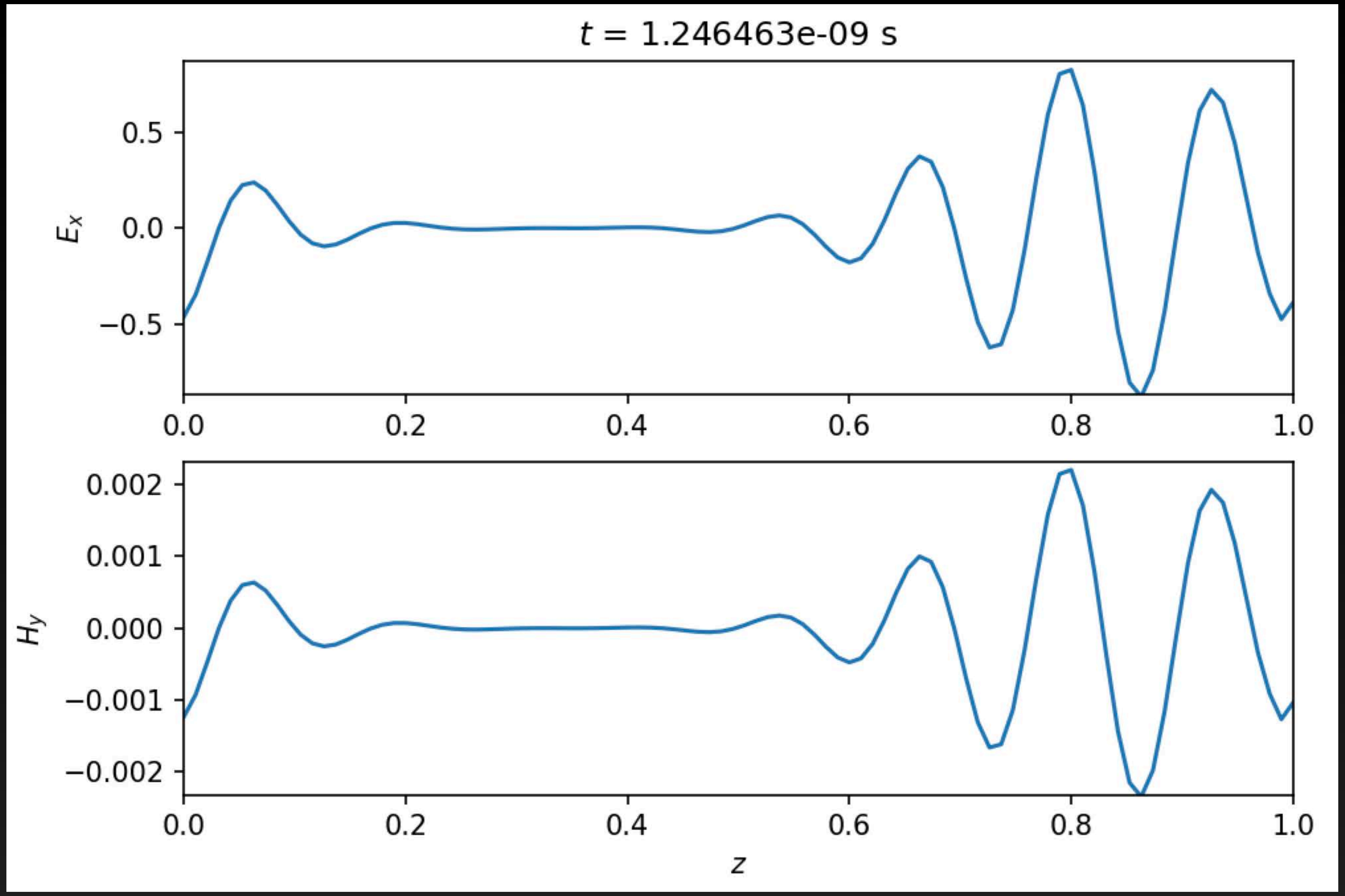
$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = 0$$

- In many regards these are the most difficult types of problems to solve. Obvious approaches are numerically unstable.
- The simplest possible stable algorithm is the upwind method *(Godunov, 1959)*:

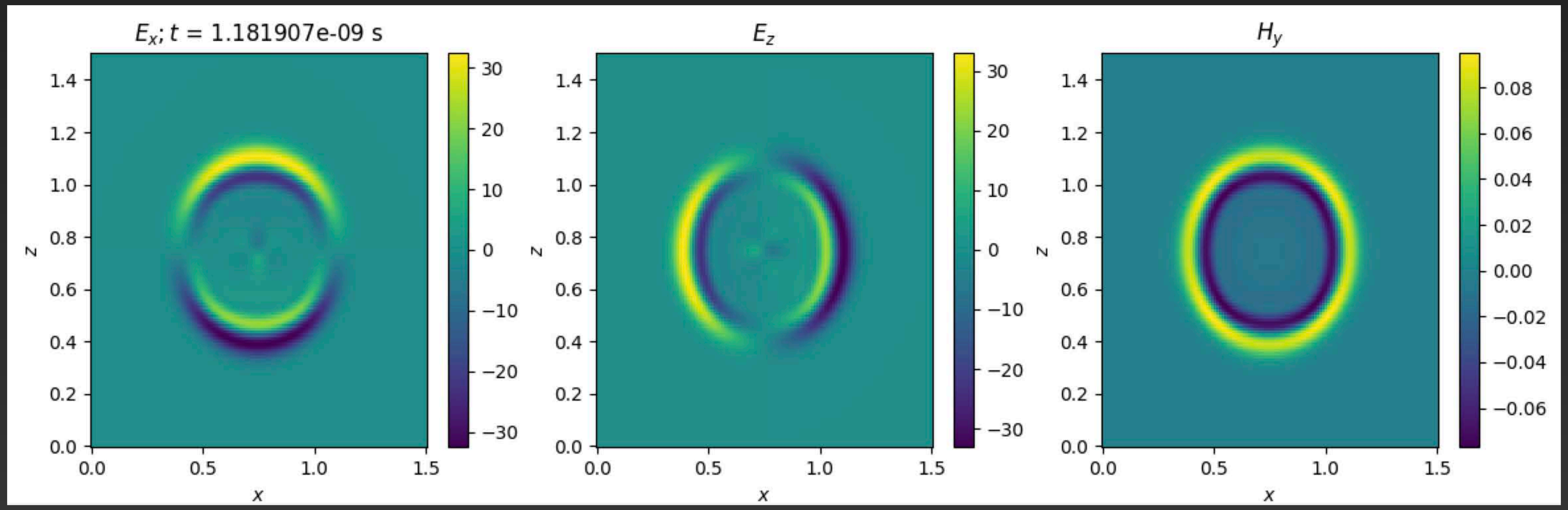
$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + v\frac{f_i^n - f_{i-1}^n}{\Delta x} = 0 \qquad v > 0$$

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + v\frac{f_{i+1}^n - f_i^n}{\Delta x} = 0 \qquad v < 0$$

- This approach is incredibly diffusive and unusable in practice but does prevent artificial oscillations and is the basis for modern shock-capturing schemes
- If you have a smooth function (i.e. no weak solutions) the Lax-Wendroff method will usually produce acceptable results. Can also try FDTD if you don't mind staggering you mesh BUT both of these will produce terrible results in systems that form shocks…



1D toy wave-packet problem: https://github.com/mattzett/numerical_electromagnetics/blob/main/waves/EMwaves1D.py

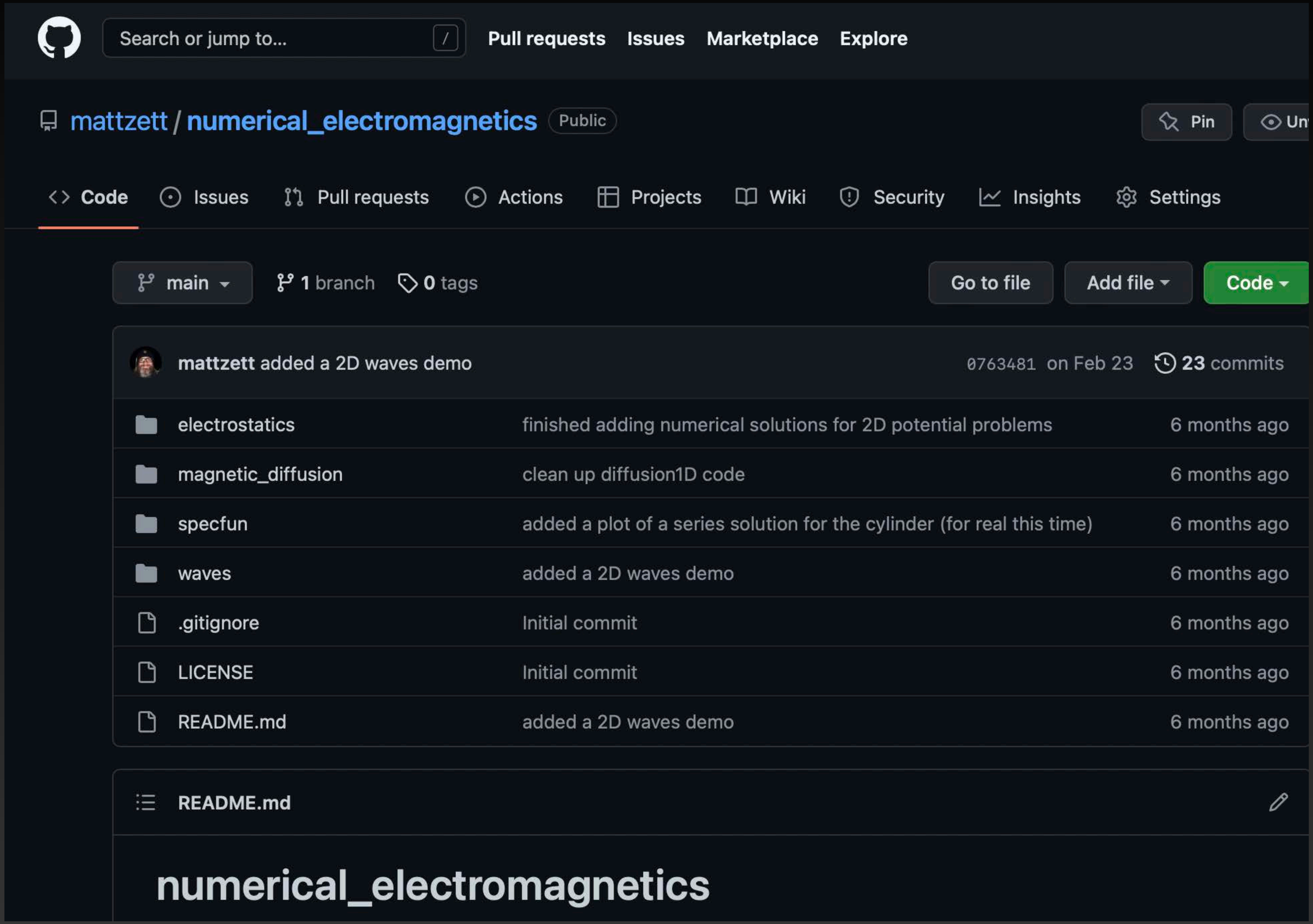


2D toy wave problem: https://github.com/mattzett/numerical_electromagnetics/blob/main/waves/EMwaves2D.py

Demos

Using electromagnetic theory as an example of how to solve elliptic, parabolic, and hyperbolic equations

These can be downloaded or viewed at: https://github.com/mattzett/numerical_electromagnetics



... But ionospheric equations are mixed type...

And we only have algorithms to deal with 3 basic PDEs

- Enter *operator splitting* — possibly the most useful and powerful technique in numerical analysis.
- Splitting allows us to separate mixed-type PDEs into constituent elliptic, parabolic, and hyperbolic equations — each can be solve sequentially using optimal approaches.
- In fact a form of this approach has been used to resolve different spatial dimensions in the example Python codes solving 2D problems at https://github.com/mattzett/numerical_electromagnetics

Example operator split: advection, diffusion, source equation

$$\frac{\partial}{\partial t}(\rho\epsilon) + \frac{\partial}{\partial z}(\rho\epsilon v_z) = -p\left(\frac{\partial v_z}{\partial z}\right) + \alpha\frac{\partial^2 T}{\partial z^2}$$

$$\frac{\partial}{\partial t}(\rho\epsilon) = -\frac{\partial}{\partial z}(\rho\epsilon v_z) \longrightarrow \left[\rho\epsilon\right]^*$$

$$\frac{\partial}{\partial t}\left(\left[\rho\epsilon\right]^*\right) = -p^*\left(\frac{\partial v_z}{\partial z}\right) \longrightarrow \left[\rho\epsilon\right]^{**}$$

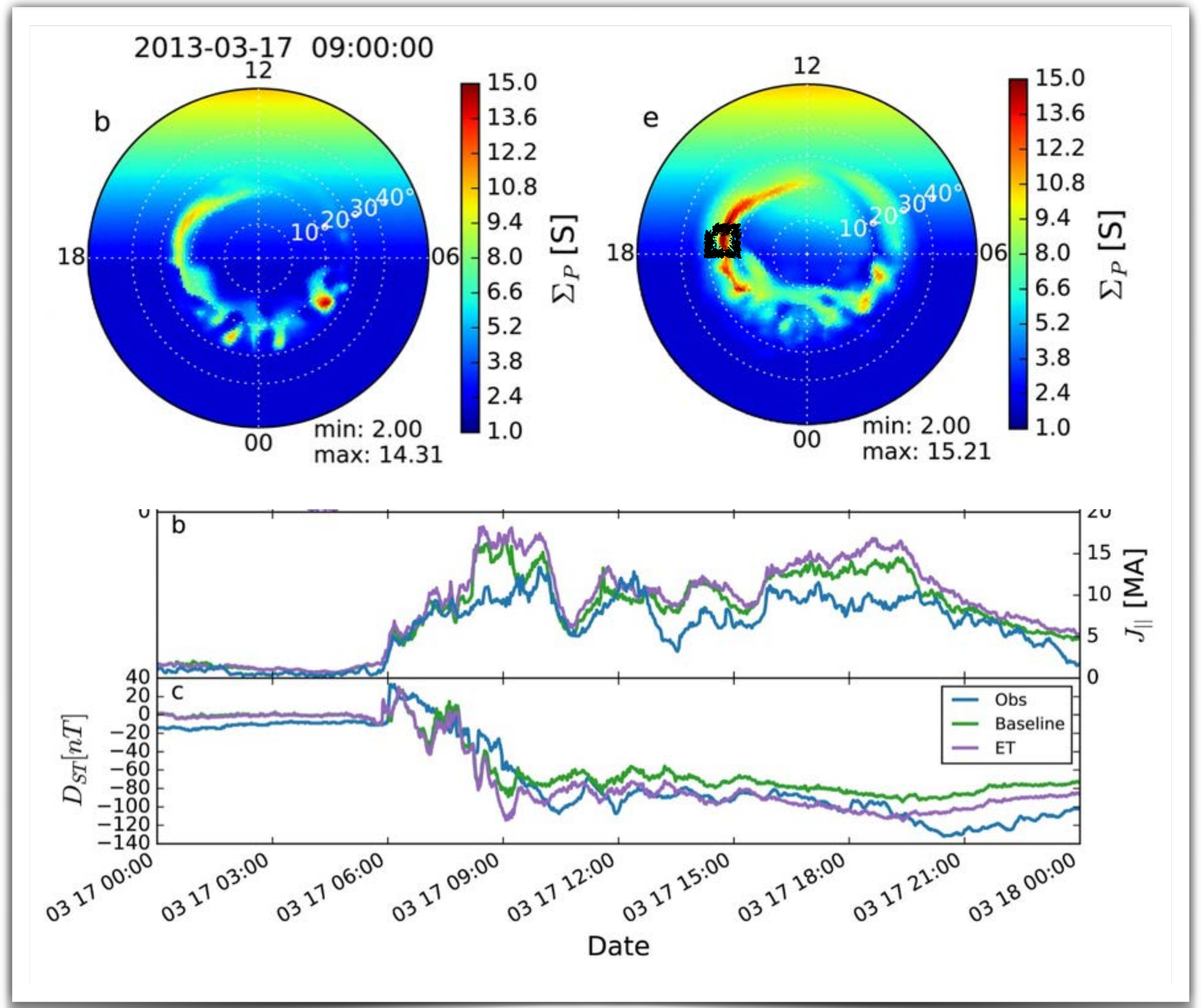
$$\frac{\partial}{\partial t}\left(\left[\rho\epsilon\right]^{**}\right) = \alpha\frac{\partial^2 T^{**}}{\partial z^2} \longrightarrow \left[\rho\epsilon\right]^{n+1}$$

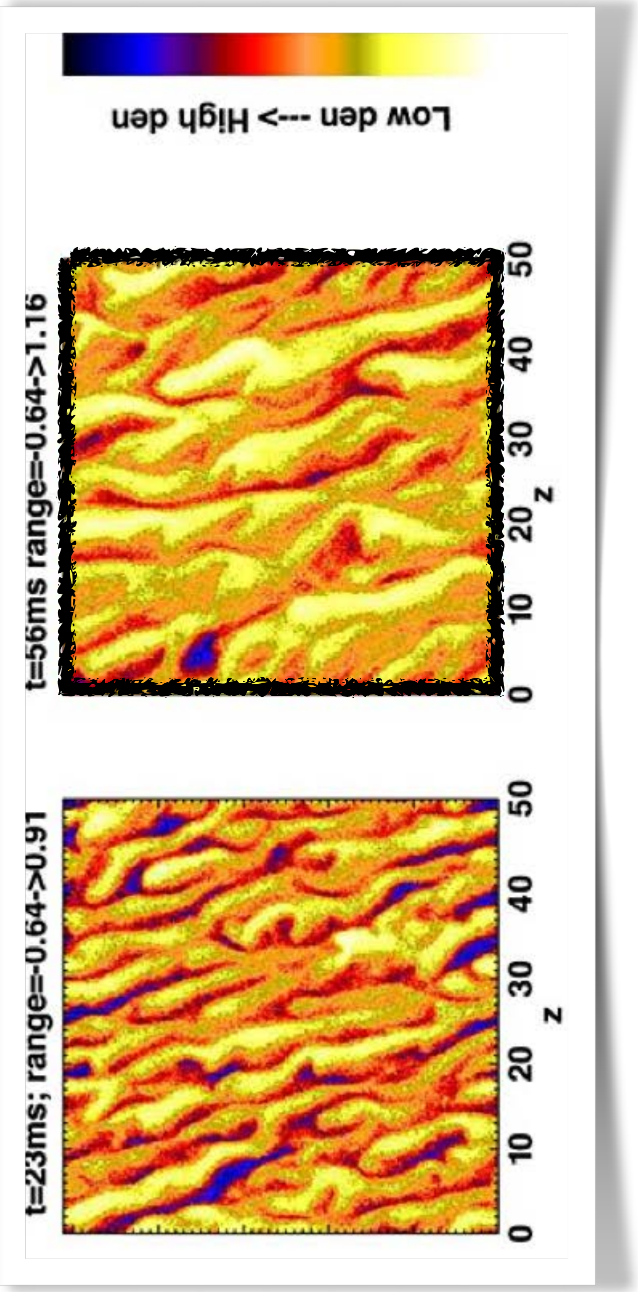
The Future

Modeling Needs (part I)

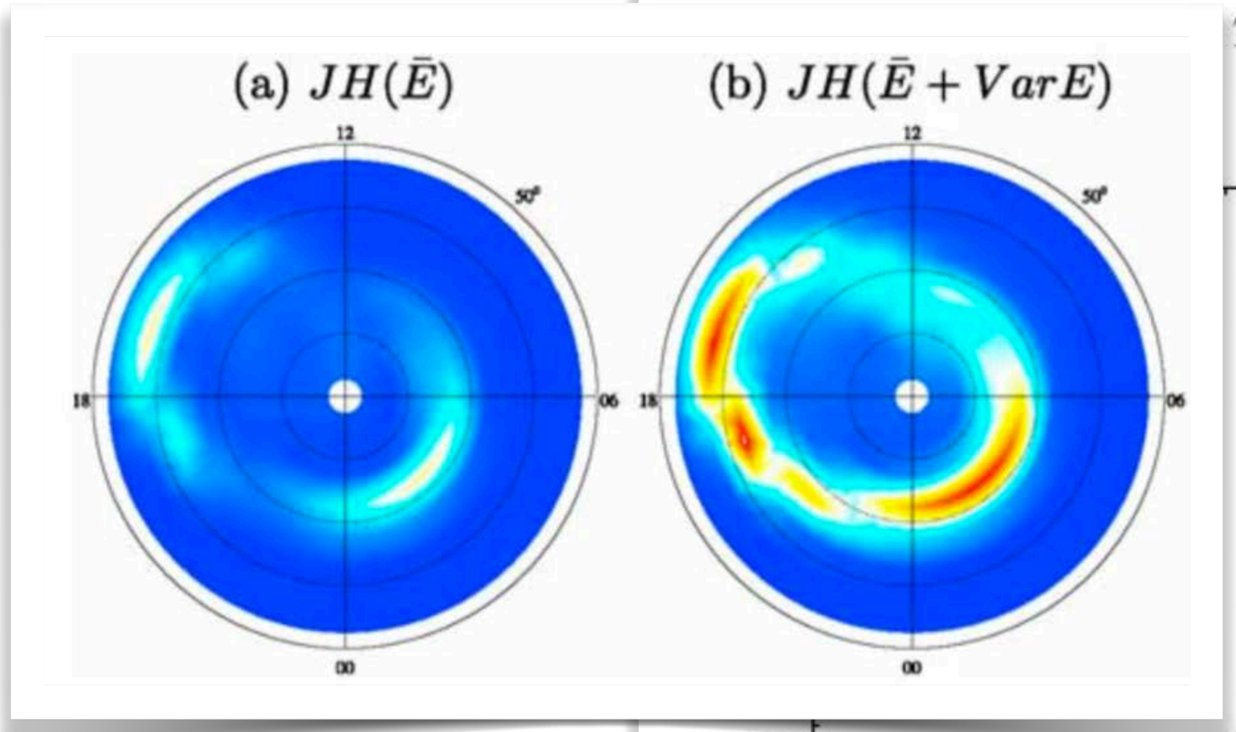
- **Develop new approaches to multi-scale physics describing coupling and feedback across scales** (coupling and parameterization strategies)
  - Plasma instabilities associated with radio disruptions depend on background state
  - Kinetic turbulence alters conductance which can have global consequences *(Wiltberger et al, 2017)*
  - Small-scale electrodynamics of MI coupling: joule heating and momentum inflow *(Deng et al, 2009)*
- **Improve predictive capability of models:** physics
  - It is challenging to predict simple day-to-day variability in IT —> smaller scale studies may be “biased” by lack of knowledge of “mean state”
  - In many cases we know physical processes are not being accounted for properly (e.g. GW dynamics in LT; Alfvenic processes mediating MI coupling)

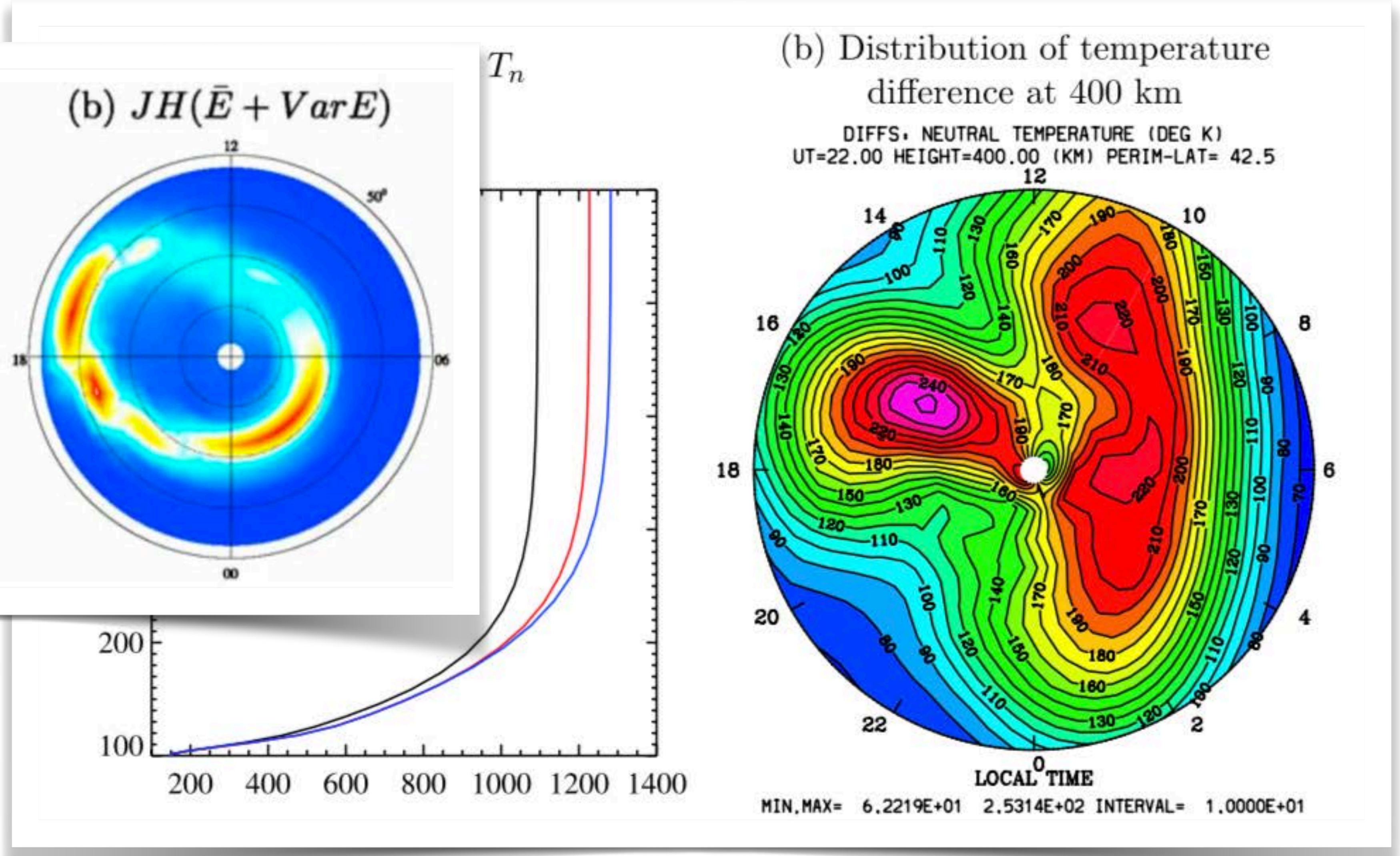
Wiltberger et al (2017)





Oppenheim and Dimant, (2013)

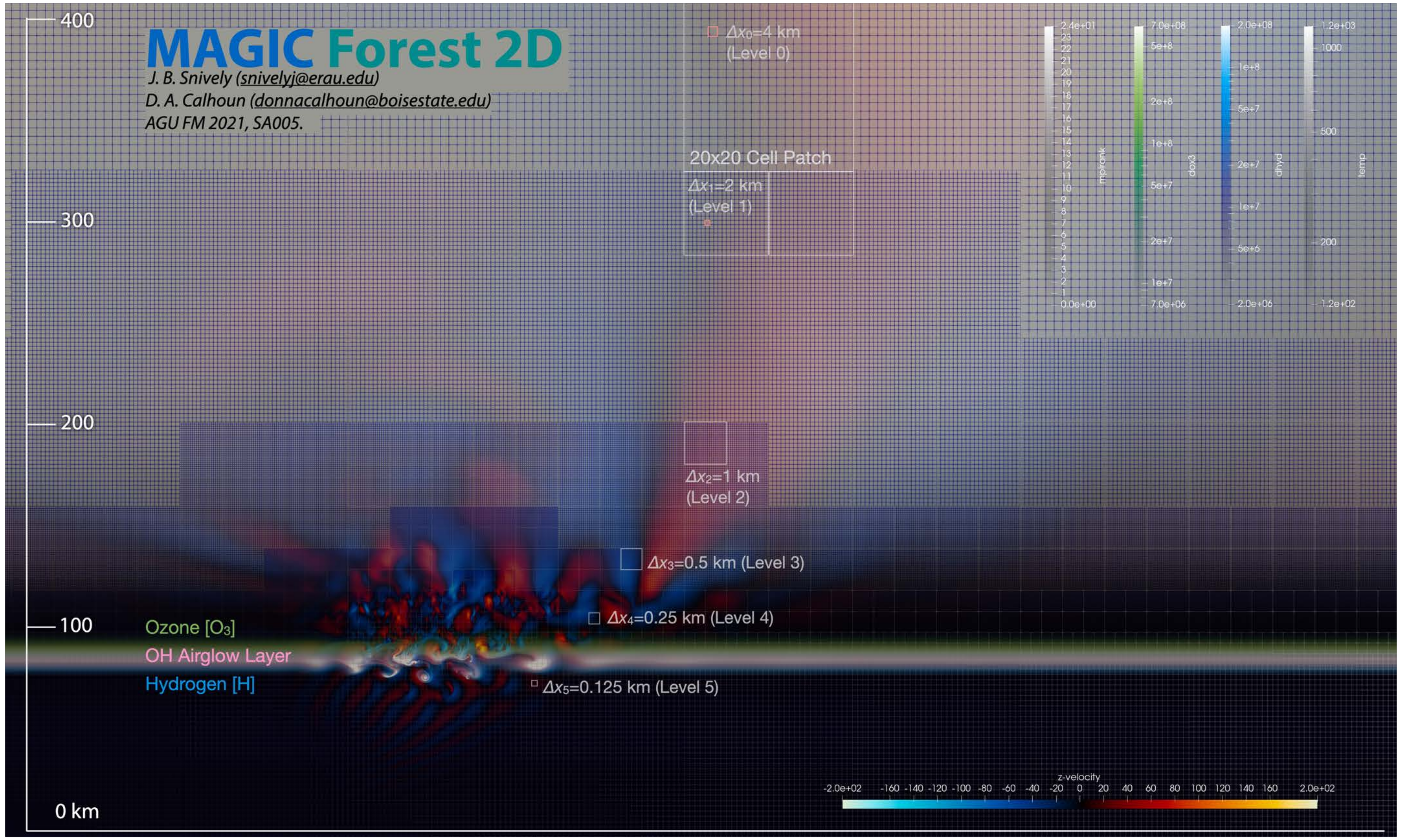


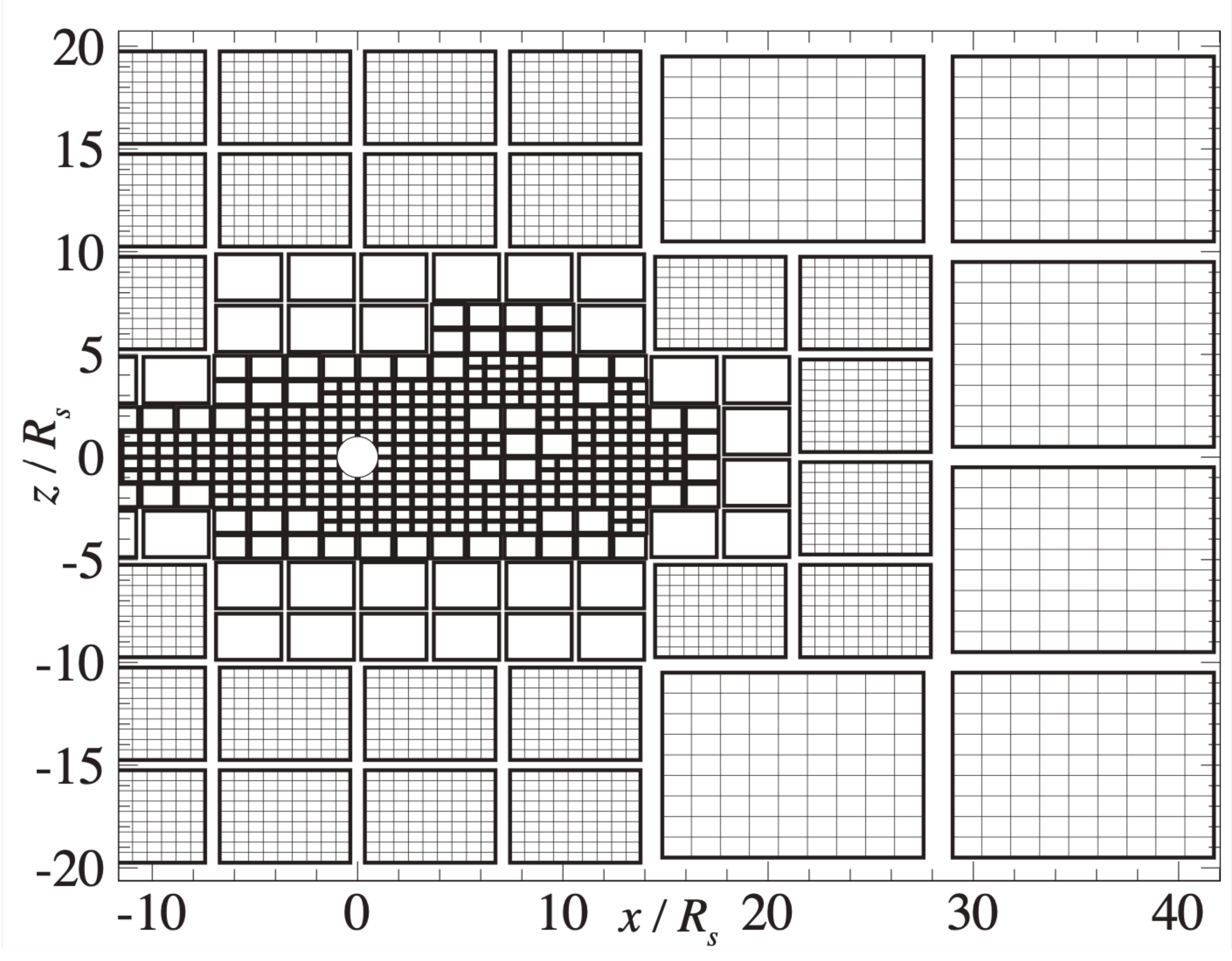


Deng et al. (2009)

Modeling Needs (part II)

- **Improve predictive capability of models:** resolution
  - Require _both_ global and local general-purpose models.
  - Leverage techniques to efficiently deal with localized processes in a global context; i.e. adaptive mesh refinement (AMR)
- **Sustain investment in general purpose codes** — can reduces time to science/application and "cost".
  - Continue ground-up development of bespoke models tailored to specific problems.
  - Modest software engineering investments to improve and promote accessibility (build/run, post processing and visualization, verification)
- **Accessibility challenges** — Computational infrastructure/resources and licensing practices.
- **Explore collaborations benefitting both science and industry**, e.g. commercial space.



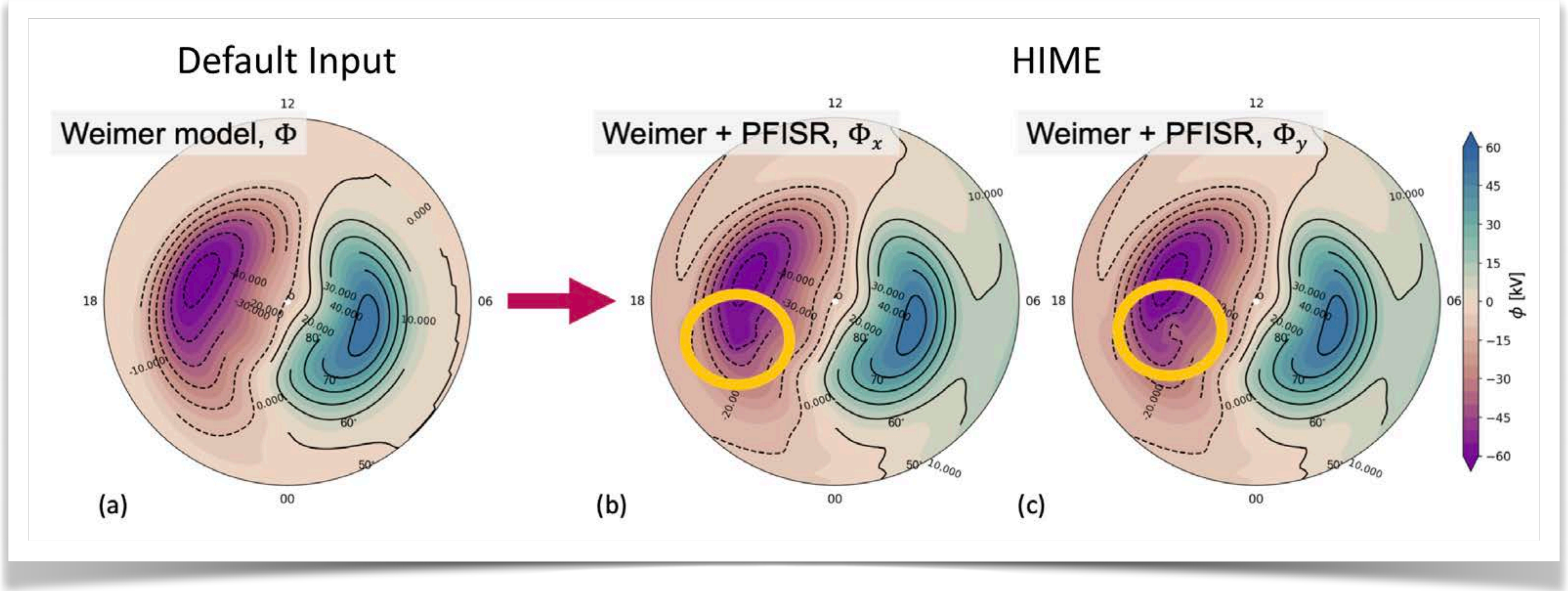


Gombosi et al (2001)

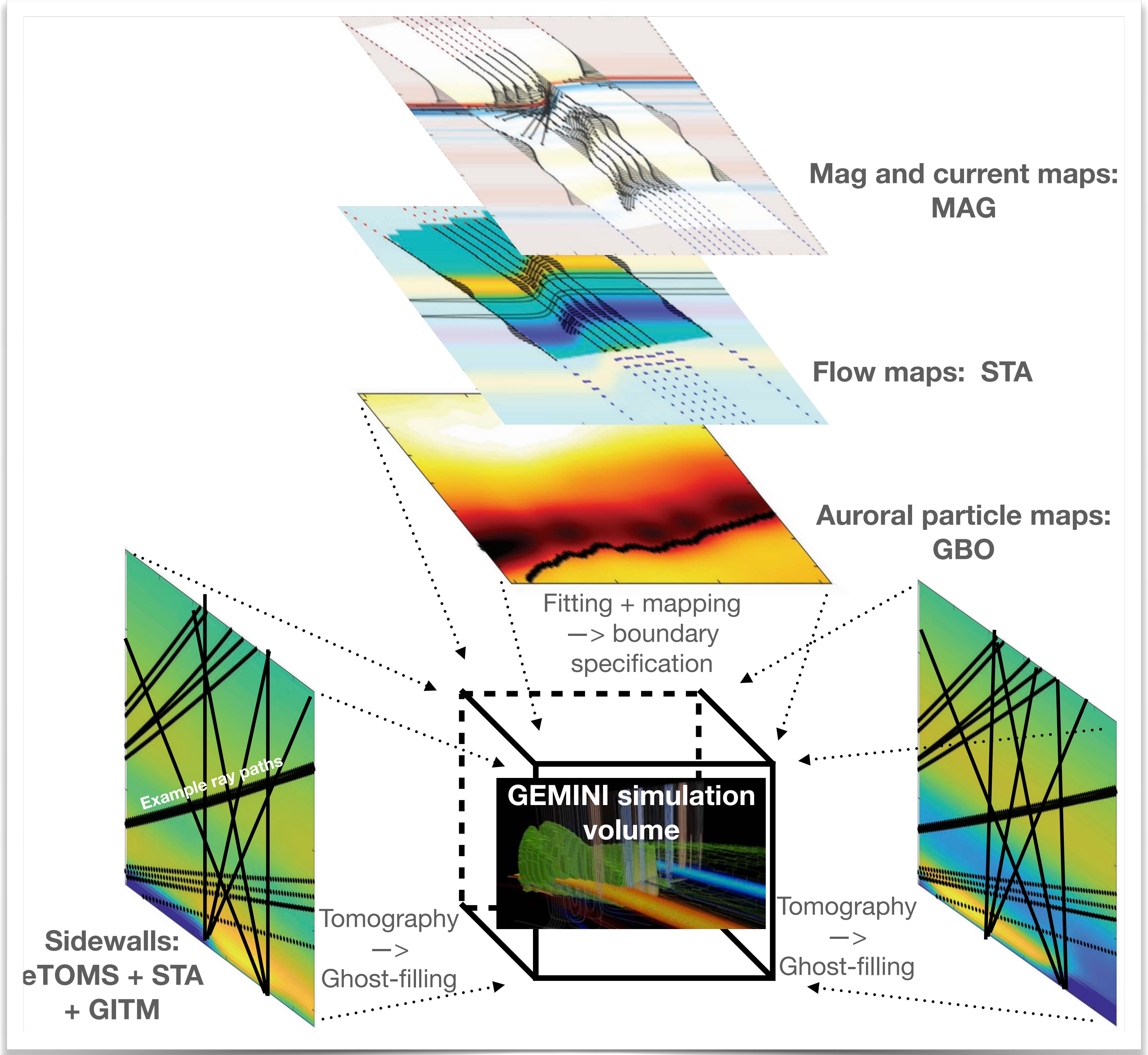
Two AMR codes: (Top) MAGIC-Forest compressible model simulation of breaking GWs. (Left) BATSRUS MHD model mesh configuration

Data constraints for models

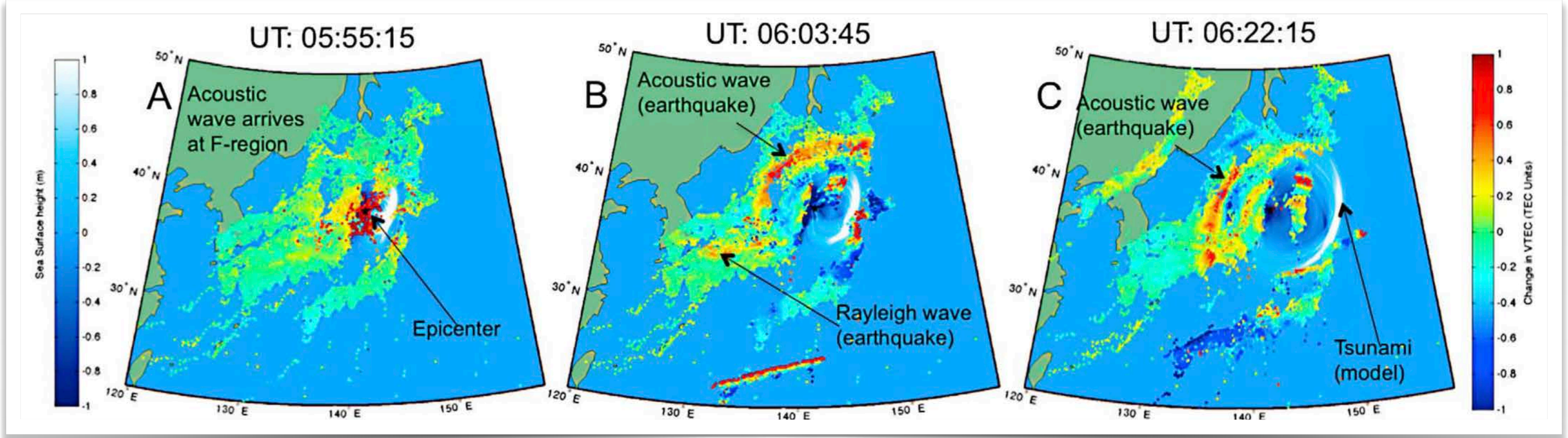
- **Model applications (as opposed to purely theoretical studies) suffer from relatively poor data constraints.**
  - High latitude ionosphere modeling - potentials, initial density, precipitating particles/conductance. Auroras, plasma patches.
  - Ground-level transient disturbances - diagnosing lower atmospheric dynamics, e.g. from seismic sources, from IT data.
  - Ionospheric plasma sources to magnetoshere - spatial distribution of energy sources affects ionospheric mass provided to the magnetosphere.
- **Tools for direct comparisons with data are needed to bring simulation outputs closer to quantities that can be compared to data.**
  - Improves quality of and realism in conclusions — improves the value of both the simulations and data products. Space mission and ground-based instrument design; planning of operations



Incorporation of local measurements into global modeling (HIME Ozturk et al 2020)



Local-scale auroral electrodynamics mission concept (ARCS; Lynch et al)



Better Visualization Tools