Data Science and Analytics: Ensemble Modeling Panel

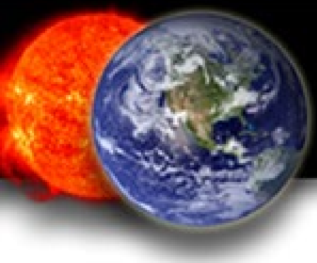
Key Questions:

1) The terrestrial weather community does multiple-model ensemble modeling, is that practical for Space Weather in the near term?
2) What data sources are needed but unavailable (proprietary, classified, etc.) that are hampering next steps? Do we work to get them available or can (ML, data curation, etc.) take care of it and how?

Moderator: Mary Hudson, Committee Member

Eric Adamson	NOAA/SWPC
Dan Welling	University of Texas Arlington
Sean Elvidge	University of Birmingham UK
Nick Pedatella	UCAR
Kent Tobiska	Spacewx SET
Edmund Henley	UK Met Office

Space Weather Operations and Research Infrastructure Workshop: Phase II, Wednesday, April 14, 2022, 1100 ET



Ensemble Modeling

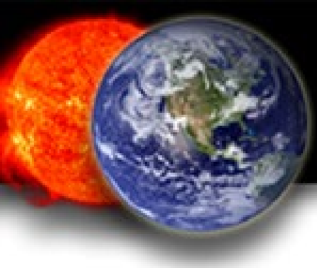
Ensembles at NOAA's Space Weather Prediction Center

- ➢ Recognized potential to constrain uncertainties and transform deterministic -> probabilistic results
- ➢ No ensembles formally in operations, but development work is ongoing
- ➢ Early focus on solar / solar wind domain
  - ✓ CME characterization
  - ✓ Ambient solar wind

Uncertainties remain largely observational

→ ***Need improved coronagraphs and new vantage points***

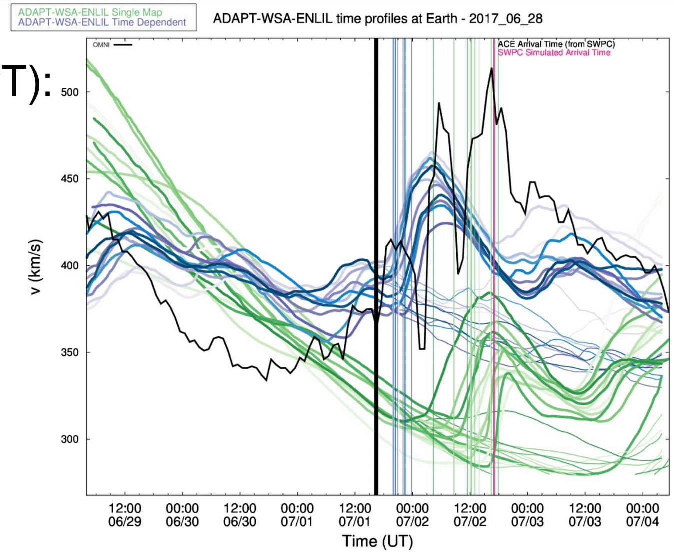
- ➢ Multi-model ensembles (MMEs) are of interest, where shown to be worth the resources

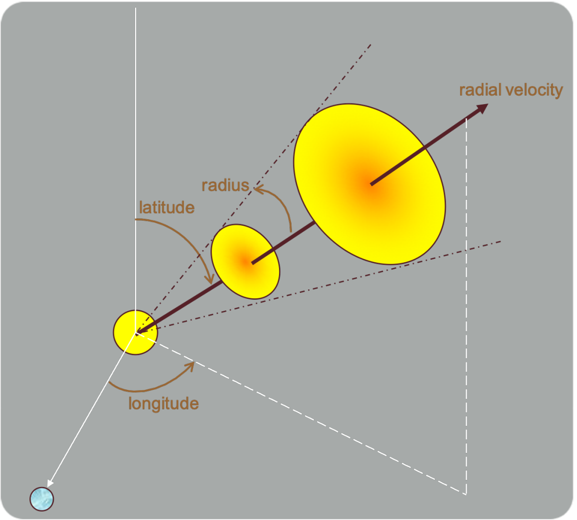


Ensemble Modeling

Air Force Data Assimilative Photospheric Flux Transport (ADAPT):

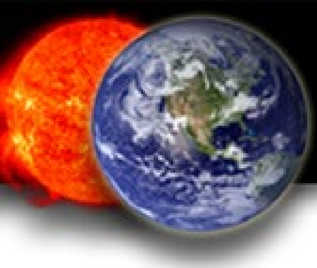
- Accounts for physical processes omitted w/in current synoptic maps
- Constrained by DA
- 12 member ensemble with IC variation in supergranulation





CME fit (cone parameters) ensemble (Pizzo et al., 2015):

- Based upon Taylor series expansion of arrival time error
- Perturbed ICs defined by maxima of input parameters
- Presumes linear relationship between IC variance and resultant parameters of interest



Ensemble Modeling

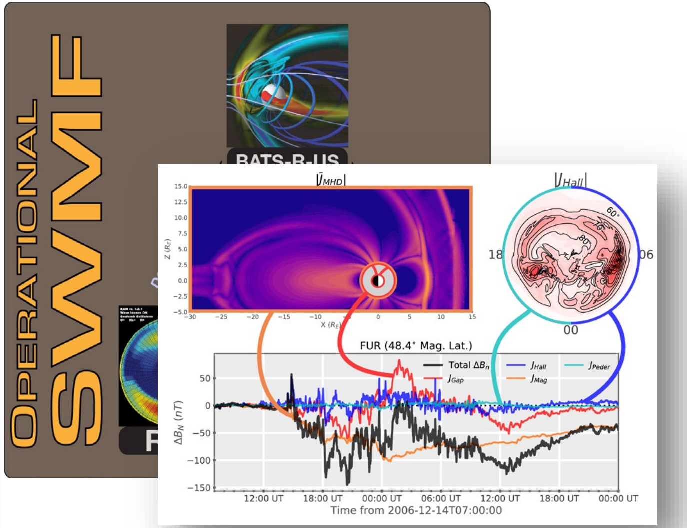
Future / Outstanding questions

- How can such ensembles be efficiently combined? Is Monte-Carlo approach best or are there more efficient methods?
- How can ensembles be effectively pruned, particularly in coupled model systems (e.g., solar-IP-geospace-…)? Combine with Data Assimilation?
- Can “submodel” MME’s afford avenue for progress in constraining magnetic structure w/in CMEs?

Summary

- Critical need for improved observational capabilities toward better characterization of CMEs
- Effective synthesis of results to meaningfully convey information to users is key
- Storage resources will be critical in laying foundation for large-scale ensemble modeling

Geospace Modeling Today

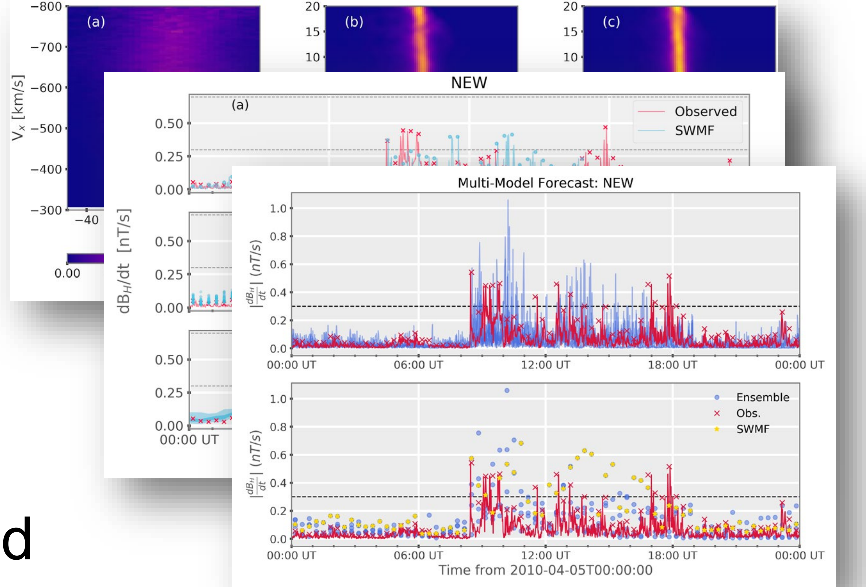


Contemporary geospace approach: global MHD coupled to ionosphere and ring current models

- Driven by L1 observations of solar wind and interplanetary field
- Used deterministically forecast ground magnetic disturbances

Currently, use of ensembles is *very* limited!

- Work has focused on perturbed input ensembles (see *Morley et al.*, 2016; current work by Toth at U. Michigan)
- Initial multi-model work in progress



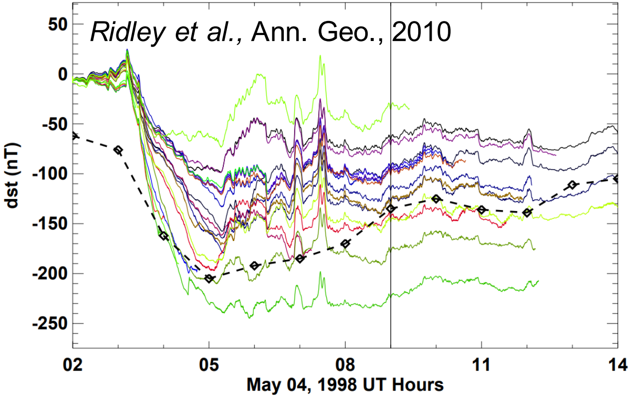
Validation efforts are not well refined

Low Hanging Fruit

We’re ready for more than the proof-of-concept

- Early work shows promise that ensembles can increase predictive skill of geospace/GMD models
- In-depth, structured studies needed to understand extent of improvement, number of ensemble members, etc.

Perturbed physics ensembles are the obvious next step



- *Many* studies demonstrate model sensitivity to IBCs, physics options, new physics features, etc.
- Many physical processes ”hidden” in input parameters
- No work to-date that fully quantifies uncertainty across the input parameter space

Required Resources

More upstream monitors required (L1 and near-Earth)

- Multiple L1 monitors help bound uncertainty in magnetospheric driving conditions, generate ensemble members
- Near-bow shock observations could provide last-moment member weighting, improve forecast accuracy

More ground magnetometers and auroral imaging are necessary to bolster validation & uncertainty analysis

- More *high time resolution* magnetometer data at more locations
- Auroral imaging allows us to validate one of our weakest points of modeling – auroral conductance and dynamics

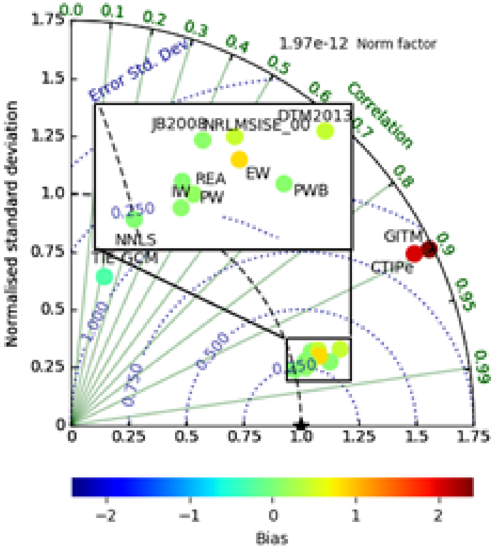
Geospace data assimilation is a huge challenge

- Large volumes, disparate physics often leads to “point source” effect of assimilation: local but not global impact
- Possibilities include assimilation of ionospheric electrodynamics, auroral observations, ground magnetometers – how viable is this?

Up and Coming Approaches - Ensembles

- Ensembles can be used in a number of different ways for space weather e.g.:
  - Data assimilation (DA)
  - Multi-model ensembles (MMEs)
  - Uncertainty quantification

- Use of MMEs is in its infancy but has demonstrated reduced errors in model specification
- Should be used in DA approaches to reduce model propagation uncertainty (“*Q*” matrix)



Skill of thermosphere models and different MME approaches compared to CHAMP derived neutral densities

Orthogonal Ensemble Members

- A key question is how to generate *independent / orthogonal* ensemble members
  - Orthogonal ensemble members in DA are needed (and usually assumed) for estimation of covariance matrices and reduction of propagation errors
  - Independent members are needed in MMEs for the assumption of error cancellation

- Ensembles often generated by perturbing (a subset of) model drivers
  - Results in ensembles with artificially small variance
  - Little work done in understanding the sensitivity of specific model drivers to specific systems/use cases - could help to understand ensemble generation

Do we have what we need?

- *N* ensemble members mean a factor of *N* increase in storage
- *N* ensemble members from *M* different models is a factor of *NxM* increase for MME storage!
    - Interesting and novel science could be investigated from this output, but we need to keep it
    - Requires investment in computational resources - crucially including data storage and associated management

- New observations
    - More data (with well quantified errors…) is always good!
        - Can be used for both validation and/or assimilation
    - There is an observational data gap for the thermosphere
    - However, there is an unprecedented launch of satellites
        - Constellations of commercial satellites could bridge the gap

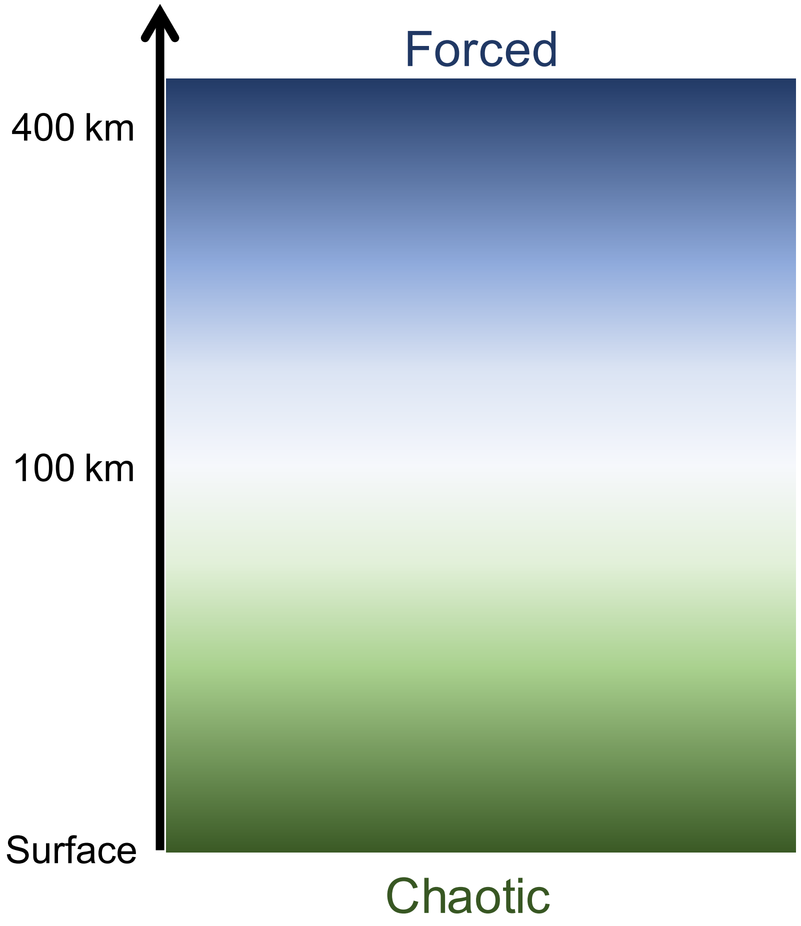
Ensemble Generation Techniques in the Ionosphere-Thermosphere

- Single model ensembles are often generated through perturbed forcing (i.e., input) parameters (F10.7, Kp).

- This approach is problematic in several ways:
  - Ensemble may not be reflective of the uncertainty in the input parameters and/or the uncertainty of the model itself.
  - Ensemble spread is deficient for some regions/times.
  - Neglects internal chaotic contributions, which may be important for short-term (< 24 h) forecasts and in the lower thermosphere and bottomside ionosphere.

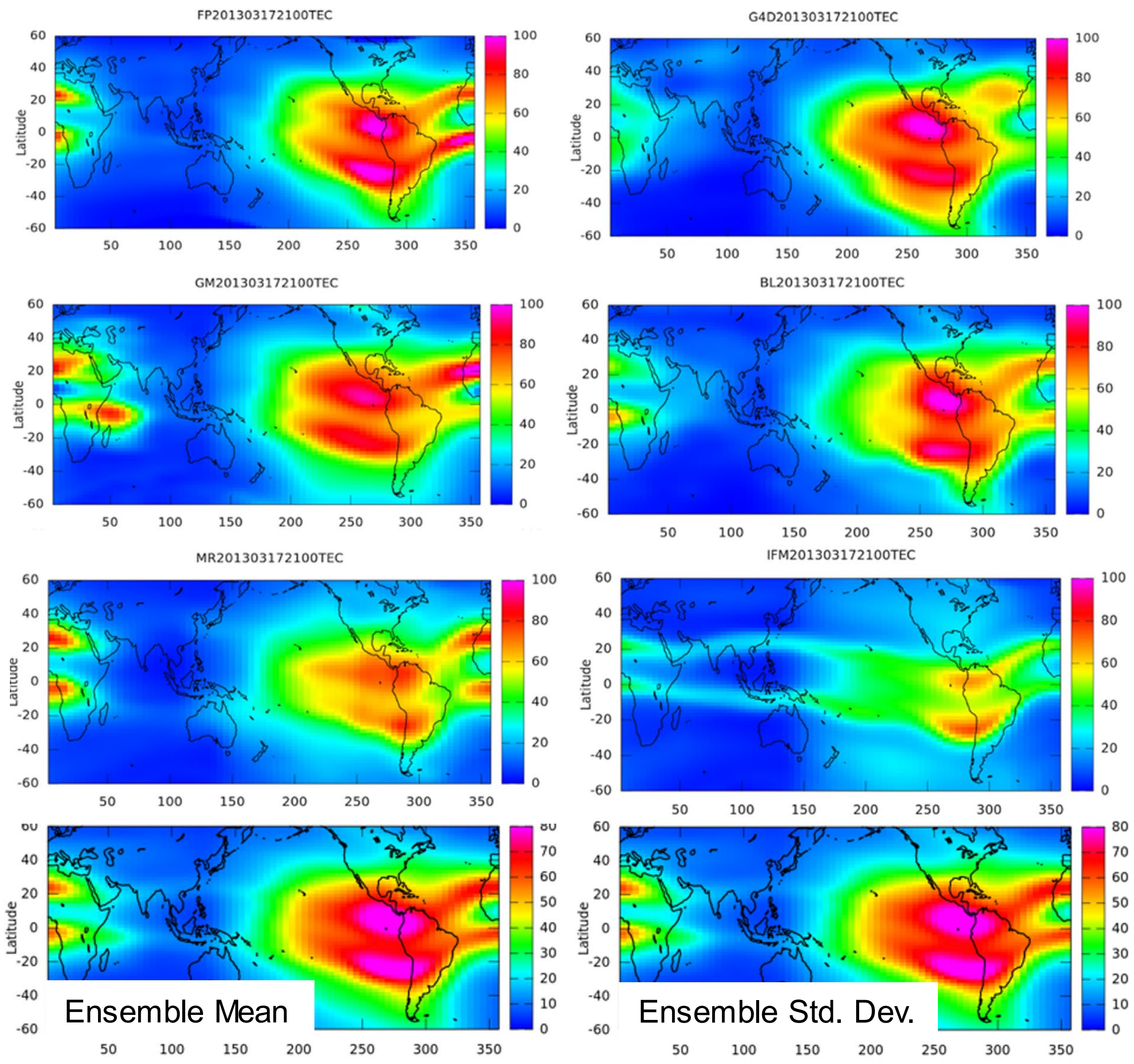
- **Need to develop and evaluate new approaches for generating ensembles that address the above shortcomings.**

- Improved ensemble generation techniques are critical for developing a better understanding of uncertainty and for ensemble data assimilation.



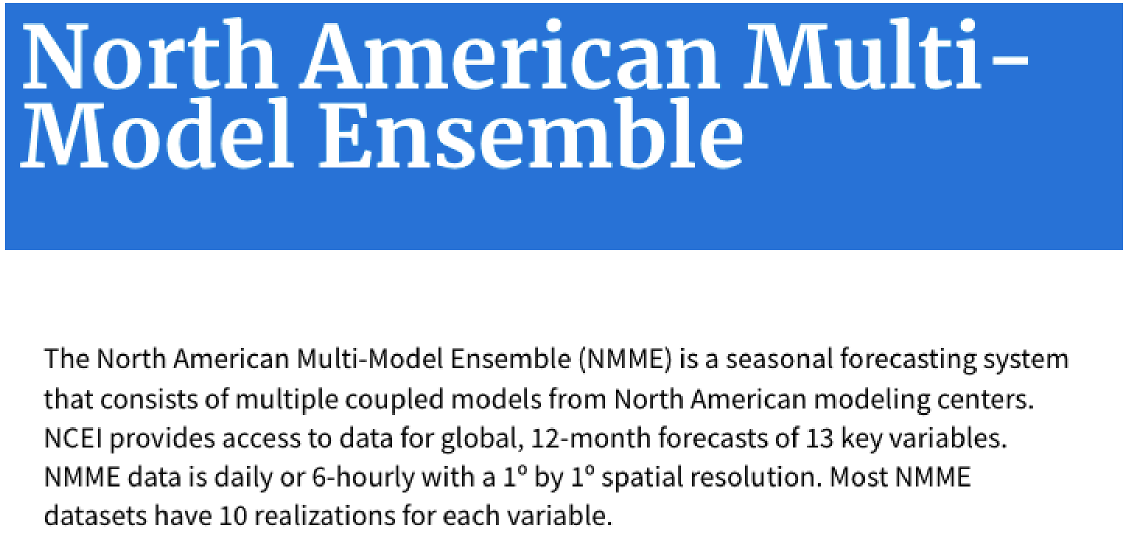
Multi-Model Ensembles

- Multi-model ensembles are widely used in climate and weather forecasting due to improvements in forecast consistency and reliability.
- Multi-model ensemble approaches have yet to be widely adopted in ionosphere-thermosphere research and forecasting.
- It remains unknown to what extent multi-model ensembles can improve current ionosphere-thermosphere forecast skill.
- **Research to understand how multi-model ensembles can be leveraged for ionosphere-thermosphere applications is needed.**
- **Enabling infrastructure would accelerate progress by making it easier to perform studies using multi-model ensembles.**



(Schunk et al., 2021; doi:10.1029/2019SW002404)

Multi-Model Ensemble Databases



North American Multi-Model Ensemble

The North American Multi-Model Ensemble (NMME) is a seasonal forecasting system that consists of multiple coupled models from North American modeling centers. NCEI provides access to data for global, 12-month forecasts of 13 key variables. NMME data is daily or 6-hourly with a 1° by 1° spatial resolution. Most NMME datasets have 10 realizations for each variable.

(https://www.ncei.noaa.gov/products/weather-climate-models/north-american-multi-model)

WCRP CMIP6

World Climate Research Programme

(https://www.wcrp-climate.org/wgcm-cmip)

- Development of databases for distribution of space weather simulations would facilitate the usage of multi-model ensembles.
- Such a database would:
  - Enable research into the use of multi-model ensembles for space weather.
  - Advance understanding of how multi-model ensembles can be used for space weather research and operations.
- **Requires an investment in computing infrastructure as well as for modelers to perform extensive simulations and make them available to the community.**

Ensemble Modeling for the Thermosphere

- A primary USSF organization that will benefit from ensemble modeling is the **USSF 18 Space Control Squadron (SPCS)**, which supports command and control of space forces.
- The 18 SPCS HASDM Astrodynamics Workstation runs the HASDM code to create the current epoch plus 72-hour predicted thermosphere density.
- This density is then used to continually update the NORAD satellite catalog several times a day.
- There is a need to improve HASDM absolute error **without modifying operational code** at USSF.
- New information can be transparently passed as added metadata lines in the JBHSGI.TXT driver files that are delivered several times a day to 18 SPCS. Examples include:
  - ✓ Historical absolute uncertainty of HASDM densities for satellite drag
  - ✓ Historical statistical variability in HASDM by altitude, solar cycle, season, and storm conditions from machine-learned analysis
  - ✓ As-run forecast absolute uncertainty in the solar & geomagnetic indices as compared to data
  - ✓ Current epoch & forecast uncertainty in densities by altitude from multi-model ensemble runs

Example models in ensemble runs

DRAGSTER/TIME-GCM using SGI
error between EXTEMPLAR:SHDB densities

EXTEMPLAR/MSIS v2 using SGI
error between EXTEMPLAR:SHDB densities

JB2008 using SGI
error between JB2008:SHDB densities

HASDM-ML using SGI
error between HASDM-ML:SHDB densities

SET HASDM Density Database (SHDB)
Absolute error between HASDM:Satellite data

SGI = solar and geophysical indices

SGI Forecast Analysis
error between SGI actual:forecast

SGI Forecast Drivers
error between SGI original:forecast

past

present

future

Science challenges that benefit from ensemble modeling uncertainties – tall tentpoles

- Oxygen–Helium transition affecting ballistic coefficients
- Carbon dioxide and nitric oxide cooling in lower thermosphere
- Coronal hole – high speed stream compounding effects
- Dst from CME/HSS magnitude and arrival effects
- Solar far-side evolution of irradiances

Ensemble Modeling for the thermosphere – summary

- The number of Low Earth Orbit (LEO) objects will TRIPLE in the next 2 years, and we expect collision hazards to increase
- We now know existing accuracies of U.S. Space Force (USSF) High Accuracy Satellite Drag Model (HASDM) from SET HASDM density database
- We can significantly reduce uncertainty in thermospheric density specification for the benefit of Space Traffic Management (STM) operations and conjunction assessment by using ensemble multi-model runs

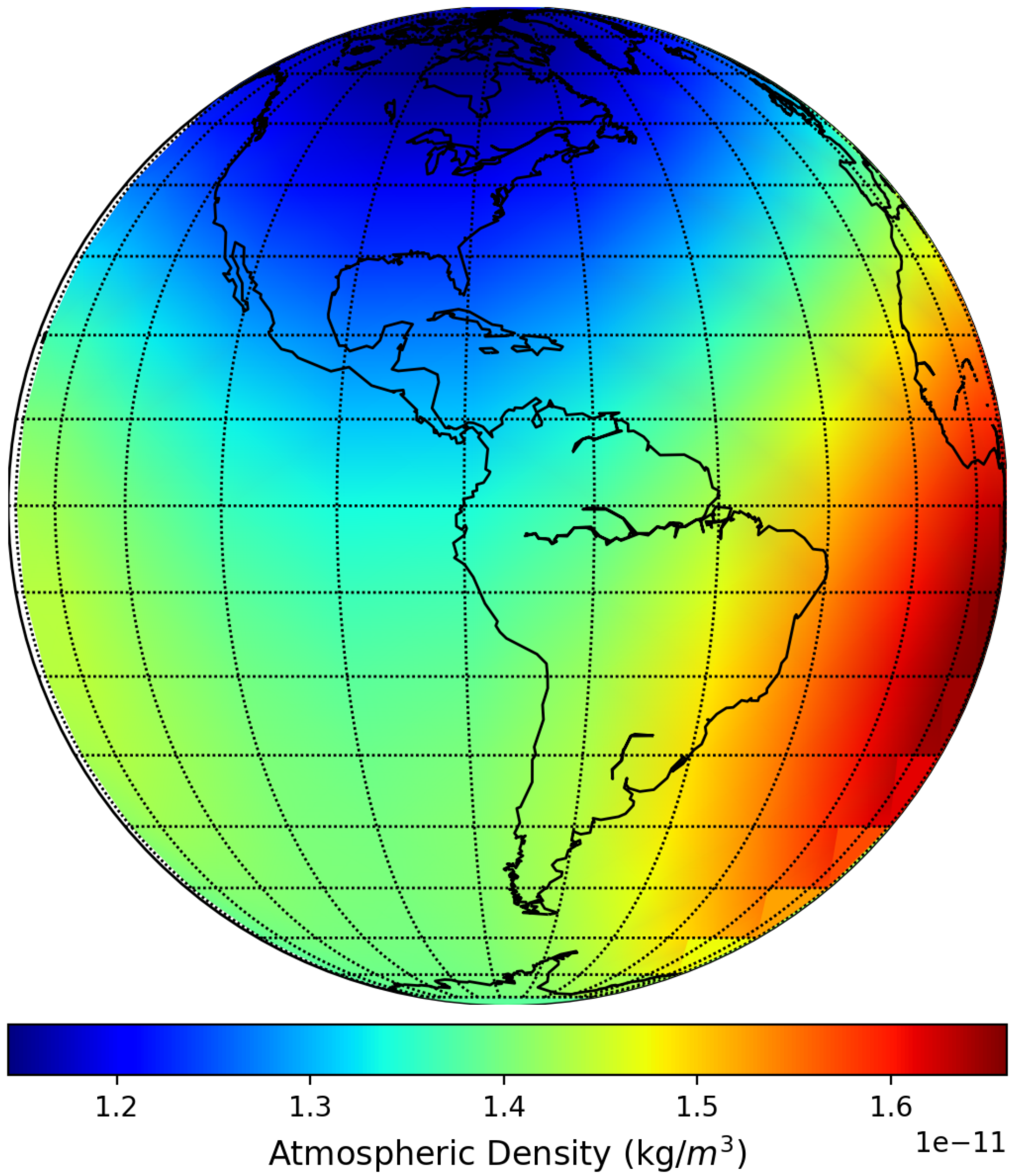
Ensemble multi-models can provide these capabilities:

- ✓ Comparative densities and their uncertainties in each altitude layer;
- ✓ Reference to absolute density uncertainty from HASDM (2–10%);
- ✓ Global density prediction variability uncertainty outside the HASDM database 20-year time frame (2000-2019);
- ✓ Dynamically calculated current epoch and forecast uncertainties using RMS uncertainties from ensemble runs and driver forecasts; and
- ✓ Improved solar and geomagnetic indices' forecasts using lessons learned from ensemble runs and statistical uncertainties.

Foundation for modeling

HASDM DataCube

Oct. 30 2003 00:00 UT at 400 km



Cheaper uncertainty quantification

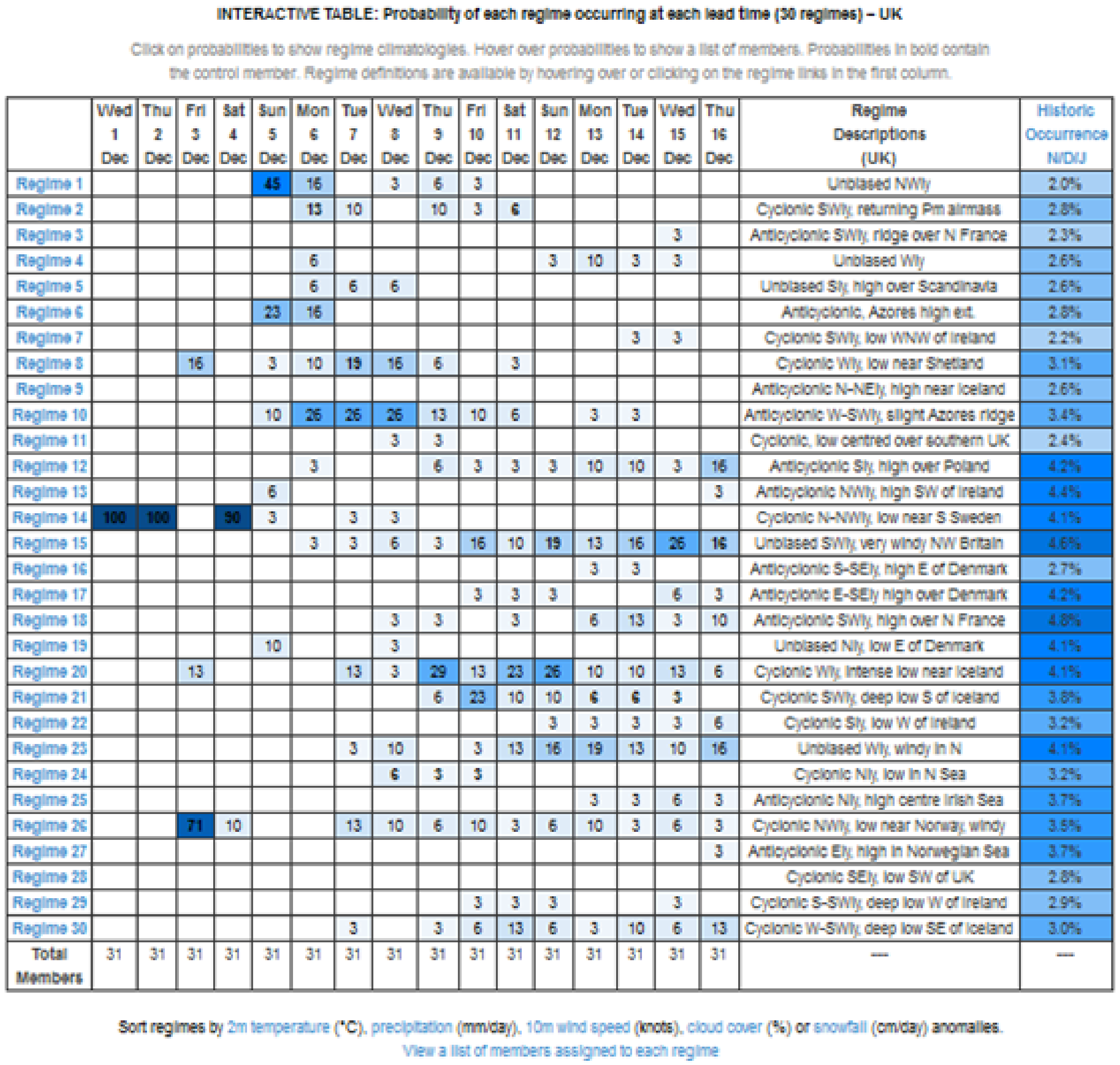
- Operationally, want weather-of-the-day / flow-dependent uncertainty: what is uncertainty given current conditions, not climatological uncertainty
- Classic ensemble approach to uncertainty is expensive: perturb a physics-based model, run different physics-based models, …
- Don’t ignore cheaper options! May suffice for uncertainty needs
  - Drag-based CME modelling – 10k members in seconds.
    Limitations: CME-CME interactions, background wind, drag parameter, …
  - Simpler physics-based models - e.g. upwind schemes
  - Reduced order models: simplify model internal dynamics
  - Surrogate/emulator approaches, used in climate science
  - ML-based modelling of model uncertainty itself (push cost to training?)

Understanding users’ uncertainty needs

- Operational resource (staff, compute, data) spent quantifying uncertainty is **useless** if uncertainty information isn’t used in users’ decision-making!
- Even if uncertainty information gets exposed to users, modeller approaches to this may not suit user needs & decision processes
  Postage stamp / spaghetti plots, RMSE, skill scores, probabilities, proportions…
- Match approaches to communicating uncertainty information to users
  - Probabilities & decision-support systems can help users who can hedge
  - Cost-loss analyses can also help keep things general, but allow user-tuning later
  - Map to user: drive impact models / use scenario-based approaches
- Involve users more in model/system design: co-production etc
- Hard! Terrestrial weather/climate rely on social science input to help

Decision-support system case study: DECIDER

- DECIDER exposes uncertainty usefully for users who can hedge
- Used historic model runs to establish k-means set of weather “regimes”
- Regimes are large-scale patterns, so more predictable
- DECIDER maps current ensemble output onto these regimes
  - Show most likely, *and* the spread
- Users can cluster *their* historic data by the *same* regimes
  - E.g. “60% of issues occur in regime 1, …”
- So can use DECIDER output as input to their internal decision-support systems
  - Avoids discarding uncertainty too early



INTERACTIVE TABLE: Probability of each regime occurring at each lead time (30 regimes) – UK

Click on probabilities to show regime climatologies. Hover over probabilities to show a list of members. Probabilities in bold contain the control member. Regime definitions are available by hovering over or clicking on the regime links in the first column.

	Wed 1 Dec	Thu 2 Dec	Fri 3 Dec	Sat 4 Dec	Sun 5 Dec	Mon 6 Dec	Tue 7 Dec	Wed 8 Dec	Thu 9 Dec	Fri 10 Dec	Sat 11 Dec	Sun 12 Dec	Mon 13 Dec	Tue 14 Dec	Wed 15 Dec	Thu 16 Dec	Regime Descriptions (UK)	Historic Occurrence N/D/J
Regime 1					45	16		3	6	3							Unbiased NWly	2.0%
Regime 2						13	10		10	3	6						Cyclonic SWly, returning Pm airmass	2.8%
Regime 3															3		Anticyclonic SWly, ridge over N France	2.3%
Regime 4						6						3	10	3	3		Unbiased Wly	2.6%
Regime 5						6	6	6									Unbiased Sly, high over Scandinavia	2.6%
Regime 6					23	16											Anticyclonic, Azores high ext.	2.8%
Regime 7														3	3		Cyclonic SWly, low WNW of Ireland	2.2%
Regime 8			16		3	10	19	16	6		3						Cyclonic Wly, low near Shetland	3.1%
Regime 9																	Anticyclonic N-NEly, high near Iceland	2.6%
Regime 10					10	26	26	26	13	10	6		3	3			Anticyclonic W-SWly, slight Azores ridge	3.4%
Regime 11								3	3								Cyclonic, low centred over southern UK	2.4%
Regime 12						3			6	3	3	3	10	10	3	16	Anticyclonic Sly, high over Poland	4.2%
Regime 13					6											3	Anticyclonic NWly, high SW of Ireland	4.4%
Regime 14	100	100		90	3		3	3									Cyclonic N-NWly, low near S Sweden	4.1%
Regime 15						3	3	6	3	16	10	19	13	16	26	16	Unbiased SWly, very windy NW Britain	4.6%
Regime 16													3	3			Anticyclonic S-SEly, high E of Denmark	2.7%
Regime 17										3	3	3			6	3	Anticyclonic E-SEly high over Denmark	4.2%
Regime 18								3	3		3		6	13	3	10	Anticyclonic SWly, high over N France	4.8%
Regime 19					10			3									Unbiased Nly, low E of Denmark	4.1%
Regime 20			13				13	3	29	13	23	26	10	10	13	6	Cyclonic Wly, intense low near Iceland	4.1%
Regime 21									6	23	10	10	6	6	3		Cyclonic SWly, deep low S of Iceland	3.6%
Regime 22												3	3	3	3	6	Cyclonic Sly, low W of Ireland	3.2%
Regime 23							3	10		3	13	16	19	13	10	16	Unbiased Wly, windy in N	4.1%
Regime 24								6	3	3							Cyclonic Nly, low in N Sea	3.2%
Regime 25													3	3	6	3	Anticyclonic Nly, high centre Irish Sea	3.7%
Regime 26			71	10			13	10	6	10	3	6	10	3	6	3	Cyclonic NWly, low near Norway, windy	3.5%
Regime 27																3	Anticyclonic Ely, high in Norwegian Sea	3.7%
Regime 28																	Cyclonic SEly, low SW of UK	2.8%
Regime 29										3	3	3			3		Cyclonic S-SWly, deep low W of Ireland	2.9%
Regime 30							3		3	6	13	6	3	10	6	13	Cyclonic W-SWly, deep low SE of Iceland	3.0%
Total Members	31	31	31	31	31	31	31	31	31	31	31	31	31	31	31	31	---	---

Sort regimes by 2m temperature (°C), precipitation (mm/day), 10m wind speed (knots), cloud cover (%) or snowfall (cm/day) anomalies.

View a list of members assigned to each regime