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Center for integrated space weather modeling metrics plan and initial model validation results

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Abstract

Metrics and model validation represent two key elements upon which the success of the Center for Integrated Space Weather Modeling (CISM) hinges. The routine calculation of important operationally- and scientifically-motivated metrics permits us to objectively measure and track the ability of coupled CISM models to predict essential space weather quantities. The rationale for CISM metrics selection is developed and the list of 29 metrics, along with the baseline models, first-generation physics models, and the data sets needed to compute skill scores, are outlined. While metrics provide a means for the objective assessment of long-term model improvement, model validation—the comprehensive, systematic quantitative comparison of model output with observations—is required for identifying and documenting model strengths and weaknesses. Two representative examples of initial validation efforts are summarized. The first uses case study analysis techniques and comparison with *in situ* observations during real events to explore the range of validity of the Lyon–Fedder–Mobarry (LFM) MHD simulation during magnetic storms. The second uses a statistical approach to compare the climatology of plasma sheet bulk properties (density, temperature, magnetic field, flows) deduced from both spacecraft observation and modeled by the LFM code.

Keywords: Space weather; Numerical modeling; Model validation

1. Introduction

In order to measure progress objectively and to make improvements in both space weather forecasting and scientific understanding, the Center for Integrated Space Weather Modeling (CISM) has incorporated metrics and model validation as critical components of the overall program. Herein, "metrics" are defined to be clearly specified and standardized quantifications of how well empirical or numerical models predict those physical measurements especially important to space weather. By analogy, tropospheric weather modeling can point to over half a century of steady progress, documented through metrics such as the 36-hour forecast of the average altitude of the 500 mbar atmospheric pressure level over the continental US (see Siscoe et al., 2004). Fig. 1 of Siscoe et al. (2004) shows the history of this meteorological metric; models' evolving prediction efficiencies reveal an upward trend

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in skill score since 1955. Tracking these metrics over time provides a quantitative record of numerical models' improving abilities to predict key quantities. Metrics inform both model developers and model users of a model's predictive capabilities.

The ability of a physics-based model to make an accurate prediction naturally relies heavily on whether the model possesses all of the most important physics, with algorithms that robustly solve the governing equations and with well-specified boundary or initial conditions. In space weather modeling, as in tropospheric weather modeling, computational limitations often constrain the scope of numerical models, forcing modelers to make simplifying assumptions in order to make a simulation tractable. Furthermore, boundary and initial values are not always well known; such input uncertainties propagate through and inevitably compromise model outputs to some degree. In order to quantify and understand the consequences of these shortcomings and, ultimately, to guide a developer's path to eliminating or reducing them, model validation is an essential tool. "Validation" refers to the broad assessment of a model's output through comparison with observations, whether statistically or via case study analysis.

The CISM metrics implementation plan and some initial, representative validation efforts are described in this paper. Section 2 outlines two distinct sets of CISM metrics, one set tracking quantities of operational space weather importance, the other of scientific importance. Section 3 details the current CISM metrics implementation plan, including a summary of the metrics and the baseline models and data that will be used to establish prediction efficiencies and skill scores. Finally, Section 4 presents specific examples of ongoing model validation that typify statistical and case study approaches to be used for all CISM models.

2. Metrics philosophy

A core set of CISM metrics will be computed routinely to quantify progress toward overall CISM modeling goals. CISM has already benefited from several studies of space weather model metrics established by the science community, including documents resulting from National Space Weather Program and CCMC studies (see e.g., Williamson et al., 2000). Several important factors influenced our selection of CISM space weather metrics. These include:

(1) the metrics must be a reasonably small collection to be able to be feasibly tracked;
(2) on the other hand, they must be comprehensive enough to assess robustly the wide range of CISM models;
(3) they must be based on direct measurements or derived quantities that will be continuously and reliably available into the foreseeable future;
(4) they must be quantities related to key space weather effects that we are trying to predict; and finally,
(5) they must be parameters that are recognized to be important by the space physics science community and/or the operational user community.

This final factor naturally divides CISM metrics into two broad categories: operational and scientific. Operational metrics will gauge the progress of our ability to predict high-priority space weather effects that are of major concern to user communities. Scientific metrics are complementary to these, chosen to assess key quantities that are important scientifically and are a critical test of a model's ultimate ability to predict, but which are not necessarily of immediate and/or direct relevance to user communities.

Guided by the five factors outlined above, CISM identified 11 metrics areas to track (six for the operational and five for the scientific metric categories) that address key phenomenon and/or regions that span from the Sun to the Earth. Operational metrics areas cover: interplanetary shocks and coronal mass ejection (CME) properties; solar energetic particle (SEP) properties; standardized magnetic indices; regional ground magnetic field variations; radiation belt energetic particle fluxes; and properties of the ionosphere/neutral atmosphere. Scientific metrics areas cover: solar and coronal hole properties; solar wind and interplanetary magnetic field (IMF) properties at 1 AU; particle and field properties of the geostationary (GEO) and medium Earth orbit (MEO) regions; properties key to magnetosphere–ionosphere coupling; and finally, ionospheric plasma properties. Section 3 contains the detailed metrics descriptions and their computation.

3. CISM metrics implementation plan

Fig. 1 summarizes the eleven different broad areas in the left-most column. The top half of the table lists those that comprise the six operational metrics types; the bottom half lists the five that broadly define the scientific metric types. Sub-categories within each type detail the specific quantities for which we will compute metrics. CISM has adopted this list of 29 individual metrics, 15 on the operational side and 14 on the scientific side, as the baseline set with which to track overall project progress. Note that every metric consists of four elements: a parameter, a "baseline" model (herein typically empirical) used to predict that parameter, an observation of that parameter for "skill score" computation, and finally, a predictive physics-based model.

		Baseline Models	Skill Score Data Sets	Physics Models
	Operational SW Community			
Operational Metrics	1 *Shocks and CMEs at L1*		ACE	MAS+ENLIL
	a Speed	Augmented Vrsnack-Gopalswamy[a]	"	
	b Arrival time	"	"	
	c Bz	"	"	
	d Duration	"	"	
	2 *SEP Properties*		GOES	UCB
	a Event/No Event	PROTONS[b]	"	
	b Rise Time	"	"	
	c Peak Flux	"	"	
	d Duration	"	"	
	e Cutoff	Shea-Smart[c]	POES	
	3 *Magnetic Indices*			
	a Dst	Temerin-Li[d]	NGDC	LFM+RCM
	b Ap/K	ARX-McPherron	"	
	4 *Regional Ground dB/dt*	Weigel-Baker[e]	IMAGE (mag)	LFM+TING
	5 *Radiation Belt EP fluxes*			
	a GEO	Li[f]	LANL	RBM
	b MEO and LEO	Vassiliadis[g]	SAMPEX	"
	6 Ionosphere/Neutral Atmosphere			
	a "State" of ionosphere	IRI[h]	Digisondes	TING
	Scientific SW Community			
Science Metrics	1 Solar/Coronal			
	a Coronal Hole Index	PFSS/Wang-Sheeley[i]	SOHO UV maps	MAS+ENLIL
	b White-light Streamer Belt Index	PFSS/Yi-Ming Wang[j]	SOHO LASCO	"
	2 *Solar Wind/IMF at L1*			
	a Density	WSA[k] + nv = constant	ACE	MAS+ENLIL
	b Velocity	WSA	"	"
	c IMF - vector	WSA + |B|	"	"
	3 *GEO/MEO Environment*			
	a Magnetic field	Tsyganenko[l]	GOES	LFM+RCM
	b Particle fluxes (ring current/rad belt)	MSM[m], CRRESELE[n]	GOES/LANL	LFM+RCM,RBM
	c M'pause crossing	Shue[o]	“	LFM+RCM
	4 *MI Coupling*			
	a Polar Cap Potential	Weimer[p]	DMSP	LFM+TING
	b Polar Cap Boundary	Weimer	“	"
	c Field Aligned Currents (2D)	Weimer	“	LFM+TING+MIC
	d Particle precipitation	AURORA[q]	“	MIC
	5 *Ionospheric Plasma*			
	a E-, F-region Heights	IRI	Digisondes +	TING
	b E-, F-region Peak Densities	"	ISRs	"

[a] Vrsnak and Gopalswamy (2002), Gopalswamy et al. (2001), Bothmer and Rust (1997), and Owen and Cargill (2002).
[b] Balch (1999).
[c] Shea and Smart (1990).
[d] Temerin and Li (2002).
[e] Weigel and Baker (2003).
[f] Li et al. (2003).
[g] Vassiliadis et al. (2004).
[h] Bilitza (2001, 2003).
[i] Wang and Sheeley (1992).
[j] Wang et al. (1997).
[k] Wang and Sheeley (1992); Arge and Pizzo (2000); Arge et al. (2004).
[l] Tsyganenko (1995, 2003).
[m] Magnetospheric Specication Model from AF-GEOSpace.
[n] CRRESradiation belt electron model from AF-GEOSpace.
[o] Shue et al. (1997,1998).
[p] Weimer (1996), Weimer (2001a, b).
[q] Air Force Statistical Auroral Models from AF-GEOSpace.

Fig. 1. Operational (top section) and science (bottom section) metrics defined for CISM are shown in the left-hand column. Baseline models, data sets, and first-generation physics models from which skill scores will be computed are shown in subsequent columns.

While many approaches to quantify metrics exist, our philosophy and approach are as follows. As discussed earlier with the 500 mbar meteorological metric, we adopt skill score as a means to quantify a model's progress. Skill score is an objective measure of how well one model predicts a measurable quantity as compared to a baseline model's prediction of that same quantity. The baseline model is a frozen, unchanging model against which all other subsequent models are compared. In our case, the baseline CISM models are empirical or semi-empirical models; these are described thoroughly in Siscoe et al. (2004) and Baker et al. (2004). As described in a companion paper (Siscoe et al., 2004), the skill score (SS) for each metric is defined as $SS = (1 - MSE/MSE_{ref}) \times 100$, where MSE is the mean-square-error between the model-derived and the observed quantity and where MSE_{ref} is the mean-square-error between the baseline model and the same observed quantity. A negative (positive) SS indicates that the tested model has less (greater) predictive capability than the baseline model, i.e., $MSE > MSE_{ref}$ ($MSE < MSE_{ref}$). We comment further on the MSE below.

For example, the fourth science metric listed in Fig. 1 is the solar wind speed at the forward Lagrange point (L1). The baseline CISM model for predicting solar wind speed at L1 is the Wang–Sheeley–Arge (WSA) model (Arge et al., 2004). The WSA model predicts solar wind speed using knowledge of the coronal magnetic field structure as an input. Comparison between WSA predictions and observed solar wind speeds measured at L1 (by ACE, WIND, etc.) provide a quantitative measure of MSE_{WSA}. Similar comparisons between observations and the predicted solar wind speed of any other tested CISM model, such as MAS/ENLIL, the combined, physics-based corona and solar wind models (Odstrcil et al., 2004), provide the quantitative model-dependent measure of MSE, from which a skill score can be derived and tracked.

Fig. 1 lists in the second column the baseline model adopted for each of the CISM metrics, both operational and scientific. Siscoe et al. (2004) describe these models, both empirical and physics-based, and their inputs extensively. The third column lists the representative data sources or sets used to compute skill scores, while the last column identifies the first-generation, physics-based, coupled CISM models to be assessed. While the specificity and refinement of the metrics and compilation of the data sets needed to compute skills scores are ongoing CISM tasks, the establishment of a frozen set of well-documented, unchanging baseline models, as captured in Fig. 1, is complete.

As noted above, the CISM team is currently in the process of defining and refining the next level of detail needed to compute metrics. Such details include specifying the relevant properties (e.g., the time cadence, the spatial location(s), the altitude extent(s), etc.) of each particular metric as well as the optimal means by which departures of model outputs from observations can be measured (e.g., MSE of a quantity versus the MSE of the logarithm of a quantity versus some other quantitative measure of error). That level of detail is beyond the scope of this paper but will be the topic of future publications. As these additional details are established and as the appropriately prepared data sets required for producing skill scores are available, CISM will compute both the operational and scientific metrics and report them to the community routinely.

4. CISM model validation

4.1. CISM validation philosophy and implementation plan

In many regards, validation of CISM models is as important to the success of CISM as is their development. A model is only useful to the extent we know how well it simulates reality. Consequently, validation and metrics define a distinct and vital research thrust within CISM carried about by a common team. Metrics provide one type of measure of model performance, specifically, one that is objectively traceable over long intervals but one that is also limited to a relatively small number of outputs. Metrics measure performance, rather than provide specifics about model deficiencies or inform modelers of how to fix them. This notion applies to the operational metrics as well as to the scientific metrics. On the other hand, the intent of model validation is to provide a deeper, more comprehensive exploration of model performance and behavior, that is unrestricted by the limitations of the five criteria listed under metrics (such as the restriction of comparing only with data sets that are nearly continuously available). Metrics and validation are both important and are complementary: metrics provide a quantitative measure of the improving predictive strength of a model, while scientific validation systematically identifies model shortcomings and strengths and informs ongoing model improvement.

CISM validation is a two-pronged effort: science validation and "end-user" validation. We outline these two aspects next. While each element is a discrete sequence of operations, both activities will be ongoing concurrently throughout the CISM effort.

Science validation occurs during the major development period of each code version. The distributed CISM validation team is working with code developers to: (1) identify key aspects of codes or code coupling which require scientific validation; (2) compile and use extant data sets to exercise and explore the ranges of validity of the codes; and (3) iteratively feedback the knowledge gained into the ongoing development of scientifically robust models. The goal of this effort is to assure that CISM scientists understand the primary science outputs of the models early enough in the process, through comparisons with the most relevant observations, so that developers will be able to adjust their codes to better model the desired regions or processes.

Once each major version of the coupled model is completed, it will be first released internally to the CISM validation team for a second regimen of unbiased validation, so called "end user" validation, before the code is released to the knowledge transfer team and thus to the wider community. This second level of validation will continue the scientific validations from the initial phase and introduce other targeted science validations identified from this first iteration. Another important element of this second phase of validation will be to exercise the codes as broadly as possible, thus to fully explore their ranges of validity and operability. Such information will be important to establish before they are made available to the wider community. The second validation stage (or "end-user" validation) will be led by CISM scientists without a significant vested interest in any of the component models. We underscore that in this "end-user" validation, it is critical to have primary responsibility in the hands of those who have not played an integral role in the code or code coupling development. During this second phase of validation, feedback to the development teams will assure the necessary fine-tuning and code documenting needed before each version is officially released to the community. While the process outlined for science validation sounds somewhat formalized, in reality, it is much less definable and structured as are the metrics computation.

4.2. *Initial representative validation efforts*

Next, we summarize two examples of initial science validation efforts. Other papers from this special issue describe additional validation efforts (see for example, Vassiliadis et al., 2004). The two examples chosen here demonstrate both traditional model validation techniques (case study analysis) as well as techniques not generally applied to the comparison of observations with large-scale simulation results (statistical "climatology"). Both explore and quantify the strengths and weaknesses of the core geospace model, the Lyon–Fedder–Mobbary (LFM) code, a global three-dimensional MHD simulation of Earth's magnetosphere (Lyon et al., 2004). While these are specific studies aimed at a specific model, the approaches described apply generically to virtually all CISM models and are representative of other ongoing and planned studies.

The goal of the first study is to quantify the degree to which the LFM code reproduces the distortions of the inner magnetosphere during the life-cycle of magnetic storms (Huang et al., 2003). It is understood that single-fluid ideal MHD codes cannot accurately model the storm-time ring current region owing to an incomplete treatment of the complicated drift physics in these regions. The pressure gradients and currents resulting from these effects are especially important during magnetic storms. For instance, the inflation and distortions of the inner magnetospheric magnetic field can greatly modify the drift paths of relativistic electrons in the outer radiation belt. Until these dynamic fields can be accurately modeled on a global scale, progress toward understanding the acceleration and losses of energetic electrons is hampered. Indeed, the lack of a proper ring current in the LFM code (as well as in all other MHD codes) and the need for a robust inner magnetosphere field motivates the ongoing coupling of the LFM model with the Rice Convection Model (RCM).

For this study, several magnetic storm intervals were selected that spanned from minor to moderate storm conditions (as measured by the Dst index). Events were restricted to those with good availability of upstream solar wind and IMF data, needed as inputs to the MHD model. They were also restricted to those having good availability of data from the inner magnetosphere (principally shown here, GOES magnetometer observations) with which to compare and quantify the model outputs.

Fig. 2 shows one result from the Huang et al. (2003) work. This figure shows the time series of a moderate magnetic storm associated with the passage of a magnetic cloud in September of 1998. The top panel shows the Dst index and subsequent panels show the vector components and magnitude of the magnetic field as well as the magnetic field elevation angle at geostationary orbit, specifically at the location of the GOES-8 spacecraft. The black curves in these panels are the measured GOES-8 magnetic fields properties. The upstream solar wind and IMF provided the inputs to the LFM model. A virtual spacecraft placed at the GOES-8 location "recorded" model output and those time series are the green curves. Finally, the CISM baseline model for geostationary magnetic fields, the semi-empirical models developed by Tsyganenko (here the 2003 storm model version; Tysganenko et al., 2003), is shown for comparison in the red curves.

Huang et al.'s case study analyses reveal and quantify the regions where, and the times when, the uncoupled LFM code performs well in addition to when it performs poorly. These analyses reveal that:

(1) MHD field lines are not stretched enough at geosynchronous orbit during storm main phase, especially on the night side (Ms in Fig. 2 indicate midnight location of GOES-8);
(2) MHD pressure in the inner magnetosphere is low compared to expected pressures during storm main phases; and

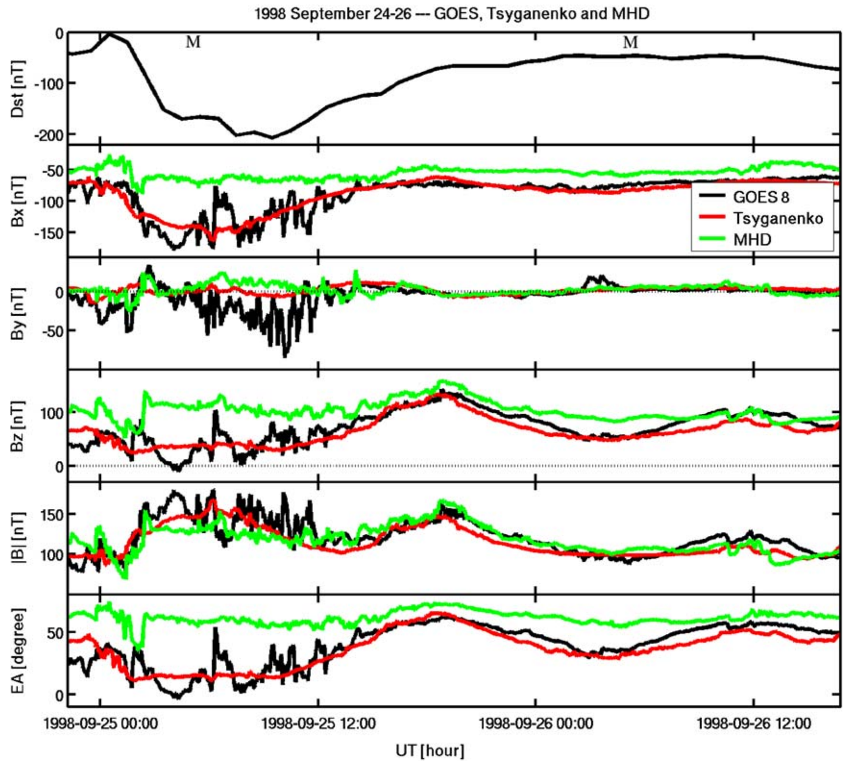

Fig. 2. Comparison of magnetic field properties at geostationary orbit as recorded by the GOES-8 spacecraft (black curve), a virtual GOES-8 spacecraft flown through the LFM model output (green curve), and the Tsyganenko et al. (2003) semi-empirical magnetic field model (red curve). The top panel shows the Dst profile of this magnetic storm, the next four panels show the vector components of the magnetic field and its magnitude, while the bottom panel shows the field elevation angle. The 'M's in the top panel indicate the universal times when GOES-8 was located at midnight.

(3) ongoing studies show that coupling the RCM with the LFM simulation leads to significantly increased pressure gradients and increased field line stretching (Lyon and Tofoletto, private communication, 2004).

An independent study by Garner (2003) showed that the RCM model, when run stand-alone with only ExB particle transport, yields high inner-magnetospheric pressures and currents. Ongoing CISM validation efforts will compare the LFM–RCM coupled results with the LFM- and RCM-only results in an effort to establish the relative importance of drift physics and the algorithms used for solving the governing equations. Such information is not only important for understanding the complexities of the global inner magnetosphere during magnetic storms, but also informs and provides critical physical insight to the LFM–RCM modelers and guides their coupling effort.

The second example represents a different form of model-data comparison: statistical climatology. Owing to the significant advancements in computer speeds and storage, it is now possible to run even high-spatial-resolution codes and produce data sets representing literally many weeks of simulation results. CISM is mining such data sets for the first time. When driven by measured solar wind inputs, the outputs of these models, sampled at high time resolution throughout the simulation volume, produce many billions of space-time data points with typically many output parameters at each point. These comprehensive data sets contain not only features testable through case study analysis, but also the long-term and sometimes critically important underlying trends. For example, the properties of a preconditioned plasma sheet might be a vital factor in determining subsequent storm size. Therefore, the ability of a model to reproduce robustly the average densities, temperatures, fields, and flows during periods between large events might be just as important as its ability to capture accurately the most dramatic dynamical events.

Guild et al. (2004) reports on one early attempt to validate the LFM code with statistical data surveys through comparative climatology of bulk magnetotail

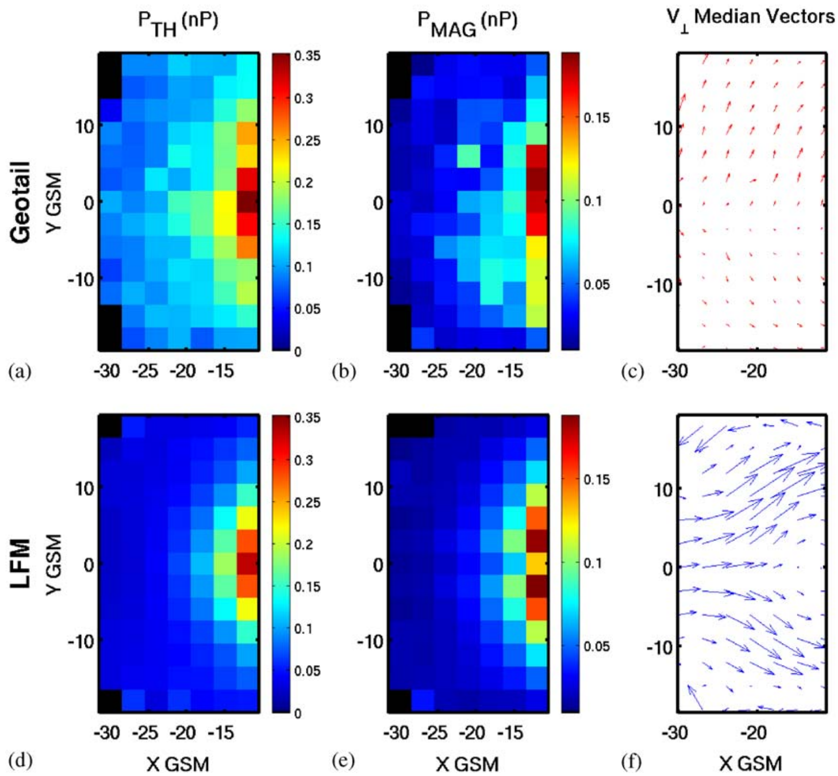

Fig. 3. Comparison of Geotail (top row) and LFM (bottom row) thermal pressure (first column), magnetic pressure (middle column), and perpendicular flows (last column) in the equatorial plane. The LFM thermal pressure (4d) falls off much steeper than the data (4a), the Geotail magnetic pressure shows a dawn–dusk asymmetry (4b), and the LFM (4f) median perpendicular flow magnitudes are much ($\sim 5\times$) higher than those in the Geotail data (4c). (From Guild et al., 2004).

plasma sheet properties. They compare more than three years of Geotail plasmasheet data (constituting nearly 800,000 data points) with 10 consecutive days of LFM simulation results (constituting over 15 million data points in the plasma sheet) driven by real solar wind and IMF inputs. Fig. 3 shows results of these initial comparisons (taken from Fig. 4 of Guild et al.), specifically, average plasma sheet properties mapped to the equatorial plane. Comparison of Geotail (top row) and LFM (bottom row) thermal pressure (first column), magnetic pressure (middle column), and perpendicular flows (last column) in the equatorial plane reveal a number of important similarities and differences. For instance, the LFM thermal pressure falls off much more steeply than the data, the Geotail magnetic pressure shows a dawn–dusk asymmetry, and the LFM median perpendicular flow magnitudes are significantly higher than those in the Geotail data. Based on these comparisons of average properties, Guild et al. (2004) reach important conclusions about model strengths and weaknesses that would not be discernable in case studies, including comparing quantitatively the degree of flow variability as well as the median flow values.

5. Summary

The CISM team believes that metrics and model validation are vital elements of a successful modeling program. Metrics provide a standard, systematic measure of how well CISM models predict space weather phenomenon of interest to operational as well as scientific users and how well their prediction improves with time. Twenty-nine metrics in eleven key areas represent a complete suite of trackable and tractable values, covering important elements of the coupled Sun–Earth system and satisfying five limiting selection criteria. Initial validation of both stand-alone and coupled models is underway. Standard case studies as well as the emerging opportunity to conduct climatology studies are already yielding new scientific insights and guiding future model development and improvements.

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