Merged Observatory Data Files (MODFs): An Integrated Observational Data Product Supporting Process-Oriented Investigations and Diagnostics

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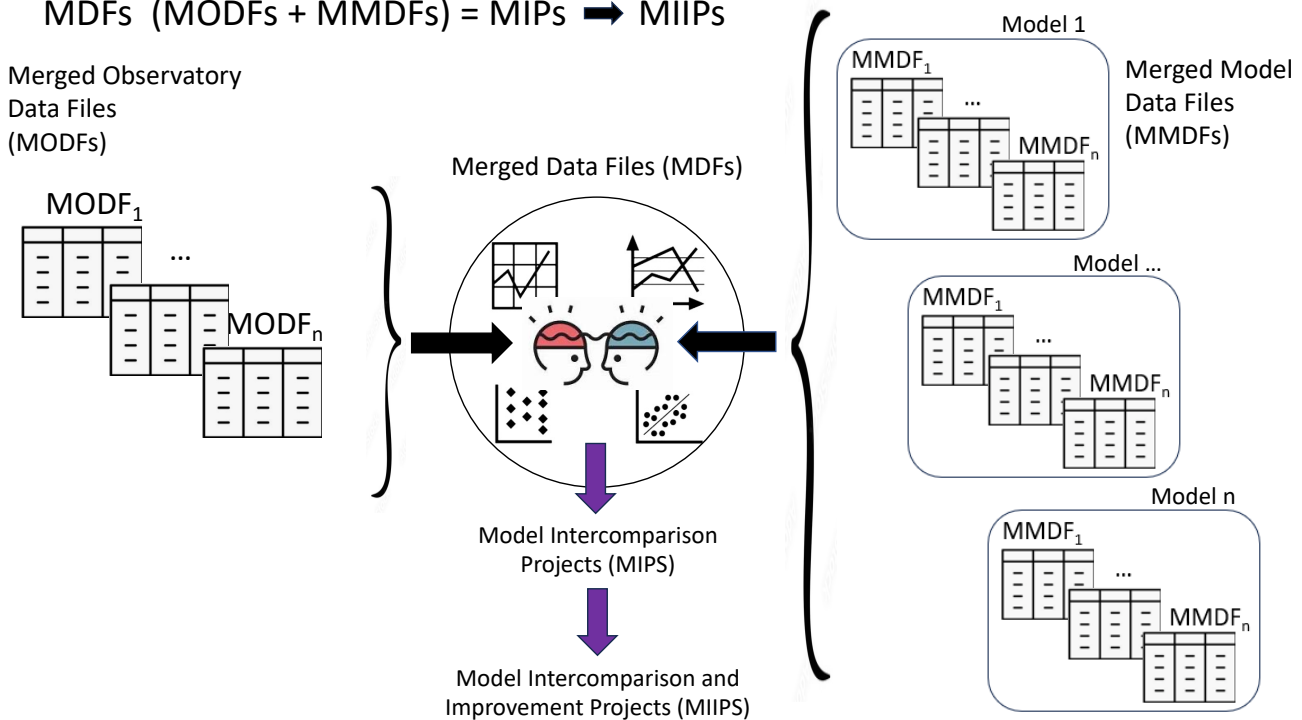
Abstract. A large and ever-growing body of geophysical information is measured on campaigns and at specialized observatories as a part of scientific expeditions/experiments. These collections of observed data include many essential climate variables (as defined by the Global Climate Observing System), but are often distinguished by a wide range of additional non-routine measurements that are designed to not only document the state of the environment, but also the drivers that contribute to that state. These field data are not only used to further understand the environmental processes through observation-based studies, but also to provide baseline data to test model performance and to codify understanding to improve predictive capabilities. To address the considerable barriers and difficulty in utilizing these diverse and complex data for observation-model research, the Merged Observatory Data File (MODF) concept has been developed. The MODF combines measurements from multiple instruments into a single file that complies with well-established data format and metadata practices and has been designed to parallel development of corresponding Merged Model Data Files (MMDFs). Using MODF and MMDF protocols will facilitate the evolution of Model Intercomparison Projects into Model Intercomparison and Improvement Projects by putting observation and model data 'on the same page' in a timely manner. The MODF concept was developed especially for weather forecast model studies in the Arctic. The surprisingly complex process of implementing MODFs in that context refined the concept itself. Thus this article explains the concept of MODFs by providing details on the issues that were revealed and resolved during this first specific implementation. Detailed instructions are provided on how to make MODFs, and this article can be considered a MODF creation manual.

1 Introduction

45   The Merged Observatory Data File (MODF) concept is based on the simple principle of combining measurements made by multiple, co-located instruments from research observatories and campaigns into a single file that complies with already established data stewardship standards. 'Observatory' here refers to a facility that measures an extensive inventory of collocated geophysical variables that have been chosen with the intention of investigating specific, usually interrelated, physical processes in order to answer hypothesis-driven science questions. In this context, an observatory could be a land site

50   or a research vessel. While it is standard scientific operating procedure to co-locate research grade instruments both continuously at observatories and episodically for field campaigns (often side-by-side with routine operational station instruments with long operational histories) there are generally no standard procedures for coordinated data management such as those that have been developed for operational data. Thus, the data from separate instruments can be scattered between separate files with different authors, formats, metadata, physical archive locations, and use restrictions.

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The specific MODF realization presented here is for Arctic observatories (Uttal et al., 2016; Mariani et al., 2022) and field campaigns that resulted from initiatives established during the Year of Polar Prediction (YOPP; Goessling et al., 2016; Jung et al., 2016; Wilson et al., 2023). One key YOPP activity was the YOPP supersite Model Intercomparison Project (YOPPsiteMIP; Day et al., submitted), which was designed to facilitate process-based validation of numerical weather

60   prediction (NWP) models at polar locations during Special Observing Periods (SOPs). The concept of MODFs and their forecasting analogs, Merged Model Data Files (MMDFs), was motivated by the YOPPsiteMIP community's desire to have the same variables from observations and models in easy-to-use files of the same structure in order to explore small-scale parameterized processes that are not represented well in the forecast models. These MODFs thus provide an integrated observation database to support model process representation through parameterization improvements for weather forecasts

65   in the polar regions. At the same time, they also facilitate comparative observational studies across Arctic sites.

The MODF concept addresses the problem that research-grade, process-level observations are currently underutilized for model evaluation of parameterization deficiencies. As weather forecasting models increase in complexity and include detailed representation of land, ocean, ice, and snow in addition to the atmosphere, it is increasingly important to evaluate

70   processes using observations recorded through the whole earth system column, including the fluxes at their interfaces, to inform model development. This requires multi-variate process-oriented diagnostic methods utilizing data that spans these multiple components to understand model error. An essential component of the MODF concept is that analogous Merged Model Data Files (MMDFs) can be developed with extracted model data near and around the observatory sites. Together, these are defined as Merged Data Files (MDFs). The MDFs, which bring together observations from different earth system

75   components as well as model output in a standard file format, provide the basis for this and will support Model Intercomparison and Improvement Projects (MIIPs) as an evolution from Model Intercomparison Projects (MIPs). The idea

of MIIPs (a new acronym that we define here) does not imply that previous MIPs did not have productive results. However, through the development of matched MODF and MMDF data sets, it is implied that what have often been intercomparison studies can be smoothly extended to model improvements.

80 ## 2 Background

Using observations and model outputs symbiotically is an area of ongoing effort and research with recognized challenges (Holtslag, et al., 2013). Many levels of MIPs have been in progress for decades (Stephens et al., 2023). In addition, existing efforts and methodologies facilitate the usage of increasingly heterogenous data sets in model–observation fusion efforts through assimilation (Gettleman et al., 2022) and for inputs into multivariate artificial intelligence analyses (Boukabara et

85 al., 2021). There are well-organized systems for managing the data from operational surface networks, upper air networks, and satellites that are uploaded into the Global Telecommunications System (GTS) that is overseen by the World Meteorological Organization (WMO) (see Global Telecommunications System (GTS), 2023; WMO, 2020). However, GTS data are only readily available directly to national forecasting centers (which presumably have developed institutionally specific reading and ingesting routines) and via products developed by WMO institutional repositories[1] (Bojinski et al.,

90 2014; Lavergne et al., 2022). The latter have necessarily gone through various quality control, formatting, averaging, and sometimes interpolation to create globally uniform products. As a result of the standardized processing, it is likely that information on high-resolution, rapid, and extreme events (Sardeshmukh et al., 2015) may have sometimes been lost.

The MODF schema has been specifically developed for managing observatory and campaign research observations as

95 opposed to operational observations. Research observations target local-scale and often rapid or extreme processes that are intended to lead to discovery of the physics within the atmosphere as well as the physics that govern the coupling processes between the atmosphere and the underlying surface. The surface can be land, ocean, ice, or any of the three, often with obfuscating layers of plant and/or snow cover that are themselves components of the system and separate objects of study. Research-grade data pose many additional challenges regarding data latency, accessibility and uptake issues, and

100 institutional ownership, compared to data that have been managed more systematically specifically for operational purposes.

The data science community is aware of these issues and in response has developed FAIR (Findable, Accessible, Interoperable, Reusable) data principles (Wilkinson et al., 2016) that can be applied to individual data sets. However, Wilkinson et al. explicitly stated that "These high-level FAIR Guiding Principles precede implementation choices, and do

105 not suggest any specific technology, standard, or implementation–solution; moreover, the principles are not, themselves, a standard or a specification." Whereas many FAIR solutions are implemented by web services (e.g., Buck et al., 2019), the MODF concept described here can be considered an alternative: an integrated data product that is based on the same

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[1] https://climatedata-catalogue.wmo.int/homepage

metadata conventions that have been developed for web service solutions. The considerations and steps described here for creating MODFs can therefore be considered a particular FAIR implementation–solution specifically for observatory and campaign data.

3 The MODF Concept

Figure 1 is a conceptual schematic of the end-to-end process involved with data collection, data quality control (QC) and processing, metadata information collection, and data amalgamation into netCDF files (Unidata, 2023) that follow the NetCDF Climate and Forecast (CF) Metadata Conventions (Eaton et al., 2022, hereafter the CF Conventions). The process for turning model forecast output into MMDFs is qualitatively similar[2], including the use of a particular set of global and variable attributes, since the specifications were developed by modellers as well as observationalists.

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[2] Differences generally arise from the fact that forecast models can produce tendencies on timestep scales that are typically not available from field instruments, and that model output is typically regularly distributed in time and space rather than coming from discrete instruments which may move irregularly in space, which operate at different optimized cadences, and which are subject to physical or power disruptions.
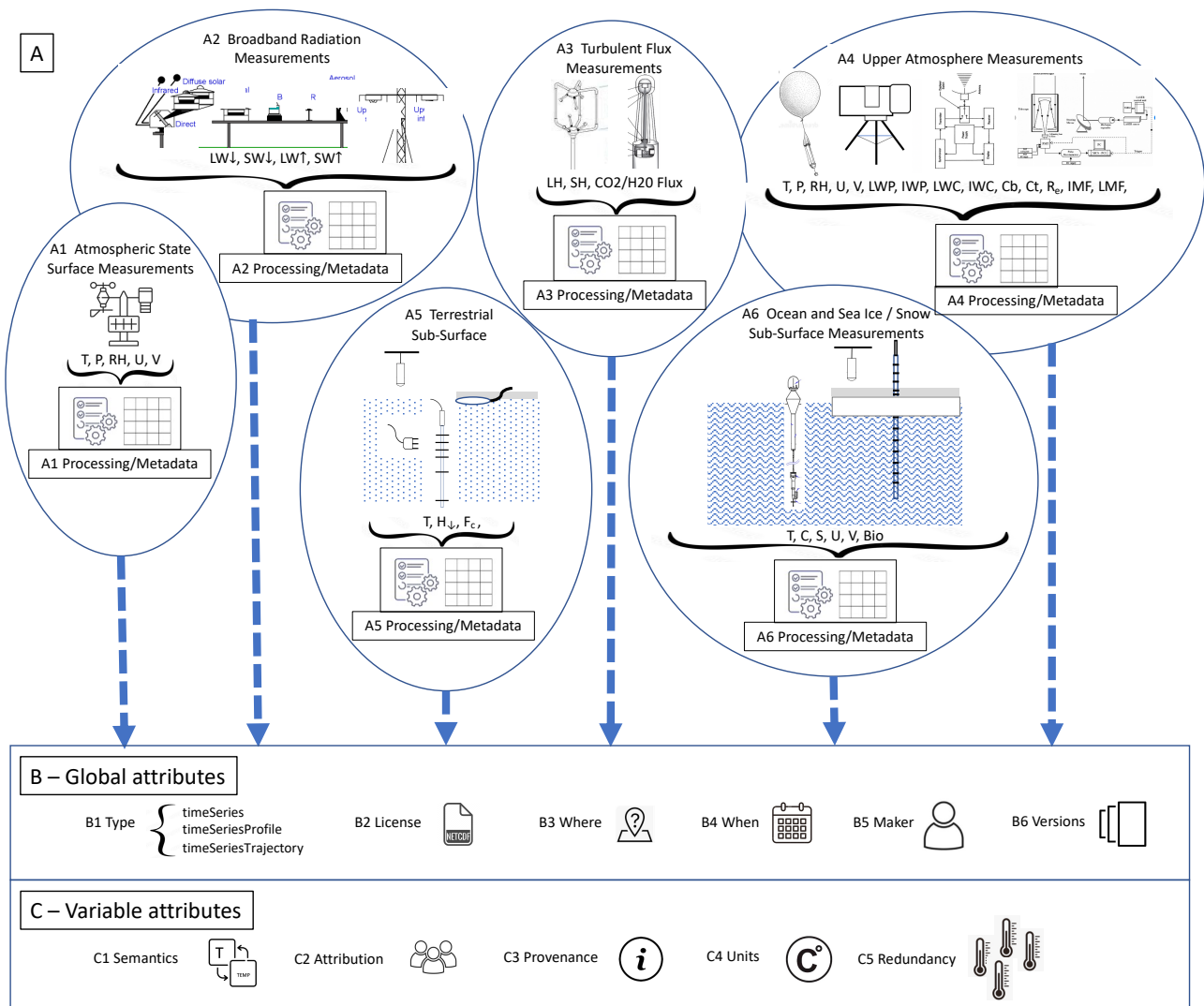
Figure 1: Instruments, measurements, data processing and metadata generation for (A1) Surface Atmospheric State, (A2) Broadband Surface Radiation, (A3) Surface Turbulent Fluxes, (A4) Upper Atmospheric Profiles, (A5) Terrestrial Sub-Surface and (A6) Ocean and Sea Ice/Snow collected into netCDF files with specified (B) Global Attributes and (C) Variable Attributes that are compliant with FAIR principles.

The different types of geophysical data (A1 thru A6) that typically can compose observatory and campaign research data are described below.

3.1 Surface Atmospheric Measurements

Surface atmospheric measurements at observatories or during campaigns are made with research-grade thermometers, hygrometers, and anemometers, which often measure at higher frequency and with more carefully calibrated sensors than operational weather stations. Such observations are sometimes side-by-side with operational weather service stations, providing context to multi-decadal operational records. Research meteorological measurements are frequently redundant, deployed at multiple locations across a site (on a scale smaller than an NWP model grid cell) or at different levels on towers to get detailed profiles in the near-surface boundary layer. Resulting variables measured are temperature, pressure, relative humidity, and the eastward and northward components of the windspeed. Both operational and research measurements of these atmospheric state variables can be considered to have well-quantified uncertainties determined by instrument calibration and tolerances.

Broadband surface radiation is measured by radiometers that measure both incoming and outgoing shortwave and longwave radiation. There are multiple commercial and experimental instrument options for measuring broadband radiation, and in the Arctic a particularly wide range of methods must be applied to keep glass domes clear of obstructions (e.g., ice, snow, dust, or sea-salt) such as heating, ventilation, and manual cleaning (Cox et al., 2021). The Baseline Surface Radiation Network (BSRN) (Ohmura et al., 1998) is a global repository for standardized radiation products that are traceable to the WMO World Radiation Radiometric Reference. However, BSRN is not designed to accommodate short-term campaign data sets and does not account for different methods for data QC and processing (Matsui et al., 2012; Long and Shi, 2006; Long and Shi, 2008).

Surface Turbulent Flux variables are calculated and inferred by a number of different methods. Eddy-correlation techniques (Kaimal and Finnigan, 1994) are based on measurements by fast-response sonic anemometers and hygrometers with built-in fast-response temperature sensors. It is often necessary to make considerable site-specific adjustments to processing methods accounting for local surface roughness, sensor height, and obstructed wind-direction sectors. In the polar regions, sensors operate near the thresholds of instrument ratings for detection and environmental conditions and have to be quality-checked for periods of riming. There are specific challenges for the cold snow- and ice-covered surface conditions over land (Grachev et al., 2018) and over the icepack of the central Arctic Ocean (Andreas et al., 2010; Cox et al., 2023). Eddy-correlation methods are only valid under stringent environmental conditions, which results in frequent data gaps. Alternatively, turbulence variables can be calculated by bulk-aerodynamic methods (Monin and Obukhov, 1954; Mahrt and Sun, 1995), but results are not as meaningful for comparing to models as it becomes a model-to-model rather than a model-to-observation comparison. Commercial packages have been developed and compared for calculating latent, sensible, and gas fluxes (Mauder et al., 2008; Fratini and Mauder, 2014), but caution must be exercised in using results and it is important to understand the basis on which variables are derived by proprietary commercial or custom software. The resulting flux

variables are latent and sensible heat fluxes, friction velocity, surface stress (momentum flux), drag coefficient, kinematic temperature scale, Monin-Obhukov stability parameter, and dissipation rate of the turbulent kinetic energy. Given the variety of physical conditions and complex methodologies for calculating turbulent fluxes, an assessment of the interoperability and consistency between flux products from different data collections is still necessary despite the existence of operational flux data networks such as FLUXNET (Baldocchi et al. 2001) and AmeriFlux (Baldocchi et al. 1996; Boden et al. 2013).

Solid and liquid precipitation are both measured at the surface but are notoriously difficult to characterize accurately. Precipitation accumulation with hourly to 6-hour frequency is traditionally measured by gauges within a surface precipitation network, usually operated by operational weather centers or hydrological agencies. Measuring solid precipitation presents a number of unique challenges; snow pillows and the Double-Fence Automated Reference (DFAR) configuration around gauges provide reliable estimations of precipitating snow. However, snow precipitation measurements from WMO standard installations with Single-Alter-shielded and unshielded gauges are affected by the undercatch of solid precipitation in windy conditions (Nitu et al., 2018; Kochendorfer et al., 2022). The WMO Solid Precipitation Intercomparison Experiment (SPICE) analyzed this undercatch and developed adjustment functions for correcting it (Kochendorfer et al., 2018; Wolff et al., 2015) which are now being used in verification practices (Køltzow et al., 2020; Buisan et al. 2020, Casati et al., 2023).

3.2 Upper Atmospheric Profiles

Radiosonde data are typically treated as if they are instantaneous vertical profiles of the troposphere by collapsing the balloon-borne trajectory of the instrument package into a profile that is time indexed with the launch time. The measurements of temperature, dewpoint temperature, pressure, humidity, and winds are high cadence (on the order of seconds) during the balloon ascent with individual launches being low cadence (every 12 hours standard launch intervals at 00 and 12 UTC). During intensive campaign periods, the launch frequency is often increased to 4–6 sondes per day. A full sounding can take 2 hours to ascend and can travel up to 200 km horizontally, and important fine-scale information is available if full, original trajectory information (time–height/pressure level–latitude–longitude) coordinates are maintained to assess the spatial displacement. Sometimes special arrangements are made to continue to capture radiosonde data during its descent after the balloon bursts (Hartten et al., 2018), although care is necessary when using descent data because key assumptions built into the instrument design are being violated. For example, the temperature and humidity sensors are positioned on the sonde so that they sample air undisturbed by the instrument casing during ascent, but those conditions may or may not be met during descent (Ingleby et al., 2022).

Many observatories and campaigns support the operation of radars, lidars, sodars, profilers, and microwave radiometers which separately and in combination can remotely infer properties through the depth of the planetary boundary layer (PBL) and free atmosphere. The systems use active (transmission and interpretation of reflected signal) and passive (detection of

natural atmospheric signal) sensing techniques. Through a significant body of research on retrieval methods, the systems can determine properties such as cloud base, cloud liquid water path, cloud ice water path, cloud liquid water content, cloud ice water content, hydrometeor sizes and shapes, snowfall rates (Matrosov et al. 2022), degree of riming, aerosol extinction coefficients, winds, temperature, and humidity. These advanced products may be obtained from diverse instrument hardware configurations and technologies as well as site-specific scanning and collection schedules. Robust site-independent retrieval methodologies that are consistent across networks such as the products produced by Cloudnet (Illingworth et al., 2007) and the ARM Active Remote Sensing of Clouds product (Clothiaux et al., 2001) have been developed, however, they may not be consistently implemented.

3.3 Terrestrial Surface and Subsurface

The terrestrial surface and subsurface is composed of complex layers of different soil, rock, ice (permafrost), and vegetation layers that can be covered with surface snow and ice with evolving density, heat capacity, conductivity, and chemistry. Thermistor strings can be co-located with tenslometers; the variables measured are gradients of temperature and moisture respectively, with thermal conductivity and heat capacity determined as fixed intrinsic properties from soil samples. Thermistor strings can also be co-located with moisture probes, providing vertical profiles of soil temperature and moisture respectively down to depths ranging from 0.1 to 2 m depending on the soil type. Snow depth, like precipitation, is a difficult quantity to measure representatively; techniques vary from using simple measurement stakes to downward-looking mast- or tower-mounted accoustic devices.

3.4 Ocean, Sea Ice, and Snow Surface and Subsurface

Ocean thermistor measurements are accompanied by conductivity and pressure measurements with resulting variables determined for salinity, temperature, and depth. Additional current meters allow determination of turbulent fluxes using eddy correlation techniques similar in principle to those used for atmospheric fluxes. Measurement of sea ice and snow macro- and microphysical properties below the atmosphere/ice or atmosphere/snow interface (i.e. subsurface) is increasingly sophisticated, with upward and downward looking acoustic devices on ice buoys determining ice thickness and snow depth (Zuo et al., 2018). Measurements are made of snow and ice density, crystalline structure, and salinity via manual sampling.

4 MODFs for the Year of Polar Prediction

The WMO Polar Prediction Project (PPP) organized the Year of Polar Prediction (YOPP; PPP Steering Group & Co-authors, 2019; Jung et al., 2016) which concluded in 2022 (Wilson et al., 2023). The YOPPsiteMIP (Svensson et al., 2020; Day et al., submitted) working group envisioned matched sets of observation and model data to support model process diagnostics. The efforts of this working group resulted in a metadata schema for MODFs and MMDFs (collectively known as MDFs) as well as an iterative production workflow. The YOPPsiteMIP effort focused on Polar terrestrial stations, but because it was

anticipated that a similar strategy would be applied to the YOPP endorsed Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) expedition (Shupe et al., 2022, Nicolaus et al., 2022), the schema was developed to also accommodate expected additional ocean and sea ice observations from ships and on-ice platforms in the central Arctic Ocean.

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The first steps in MODF production are to assemble the available data files that will feed into the MODF, extract the desired data, and acquire the corresponding metadata.During these steps each individual instrument and instrument group requires both unique quality control and processing, together with attribution tracking, in order to produce the geophysical variables and to document their provenance. Given the heterogeneity and often research-grade nature of campaign data, the amount

230 and quality of metadata for different variables is likely to be inconsistent. Although required metadata are ideally harvested from the internally documented data files, it is likely that many data sets will need additional metadata that will require interviewing original data collectors. (For an example of this other than our own, see Papoutsoglou et al., 2023). Once individual data and any available metadata from individual instruments and instruments suites are created and/or assembled, the merging process can begin.

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As we developed the schema and workflow, we identified the following challenges and solutions.

Semantics: Data semantics address the issue of the same variable being given different names drawn from multiple or ad hoc naming conventions. A significant part of the MODF solution has been the development of an extensive schema based on

240 already existing vocabulary standards.

Units: Variables' units are frequently absent entirely from data sets or expressed with nonstandard abbreviations (Hanisch et al., 2022). The MODF solution is to associate each variable with recommended units, typically as identified in the CF Standard Name Table (2023). Eaton et al. (2022) explain how these are meant to be compatable with and generally

245 recognized by the Unidata (2020) UDUNITS package.

Attribution: Perhaps the greatest MODF challenge is not technical but rather cultural. When data for a single MODF product come from instruments operated from multiple institutions and researchers, there are complex issues with acknowledging the original sources of the data (Pierce et al., 2019; Nature Editorial, 2022). Data from campaigns or

250 programs usually have multiple institutions and individual researchers involved, all of whom have different performance metrics for original research. This often leads to official or implicit data embargos so that the researchers who collected the data will have the first opportunity to publish research results. The design of MODFs is responsive to these issues by providing a high level of attribution metadata including links to original data and data producers, thereby supporting copious data citations (Vannen et al., 2020).

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Data Heterogeneity: Measurement heterogeneity is generated by how data are collected and processed. The MODF solution is to document variable derivation as much as possible from original data metadata: type of instrument, calibration information, method of deployment, quality control and processing histories, and original licenses.

260 Inconsistent Cadences: Different variables are collected on a range of native cadences varying from Hz for the fast response sensors needed to record phenomena that can change on short time scales (typically in the atmosphere) to sensors for which it is sufficient to sample on hourly or even daily time scales (typically in the terrestrial sub-surface) with a wide range in-between (typically for the ocean and ice sub-surfaces). The MODF solution is for each variable to retain its native recording cadence and to minimize any temporal averaging beyond that necessary for sensible data processing. In addition, original 265 data sets are not interpolated to fill data gaps.

Redundancy: It is common during campaigns or at intensive observatory sites for there to be multiple measurements of the same variable (e.g., temperature). There is important information contained in redundant measurements when evaluating how representative a variable is of site characteristics or when comparing the in-situ observations to model grid cells and 270 satellite footprints to evaluate local variability. The MODF solution is to include as many redundant measurements as possible, maintaining high-accuracy location information that help define the observations' microclimates, including for example soil and vegetation characteristics.

Processing Levels: Research-grade data sets typically require unique quality control and often extensive post-processing 275 which rarely can be fully automated. Frequently the state variables (e.g. temperature) are readily available in near real-time, whereas more complex variables such as turbulent fluxes can have a wide range in availability depending on whether they are output by commercial software (Fratini and Mauder, 2014), calculated from bulk variables, or based on customized calculations for complex environments. The MODF solution is to include full processing, data quality, and usability metadata.

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Versions: Since it is common for observed data to have versions, the MODF concept accommodates multiple product releases. Examples of data versions are raw (sometimes just voltages); minimally quality checked by automated elimination of extreme physically unrealistic outliers; subjectively curated for unusual and if possible correctable operational or environmental conditions; and different levels of processing to produce retrieved variables (those based on more direct 285 measurements). Frequently, highly processed and certified data are available months or even years after the original collection period. In some cases, all processing levels of data are available and archived. Two obvious ways of handling the situation are to either replace original data with more processed data as it becomes available (Figure 2A) or to keep all

versions of data (Figure 2B). MODFs' rich metatdata includes careful version tracking for individual variables which encourages the latter.

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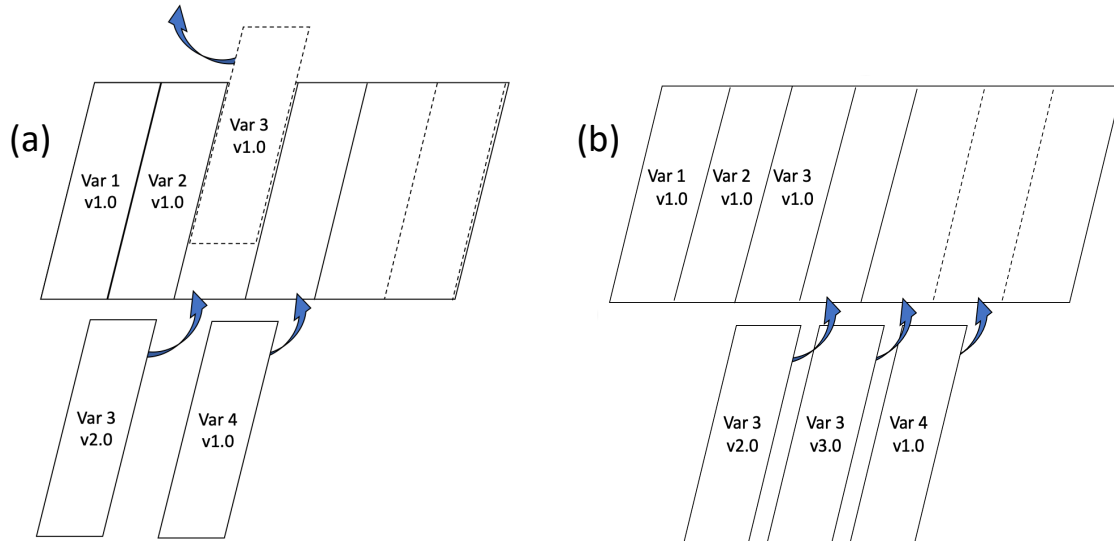
Figure 2: There are 2 approaches for MODF augmentation (as new variables become available) and modification (as variables proceed through processing levels). In both approaches, variables that are immediately available (Var 1, Var 2) can be immediately ingested and variables can be added as they become available (Var 3, Var 4). The 2 approaches accommodate two strategies for variables that undergo post processing resulting in products with quality-control (QC) levels. In (a), original data (Var 3 v1.0) can be replaced with QC'ed data (Var3 v2.0). In (b), original data (Var3 v1.0) can be retained in the MODF and QC'ed data (Var3, 2.0) can be added.

5 The H-K Variable Schema Table

The H-K Variable Schema Table, developed for the YOPPsiteMIP (Hartten and Khalsa, 2022, hereafter the H-K Schema), provides guidelines for creating both MODF and MMDFs as netCDF files (Unidata, 2023) with consistent variable names and metadata. Hereafter the discussion in this paper centers on those entries which are relevant to MODFs, although most of them are also relevant to MMDFs. The H-K Schema follows the Attribute Convention for Data Discovery (2022; hereafter ACDD), the NetCDF Climate and Forecast (CF) Metadata Conventions (Eaton et al., 2022), and the ISO/TC 211 19100 series of standards for digital geographic information. Short variable names are compliant with the World Climate Research Program (WCRP) Coupled Model Intercomparison Project, Phase 6 (CMIP6; Taylor et al., 2022) whenever possible as these are in wide use in the geophysical research community.

For global attributes, the H-K Schema requirements include identifying the file feature type, the file maker, the license, the location, information on when data was collected, and a permanent identifier. The global attributes listed in the H-K Table

are minimum requirements, and may be augmented by others from the ACDD or the CF Conventions in order to include other metadata deemed important for provenance or useability. In particular, *product_version* global attribute can be used to help clearly identify when an MODF has been augmented by new or reprocessed variables, and *comment* can always be used for free-text metadata or stable URLs linked to additional metadata files. For variable attributes, the H-K Schema specifies identifying vocabularies, units, individual variable attribution (who originally collected the data) and variable provenance, and also presents a method for differentiation of multiple measurements of the same geophysical variable (redundancy). The H-K Schema is available in both json (machine readable) and pdf (human readable) formats.

5.1 Global Attributes

Global attributes are the descriptive metadata that are relevant for the entire MODF file. Table 1 lists recommended global attributes for MODFs. Some were chosen because they are highly recommended by ACDD. Others are merely recommended by ACDD, but they made sense for our purpose and seemed not overly burdensome for those most likely to be making MODFs. We chose additional attributes from metadata standards other than ACDD (e.g. the CF Conventions, the DataCite Metadata Kernel v4.4 (DataCite Metadata Working Group, 2021)) because we felt they would help MODFs be FAIR. Some global attributes whose inclusion and consistent use is particularly important are described below. We use italics for the names of attributes and single quotes around variable names.

id: The global unique Persistent Identifier (PID). This global attribute does not supersede references to the PIDs associated with individual variables (Prakesh, et al., 2016), which can be provided within the variable attribute *references*. The MODF *id* remains constant as modifications or additions are made to the MODF file.

license: Specifies terms of distribution. As with *id,* individual variables and groups of variables in the MODF may have unique license requirements that can be recorded in the variable attribute *comment*.

creator_name: The names of individuals who should be in the citation for the MODF (Jones et al. 2020, see §2.2.7.3.3). The DataCite Metadata Kernel v4.4 (DataCite Metadata Working Group, 2021) defines creators in this context as the main producers of the MODF file and also links them to authorship. (Note that the main producers of component data sets are credited within the variable attributes coming from their individual data sets.) Enabling those who create MODFs to receive appropriate credit for their work is a key element of making MODFs FAIR; data reuse depends in part on data accessibility, which in turn is more likely when data are "considered legitimate, citable products of research" (Data Citation Synthesis Group, 2014).

featureType: Although the original vision was to have a single MODF for a site during a campaign that would include all relevant variables, when considering the practicalities of archive submission, it became apparent that file *featureType* needed

to be specified to facilitate data services such as visualization tools. Most observatory data fits into *featureTypes* timeSeries, timeSeriesProfile and timeSeriesTrajectory. These *featureTypes* are defined by the temporal-spatial dimensions that are

345   associated with individual variables: time only for timeSeries, time and height (or depth) for timeSeriesProfile, and time–height (or depth)–latitude–longitude for timeSeriesTrajectory.

missing_value: Establishes one consistent *missing_value* for all data in the MODF.

350   *history:* Provides an audit trail for the MODF file, documenting its provenance. Initially, this should include information about how it was created. Later, if the original file is modified (e.g. variables are corrected or added), information about what has changed should be added to the original information. The CF Conventions recommend that each step be documented by a line containing a datestamp, the name of the person or entity who did the action, a brief description of the action, and any program(s) which accomplished the action (including relevant settings or command arguments). If the modifications involve

355   the addition of a new version of an existing variable, the variable attributes associated with the new version, and the earlier version if it is not removed, should thoroughly document the change.

Table 1: H-K Schema Recommended Global Attributes (adapted from Hartten and Khalsa, 2022)

Attribute	Description of Required Information
title	Short human-readable phrase or sentence describing the MODF
date_created	Date on which current version of the MODF was created or modified
Conventions	List of the conventions that are followed by the MODF
standard_name_vocabulary	Name and version of the controlled vocabulary from which variable Standard Names come
creator_name	Name of the main individual(s) involved in producing the MODF, or the authors of the publication, in priority order
creator_email	Email of the main individual(s) involved in producing the MODF, or the authors of the publication (if there is one) describing the MODF
institution	Institution where the original MODF was produced
id	Persistent Identifier (PID) for the MODF
naming_authority	Naming authority for PID (preferably using reverse-DNS naming, e.g. 'edu.ucar.unidata', although URIs may be used)
license	Terms of distribution and use
time_coverage_start	Time of the first data point in the MODF
time_coverage_end	Time of the last data point in the MODF
featureType	One of the following: 'point', 'timeSeries', 'trajectory', 'profile', 'timeSeriesProfile', or 'trajectoryProfile'
contributor_name	Name of any individual(s) responsible for collecting, managing, distributing, or otherwise contributing to the development of the MODF; may indicate those who helped with the development but who were not so "key" as to be listed as an author
contributor_email	Email of any individual(s) responsible for collecting, managing, distributing, or otherwise contributing to the development of the MODF
project	Name of the project(s) principally responsible for originating this MODF
summary	A paragraph describing the MODF
source	The method of production of the MODF; may include line breaks to enhance readability
metadata_link	URL to detailed documentation (DOIs expressed as https://doi.org/...)
history	Provides an audit trail for modifications to the MODF
references	Published or web-based references that describe the MODF or methods used to produce it
keywords	Comma-separated list of key words and/or phrases, preferably drawn from a controlled vocabulary, e.g. the GCMD at https://earthdata.nasa.gov/earth-observation-data/find-data/gcmd/gcmd-keywords

5.2 Time, Space and Site Variables

In the H-K Schema, variables have been divided into subgroups. There are three subcategories with time, space, and site information: temporal dimensions and variables; spatial dimensions and variables; single level fixed variables. Per the NetCDF Users Guide (Unidata, 2023), dimensions "may be used to represent a real physical dimension, for example, time, latitude, longitude, or height.... [or] to index other quantities, for example station or model-run-number." Examples of these indexing variables are listed in Table 2 and discussed further below. Per the H-K Schema, all dimensional and geophysical variables are given a short CMIP or CMIP-like variable name and are characterized by variable attributes *long_name*, *standard_name*, *units*, additional recommended attributes, and any other attributes the MODF creators feel necessary to fully document the data.

Table 2: Examples of dimensions and variables related to time, space, and site information, together with the associated *long_name*, *standard_name*, *units* and recommended attributes (extracted from Hartten and Khalsa, 2022). A solid grey line to the left of each "Minimum Recommended Additional Attributes" entry indicates the rows to which each list applies; not all rows have additional recommended attributes.

Variable Name (CMIP or CMIP-like)	*long_name* Attribute	*standard_name* Attribute	*units* Attribute	Minimum Recommended Additional Attributes
TEMPORAL DIMENSIONS AND VARIABLES				
time	Valid Time	time	hours since ...	
time15	Valid Time for Observations with 15-Minute Cadence	time	hours since ...	*delta_t*; *calendar*
time_sonde	Radiosonde Valid Time	time	hours since ...	
SPATIAL DIMENSIONS AND VARIABLES				
height_tower	Tower Observation Height	height	m	
lat_sonde	Radiosonde Latitude	latitude	degrees_north	*missing_value*;
lon_sonde	Radiosonde Longitude	longitude	degrees_east	*actual_range*;
alt_sonde	Radiosonde Altitude	altitude	m	*instrument*; *source*
SINGLE-LEVEL FIXED VARIABLES				
orog	Surface Altitude	surface_altitude	m	*missing_value*; *source*; *references*; *comment*

'time', 'time15', 'time_sonde': MODFs are intended to retain as much high-resolution information from the original data collection as possible. Averaging is limited to that necessary for processing (e.g. for eddy-correlation flux calculations) and data are not interpolated. Therefore, temporal dimensions support maintaining original data collection cadences for individual variables. For instance, in MODFs 'time' is a generic temporal dimension whereas 'time15' is a time dimension associated with variables collected at 15 min intervals and 'time_sonde' is the time dimension associated with the data collected during a radiosonde ascent. In the YOPPsiteMIP implementation of MODFs, we have chosen to append 'N' or '_platform' to a generic CMIP name such as 'time' in order to indicate a time array with a particular cadence in minutes or a time array tied to a particular instrument or platform. In keeping with CF Metadata guidelines, all the differently named time variables can and should have the same long_name attribute.

'height_tower': A spatial coordinate can be a single scalar value or a set of values (a dimension) that describes the location where geophysical measurements are collected. This can be an array of fixed values in the case when measurements are made at set levels, for instance on an instrumented tower. A tower may also consist of multiple measurements of the same geophysical variable collected at different heights above the ground. For instance, observations of air temperature collected by three sensors located at the surface (2 m AGL), on a pole (10 m AGL), and on top of a building (20 m AGL) could be combined into a single array designated as '_tower' so long as the sensors' horizontal positions were co-located.

'lat_sonde', 'lon_sonde", "alt_sonde": Spatial coordinates can also be a dimension variable. For instance, if information is retained on the latitude, longitude, and/or altitude of a radiosonde during its ascent, this information should be put into auxilliary coordinate variables that provide the location in space for the geophysical variables collected by the sonde. If the sonde output includes only varying altitudes and a fixed launch time, the geophysical data from each sonde flight should be put into a file with the *featureType* "profile". If the sonde output includes varying altitudes and associated times, the geophysical data should be put into a file with the *featureType* "timeSeriesProfile". In both cases a scalar altitude variable should be used as the vertical dimension for each flight. However, if varying latitude and longitude are also provided, the geophysical data from each sonde should be put into a file with the *featureType* "timeSeriesTrajectory" with the reported altitude, latitude and longitude being provided as coordinate variables for each flight. Finally, the "profile", "timeSeriesProfile", and "timeSeriesTrajectory" *featureTypes* all require that times be monotonically increasing. It would be tempting (and not against the *featureType* requirements) to put geophysical data collected during radiosonde descent and their accompanying spatial coordinates into the same variables used for the values collected during ascent. However we would recommend using a separate set of variables instead, with a clearly different suffix and *long_name* set. Data collected during descent has different statistical characteristics than data collected during ascent (Stephan et al., 2021; Ingleby et al., 2022) and we think users should affirmatively choose, rather than accidentally use, such "off-label" data.

'orog': Certain fixed variables are descriptive of the site or the platform from which measurements are taken. An example of the former is the variable with the surface altitude (CMIP name 'orog'), which describes the site's altitude above the surface defined as the lower boundary of the atmosphere. Other common single-level fixed variables are the 'lat' (latitude) and 'lon' (longitude) which identify a site's general location. If the site has distributed measurements, individual variables may have more refined 'lat_platform' and 'lon_platform' variables or dimensions.

5.3 Geophysical Variable Attributes and Examples

There are six categories of geophysical variables: Single-level atmosphere variables; surface and Top-of-Atmosphere (TOA[3]) variables; atmospheric variables on model or instrument levels; sub-surface terrestrial variables; oceanic variables on model or instrument levels; sea ice variables. Examples of *long_name*, *standard_name*, and *units* attributes for observed geophysical variables that have been catalogued in the H-K Schema are shown in Tables 3 and 4. A full listing of all the single-level atmospheric variables, the surface and TOA variables, and the atmospheric variables on instrument levels in the H-K Schema version 1.2 is presented in Table A1, while a listing of the current H-K Schema oceanic variables on model or instrument levels, sub-surface terrestrial variables, oceanic single-level variables, and sea ice variables is found in Table A2. Some discussion of the examples in Tables 3 and 4 follows.

CMIP name: The Coupled Model Intercomparison Project (CMIP) names are taken from the CMIP6 Participation Guidance for Modelers, a program supported by the NASA Program for Climate Model Diagnosis & Intercomparison. CMIP names prioritize terse, presumably code-efficient abbreviations such as 'ta' (air temperature). To clearly identify the variables that were observed or derived redundantly from different methods or platforms, a suffix can be appended (e.g., _tower, _radar, _8m). Some standard measurements, such as 2m temperature and 10m winds, have unique CMIP names such as 'tas', 'uas' and 'vas' (near-surface air temperature, eastward wind, and northward wind, respectively). In the case where a CMIP variable name has not been defined in the CMIP6 vocabulary, a CMIP-like name has been composed.

long_name: Fully describes the physical quantity and can be thought of as useful attribute for labeling plot axes; in other words, it is the name that best communicates with humans about what the variable is. (Note that the *long_name* does not necessarily need to be in English.) The H-K Schema provides ad hoc *long_name* definitions for all variables.

standard_name: Taken from the CF Standard Name Table (2023), which is periodically updated based on community requests and discussion (see the "Discussion" link at CF Metadata Conventions (2024)). Standard names are constructed in conformance with the CF Conventions (Hassell et al., 2017; Guidelines for Construction of CF Standard Names, 2024). Different variables can have the same standard name. For instance, 'albs' and 'albsn' both have the *standard_name* of

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[3] TOA variables are only relevant to MMDFs, but are grouped with surface variables in the H-K Schema and therefore included for completeness.

surface_albedo, but 'albsn' is restricted to use over snow-covered areas. Redundant variables (such as multiple measurements of temperature, or fluxes computed by bulk versus eddy-correlation methods) will have the same standard name and will require differentiation by a suffix added to the CMIP name, additional descriptors in the *long_name*, and

440   possibly accompanying spatial-temporal indices. The *standard_name* of a variable sometimes implicitly gives information about the directionality of a flux or similar variable, information which is explicitly given in the CF Standard Name Table and replicated in the Notes column of the full H-K Schema. Specifically, to continue with the example of fluxes, "The sign convention is that "upwelling" is positive upwards and "downwelling" is positive downwards" is part of the definition of any variable with those four up/down words in its *standard_name*.

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Table 3: Examples of atmospheric variables, together with the associated *long_name*, *standard_name*, and *units* attributes (extracted from Hartten and Khalsa, 2022).

Variable Name (CMIP or CMIP-like)	*long_name* Attribute	*standard_name* Attribute	*units* Attribute
SINGLE-LEVEL ATMOSPHERIC VARIABLES			
tas	Near-Surface (2m) Air Temperature	air_temperature	K
tas_site1	Near-Surface (2m) Air Temperature at Site1	air_temperature	K
uas	Near-Surface (10m) Eastward Wind	eastward_wind	m s-1
SURFACE AND TOA VARIABLES			
snd	Surface Snow Thickness	surface_snow_thickness	K
ts	Surface (Skin) Temperature where Land or Sea Ice	surface_temperature	K
rsds	Downward Shortwave Radiation at the Surface	surface_downwelling_ shortwave_flux_in_air	W m-2
ATMOSPHERIC VARIABLES ON MODEL OR INSTRUMENT LEVELS			
ta	Temperature	air_temperature	K
rsd	Downward Shortwave Radiation	downwelling_ shortwave_flux_in_air	W m-2
ua	Eastward Wind Component	eastward_wind	m s-1

Table 4: Examples of non-atmospheric variables, together with the associated *long_name*, *standard_name*, and *units* attributes (extracted from Hartten and Khalsa, 2022).

Variable Name (CMIP or CMIP-like)	*long_name* Attribute	*standard_name* Attribute	*units* Attribute
SUB-SURFACE TERRESTRIAL VARIABLES			
gtsl	Bulk Soil Temperature	soil_temperature	K
mrlsl	Layer-Average Soil Moisture	moisture_content_of_soil_layer	kg m-2
OCEANIC SINGLE-LEVEL VARIABLES			
tos	Sea Surface Temperature	sea_surface_temperature	K
mlotst	Ocean Mixed-Layer Depth	ocean_mixed_layer_ thickness	m
rsntds	Net Downward Shortwave Radiation at Sea Water Surface	net_downward_ shortwave_flux_ at_sea_water_surface	W m-2
OCEANIC VARIABLES ON MODEL OR INSTRUMENT LEVEL			
to	Ocean Temperature	sea_water_temperature	K
so	Sea Water Salinity	sea_water_salinity	1e-3
SEA ICE VARIABLES			
sithick	Sea Ice Thickness	sea_ice_thickness	m
sisali	Sea Ice Salinity	sea_ice_salinity	1e-3

Table 5 lists the other attributes that should be included in MODFs for geophysical variables. Some of the variable attributes in Table 5 are listed in the CF Conventions as being for use as either global or data attributes, but the *history* attribute is listed as for global use only. We have encouraged its use with variables (data) in MODFs because we believe that maintains the spirit if not the letter of the CF Conventions; like *institution*, *references*, *source*, and *title*, *history* helps document the provenance and nature of the data included in these multi-institution, multi-sourced files. We also encourage MODF (and MMDF) makers to make use of additional variable attributes to share information about the variable contents with users. Brief explanations of some of the attributes in Table 5 follow, but those interested in creating MODFs should also review the definitions and explanations of attributes in the ACDD and the CF Conventions.

original_name: Refers to the name of the variable in the original file from which it was extracted. This provides an important cross reference in the case where a user may need to refer back to the original source data set.

465 *instrument:* Tracking instrumentation characteristics and in many cases calibration coefficients is critical to provide information for users who may be in the process of developing refined data processing, developing higher-order products, or doing instrument intercomparison studies.

references: Published material that describes either the data or the methods used to produce it should be listed here. Best practice is to include a URI (a DOI for a paper, or a URL for a website).

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source: Both the CF Conventions and ACDD describe this as "the method of production of the original data", by which they mean either the model that produced it or the instrument that gathered it. In either case, the idea is to give the user information that will help them understand what they're working with, what assumptions or methods are inherent to the data. Therefore, the name and version of a numerical model, or the type and perhaps make and model of an instrument, would be

475 appropriate here.

history: Provides an audit trail for the data, documenting its provenance. When used as a variable attribute, this should trace what has been done to the data from its raw state until it was put into this file. We recommend that each step be documented by a line that starts with a datestamp and the version number of the variable, the person or entity who did the action, a brief

480 description of the action, and any program(s) which accomplished the action (including relevant settings or command arguments).

Table 5: Minimum recommended additional variable attributes for geophysical variables (adapted from Hartten and Khalsa, 2022)

Additional Variable Attributes	
missing_value	contributor_name
actual_range	contributor_email
instrument	creator_name
source	creator_email
references	institution
history	comment
original_name	

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Figure 3 describes the work flow and process that developed through the efforts of the YOPPsiteMIP team of observers, modellers, data scientists, and data managers. Key components include both the H-K Schema and the A-M Variable and Attribute Template Table (Morris and Akish, 2022). The A-M Table was developed for collating metadata that was not already encoded into the individual data files being used as input to MODFs, and was used as a direct input to the MODF creation process. The development of the H-K Schema and the A-M Table was a highly iterative process, as indicated by the two-way arrow between **C** and **D** in Figure 3, and is expected to continue to be so .
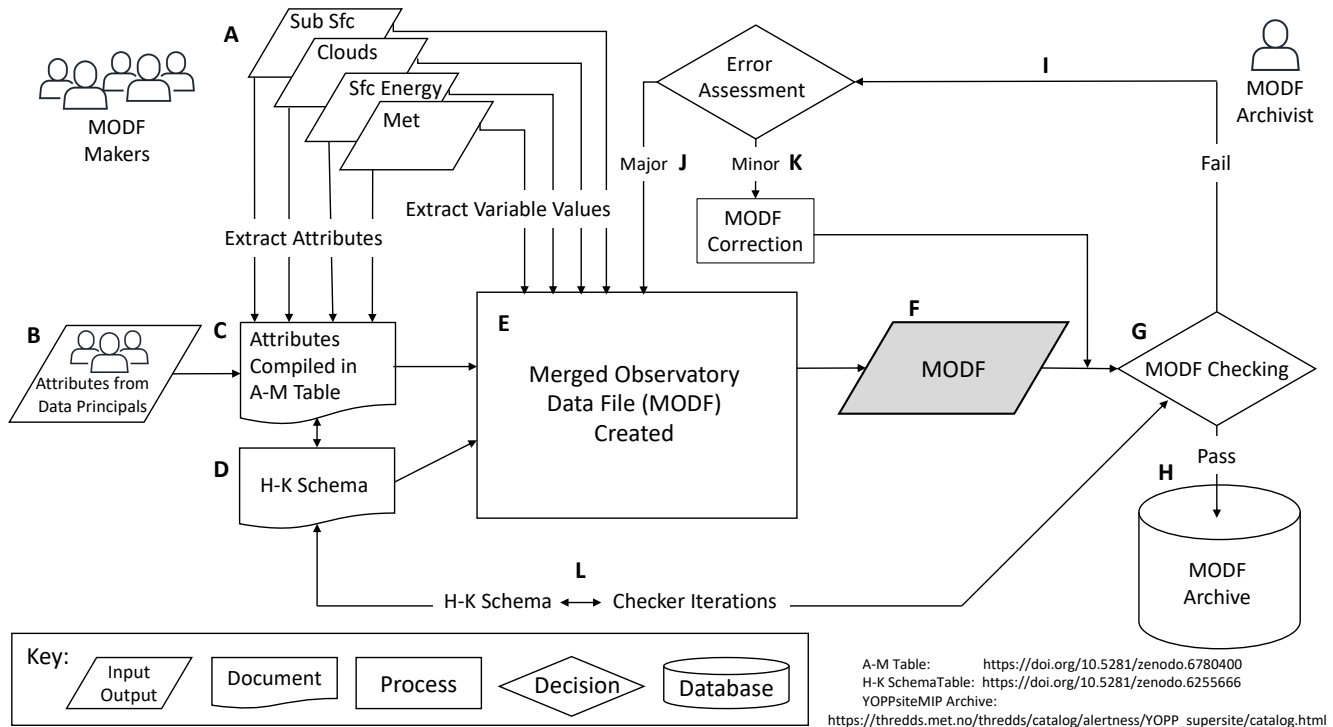
Figure 3: The MODF workflow process. A: Gather input files, B: Interview contributing data principals for necessary metadata not digitally encoded in data files, C: Utilize the A-M MODF template to construct the specific MODF framework based inputs from A and B compliant with the H-K Schema (D). MODF Makers create the MODF (E) with inputs from (C) and the data values from individual files collected (A). F: MODF file. G: MODF checking. H: Upon 'pass', send MODF to archive. I: Upon 'fail' assess MODF. J: Major fails, return MODF Makers. K: Minor fails, archivist corrects and sends MODF to archive after rechecking (G). L: Iterative developments between H-K schema (D) and MODF checking (L). People icons adapted from one designed by vectorstock (Image #45970079 at VectorStock.com).

6 Discussion

We have presented the H-K Schema (Hartten and Khalsa, 2022) and a production framework for organizing complex campaign and observatory data from multiple instruments into Merged Observatory Data Files (MODFs). The H-K Schema also enables formatting forecast model output into corresponding Merged Model Data Files (MMDFs). MODFs and

505   MMDFs, i.e. Merged Data File (MDF) collections, are compliant with existing metadata and data standards that support FAIR principles. The Schema and the framework were developed by a YOPPsiteMIP working group of observers, modelers, and data managers. MODFs address the mundane but complex issues that arose from the YOPPsiteMIP vision of confronting polar weather forecasting models with observations from richly instrumented sites during special observing periods. The issues addressed include data semantics, attribution for original data, data provenance, different cadences, multiple

510   measurements of the same variable from the same site (including local, subgrid-scale spatial distribution), versioning strategies to account for different levels of data processing, unit conventions, and missing data indicators. Because of the high cadence of many measurements (seconds to minutes), MODFs can be used to evaluate accumulating biases at model timestep increments, which are typically shorter than model output increments.

515   Although providing site, instrument, processing, and attribution metadata documentation is good practice, it is often neglected. Since we discovered that this essential MODF information was difficult to assemble after the fact, we recommend that as part of the routine MODF development process observers use datagrams during development, deployment, and operation of sensors as a standard practice. Datagrams "are designed to document the life story of a data value from start to finish and provide a guide for humans to design, deploy, troubleshoot, repair, record, transmit, process, and archive data

520   collected with measuring devices." (Morris and Uttal, 2022). In addition to proactively gathering observation metadata, the MIIP strategy would also be significantly supported if model output were extracted in the vicinity of observatories in real-time; this can be a difficult after the fact for routine output, and impossible for timestep output. Furthermore, while we strongly encouraged YOPPsiteMIP MODF and MMDF makers to check their files for compliance before submitting, we have found it incredibly useful that the data manager at the host archive we worked with actively participated in checking the

525   files (Tjernström, 2022) and in some cases making editorial corrections to bring the MODFs and MMDFs into full compliance with the H-K Schema. This sort of effort at the data archive can be necessary when MDF providers do not have the resources to support the level of data management required to create fully compliant files.

     Currently the H-K Schema includes geophysical variables across the atmosphere, snow, ice, terrestrial, and ocean systems.

530   Appendix A lists the MODF (and MMDF) values that are currently in the H-K Schema (version 1.2). These are not exhaustive, and we expect that MODF users and makers will augment their MODF files to accommodate individual campaigns by including, for example, atmospheric aerosols, constituent gases, additional ocean and terrestrial variables, and ecosystem and biogeochemical data. Any additional variables should be incorporated for specific applications using the metadata standards described here. Some MODF variable collections (e.g. precipitation from different sensor systems, or

535   profiler data with sensor-to-sensor and/or range dependent measurement volumes) may require discovery or creation of special variable attributes. If no standard exists we recommend that the custom variable attribute be submitted for consideration as a standard; directions are available via the "Discussion" link at CF Metadata Conventions (2024). However,

MODF makers should keep in mind that additional variable metadata for complicated variables can also be shared via the *reference* and *comment* attributes.

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A first set of MODF files (Mariani et al., in review) implementing the H-K Schema from concept to production for YOPP Special Observing Periods has been archived by the Norwegian Meteorological Service where a collection[4] of matched MODF and MMDF files are available for several Arctic ground stations. As of March 2024 these MODFs are not yet available for all the Arctic YOPP Supersites, nor for any of the Antarctic YOPP Supersites; those which are available do not

545 yet contain all the observed variables from the individual sites. This situation reflects the difficulty involved with amalgamating data into MODF files. An initial analysis (Day et al., submitted) using the YOPPsiteMIP MODF–MMDF collection demonstrates through a number of examples and case studies how process-describing variables such as surface fluxes (longwave, sensible, and latent) and ground fluxes can be used to gain deeper understanding into the nature of forecast errors.

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The main motivation for the creation of the MODF and MMDF file format is to accelerate improvements of process description in numerical models by facilitating evaluation using suitable observations. The main strength is that the concept and format is co-developed by and has purpose for both the modelling and observational communities. Another beneficial aspect is that what we have presented here is a structure that could be built upon by the data management community and

555 incorporated into data center operations. The format is intentionally designed with growth in mind, allowing for new variables and feature types together with the possible development of community platforms for interaction. These aspects pave the way for widening the concept to include more sites as well as extending the time coverage for existing sites, and also to include more processes and additional research areas. While the material presented here is intended to help explain MODFs and how to create them, we encourage those making MODFs to explore the ACDD, the CF Conventions, and the

560 DataCite Metadata Kernel to more fully understand the possibilities for expansion.

We acknowledge that model–observation interoperability is based on standards that may be limiting for specific applications, so we expect that custom MODFs will be developed as necessary. In other words, the MODF concept is meant to be flexible while remaining within proscribed protocols. While there are few limitations to the MODF concept, currently the types of

565 data that are encompassed are designed for the YOPPsiteMIP goals (Jung et al., submitted). Further development depends on the engagement by communities and their interest to grow and expand the format based on other research needs. The success of the MODF format is and will be dependent upon the interest of those data producers.

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[4] https://thredds.met.no/thredds/catalog/alertness/YOPP_supersite/catalog.html

The concept of organizing multivariate observational data sets from a single site or platform into a unified product is not unique. Wei et al. (2021) describes how ICARTT data format conventions (Aknan et al., 2013) can be used to create merged in-situ data products from research aircraft carrying multiple sensors. The U.S. DOE ARM program (Stokes and Schwartz, 1994) creates Climate Modeling Best Estimate (CMBE) data files (Xie et al., 2010) for their Climate Reference Sites. Hogan and O'Connor (2004) describe how the Cloudnet project preprocesses cloud data from multiple remote sensors using appropriate ancillary observations and model forecasts, then makes the output available in netCDF format with rich metadata about the preprocessing. What is unique about MODFs is the strategy of *simultaneously* creating corresponding matched MMDF data files to support modeling verification and process evaluations. This addresses a long-standing issue with communication silos between observing and modeling sciences (Holloway et al., 2014, Sprintall et al., 2021, Neang et al., 2021).

We also expect that MODFs will be used to facilitate studies of *interdisciplinary* observation-based system science. The NSF workshop report Opportunities and Challenges of Arctic System Science (Vorosmarty et al., 2018) introduced the concept of "… multiple 'currencies' that link the Arctic climate and environment—geophysical entities such as water, energy, carbon, and nutrients with quantifiable properties—and how they interact to produce and illuminate systems-level behaviors". MODFs, by quantifying the currencies throughout a system with internally consistent standards, can serve to break down barriers between individual studies of separate components of the system that are typically divided along disciplinary lines, thereby advancing multidisciplinary process studies.

Generating MODFs will expand usage of data from field campaigns by increasing data uptake and decreasing data latency. This will promote usage of non-operational data that are currently underutilized and difficult to access comprehensively, specifically for environmental services requiring near real-time environmental intelligence. The U.S. Interagency Arctic Research Policy Committee (IARPC) has defined environmental intelligence as "a system through which information about a particular region or process is collected for the benefit of decision makers through the use of more than one inter-related source". Furthermore, IARPC notes that "Traditionally, researchers collect data, develop models, and communicate results through well-established channels that are often slow and inefficient. While the vetting of scientific results ensures that the conclusions are of highest quality, the process is not well-aligned with the need for rapid information delivery in the face of environmental transitions that are putting stress on ecosystems and human populations." MODFs will not only accelerate timely and relevant data access and scientific results for the primary researchers that collected the data, but will also support the iterative observations, modeling, and data systems that connect researchers, stakeholders, and decision-makers to allow informed responses to environmental events. To this end, MODFs are designed to be living files that can be created in a timely manner with near real-time variables and then augmented when additional variables become available. This is particularly important for situations in which observational data becomes obsolete before it can be utilized by environmental awareness and short-term prediction services for extreme events. MODFs can then be augmented with variables that are only

available after extensive human-assisted processing (e.g., surface energy balance fluxes) for research purposes, as well as with new versions of variables that require detailed quality control to produce higher-level and higher-reliability products.

605 This addresses the concern that many data providers express about only releasing the most highly curated values (often resulting in data embargos and release time lags) and recognizes that the level of necessary post-processing depends on the application, while still reducing data latency so that rapid climate change events might to be addressed in a timely manner.

Creating merged data products that are also Findable, Accessible, Interoperable, and Reusable is easy to say and hard to

610 implement; it is expensive in any currency, be it time or people or computing. In developing the concept of MODFs and MMDFs we have struggled over whether there is a realm between "nothing" and "everything", of how to keep the quest for perfect compliance from preventing a good or even very good improvement. In the end, we think the guiding principle must be this: to remember that FAIR data is an ideal, and the implementation involves tradeoffs; some metadata is better than none, and anything that moves along this path is good.

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Appendix A: Current Measurable Geophysical MODF and MMDF Variables and Their "Essential Climate Variable" Status

The H-K Schema is a set of tables that is expected to be expanded and adjusted as the need arises for additional MODFs and MMDFs and for additions to existing ones. Therefore, researchers interested in using the H-K Schema to guide file creation should always refer to the current online version; the DOI listed in the References of this article will always land on the most recent vesion of the Schema, and when a new version of the H-K Schema is published the earlier versions will be prefaced with a note including a link the the latest version.

In this Appendix we list the *long_name* attribute for all atmospheric (Table A1) and non-atmospheric (Table A2) geophysical variables, current as of the time of this manuscript's submission. We do this for two reasons: to show the variety of variables incorporated in the H-K Schema so far, and also to highlight the variables in the Schema which the WMO has identified as Essential Climate Variables (ECVs; Essential Climate Variables, 2023). Note that some of the ECVs are defined by the Global Climate Observing System (GCOS) in a manner other than the point measurements typically made at field sites. Those details are identified by footnotes in the tables. Lavergne et al. (2022) have proposed expanding the list of ECVs related to sea ice; proposed sea ice ECVs that are in the H-K Schema are separately highlighted in Table A2.

Table A1: Atmospheric variables (extracted from Hartten and Khalsa, 2022) that are measured at Arctic YOPP supersites or included in Arctic YOPP MMDFs (prefaced by "•"). Underlined variables are ECVs.

Variables' *long_name* Attribute	
SINGLE-LEVEL ATMOSPHERIC VARIABLES	
Surface pressure	Height of atmospheric boundary layer
Mean sea level pressure	Total precipitation of water in all phases per unit area
Near-surface eastward wind	Total cloud cover
Near-surface northward wind	Cloud optical thickness
Near-surface wind speed	Total column water vapour
Direction near-surface wind from	Total column cloud water in liquid phase
Near-surface wind gust	Total column icewater
Near-surface air temperature	Surface horizontal visibility
Near-surface dew point temperature	Ozone concentration in air[a]
Near-surface specific humidity	Photosynthetic photon flux density
Near-surface relative humidity	Reflected photosynthetic photon flux density
Surface roughness for momentum	
Surface roughness for heat	
SURFACE AND TOP-OF-ATMOSPHERE VARIABLES	
Surface snow thickness	•Top-of-atmosphere incoming shortwave radiation
•Surface snow area fraction	•Top-of-atmosphere outgoing shortwave radiation
Snow water equivalent	•Top-of-atmosphere outgoing long wave radiation
Snow density	Upward surface shortwave radiation
Surface (skin) temperature where land or sea ice	Downward shortwave radiation at the surface
Snow surface skin temperature	Net shortwave radiation at the surface
Snow temperature	Upward surface longwave radiation
Ground skin temperature	Downward surface longwave radiation
Surface albedo[b]	Net longwave radiation at the surface
Snow albedo[b]	•Surface turbulent latent heat flux
Surface downward heat flux in snow	Surface turbulent latent heat flux[c] (bulk method)
Downward heat flux at snow botton	Surface turbulent latent heat flux (eddy covariance method)
•Canopy area fraction	•Surface turbulent sensible heat flux
Time-average eastward turbulent surface stress	Surface turbulent sensible heat flux (bulk method)
Time-average northward turbulent surface stress	Surface turbulent sensible heat flux
	(eddy covariance method)
	Ground heat flux

[a] Total column ozone is the listed ECV, while observations from a site are typically point values.
[b] The ECV listing is for maps, not point measurements, of albedo; snow albedo is not explicitly listed.
[c] The ECV listing specifies "Land-Biosphere Evaporation from Land".

Variables' *long_name* Attribute

ATMOSPHERIC VARIABLES ON MODEL OR INSTRUMENT LEVELS

•Geopotential height

Geopotential height on half levels

Atmospheric pressure

Pressure on full levels

Pressure on half levels

Eastward wind component

Northward wind component

Wind speed

Direction wind from

Vertical velocity

•Vertical large-scale wind in pressure coordinates

Air temperature

Dew-point temperature

Specific humidity

Relative humidity

Wet-bulb potential temperature

•Tendency of air temperature

•Tendency of air temperature due to advection

•Tendency of specific humidity

•Tendency of specific humidity due to advection

•Tendency of eastward wind

•Tendency of northward wind

Upward longwave radiation

Downward longwave radiation

Upward shortwave radiation

Downward shortwave radiation

•Vertical eddy diffusivity coefficient for momentum
due to parameterized turbulence

•Vertical eddy diffusion coefficient for temperature
due to parameterized turbulence

Turbulent sensible heat flux based on
virtual potential temperature

Turbulent moisture flux based on vapor content

Eastward turbulent momentum flux

Northward turbulent momentum flux

Turbulent kinetic energy

•Percentage cloud cover, including both
large-scale and convective cloud

Mass fraction of cloud liquid water

Mass fraction of cloud ice

Snowfall flux per unit area

Cloud base height

Table A2: Non-atmospheric variables (extracted from Hartten and Khalsa, 2022) that are measured at Arctic YOPP supersites or included in Arctic YOPP MMDFs (prefaced by "•"). Underlined variables are ECVs, with a dashed underline used for newly proposed sea ice ECVs (Lavergne et al., 2022).

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Variables' *long_name* Attribute	
SUB-SURFACE TERRESTRIAL VARIABLES	
Temperature of soil	Average layer soil moisture
OCEAN SINGLE LEVEL VARIABLES	
Sea surface temperature	Atmosphere-ocean sensible heat flux
Ocean mixed-layer depth	Atmosphere-ocean latent heat flux
Ocean surface x-stress	Net downward shortwave radiation at sea water surface
Ocean surface y-stress	Net downward longwave radiation at sea water surface
Significant wave height[d]	Fresh water flux into sea water
	•Water flux into sea water due to sea ice thermodynamics
OCEAN VARIABLES ON MODEL OR INSTRUMENT LEVELS	
Ocean temperature	Ocean u-velocity
Sea water salinity	Ocean v-velocity
	Ocean w-velocity
SEA ICE VARIABLES, REPORTED ON ATMOSPHERIC GRID	
Sea ice concentration (area fraction)	Rainfall rate over sea ice
•Sea ice concentration (area fraction) in categories	Sea ice surface temperature
	(at the interface of sea ice or the snow on it
	and the overlying air)
Sea ice thickness	Temperature at snow-ice interface
•Sea ice thickness in thickness categories	Temperature at ice-ocean interface
Snow thickness on sea ice	Sea ice/snow albedo
Sea ice age	Ocean-ice net sensible heat flux
Sea ice u-velocity	Net upward sensible heat flux over sea ice
Sea ice v-velocity	Net upward latent heat flux over sea ice
Sea ice salinity	Downwelling shortwave flux over sea ice
•Sea ice normal stress (pressure)	Upwelling shortwave flux over sea ice
•Compressive sea ice strength	Downwelling longwave flux over sea ice
Fast ice concentration (area fraction)	Upwelling longwave flux over sea ice
Fast ice thickness	Net conductive heat flux in ice at the surface

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[d] ECV listing is for just wave height.

Author Contributions

TU conceptualized the original MODF vision; CJC and MM participated in conceptualization by providing valuable perspectives on the practicality, utility and application of the MODF concept. BC, GS and JD provided methodology requirements from a numerical modeling perspective. LMH and SJK, in developing the H-K Schema, provided methodology requirements from an observational perspective and also enhanced data curation. JT and OG guided development of the H-K Schema and MODF formats by providing methodology requirements from a data repository standpoint.

Software contributions were provided by JH and JT, who wrote python code functions to facilitate MODF creation, checking and modification. Data curation, investigation, and software contributions were provided by EA, SM, NH, LXH, RC, ZM, EO, RP, JH and MM, who served as MODF Makers and through that practical application of the MODF concept developed the workflow indicated in Figure 3. They also iteratively worked with LMH and SJK to further develop the H-K Schema. JT contributed to data curation, software, and validation by serving as the MODF Curator and by iteratively working with LMH and SJK to further develop the H-K Schema. GP and NH enhanced data curation by developing strategies to have MODFs include comprehensive formal attribution for individuals and institutions.

TU drafted the original manuscript, and TU, LMH, and SJK revised the draft, with commentary and revisions from BC, GS, JD, SM, EO, RP, ZM, JT, MM, and CJC. Visualizations, in the form of figures and tables, were drafted by TU and revised by TU and LMH.

Competing interests

The authors declare that they have no conflict of interest.

Code and data availability

The H-K Variable Schema Table developed for the YOPPsiteMIP is archived on Zenodo (https://zenodo.org/records/6463464) under the Creative Commons Attribution 4.0 International License (https://creativecommons.org/licenses/by/4.0/).

The A-M Variable & Attribute Template Table developed for the YOPPsiteMIP is archived on Zenodo (https://zenodo.org/records/6780400) under the Creative Commons Attribution 4.0 International License.

A preliminary set of MODF and MMDF files developed for the YOPPsiteMIP is available at https://thredds.met.no/thredds/catalog/alertness/YOPP_supersite/catalog.html. The catalog link provides information on licensing and crediting which is not repeated here as the example files are not the subject of this manuscript.

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