Chapter 7

Generic Strategy for Consistency Validation of the Satellite-, In-Situ-, and Reanalysis—Based Climate Data Records (CDRs) Essential Climate Variables (ECVs)

Yijian Zeng, Wim Timmermans, and Zhongbo Su

Abstract The Climate Data Record (CDR) is a time series of measurements of sufficient length, consistency and continuity to determine climate variability and change. The generation of ECVs (Essential Climate Variables)/CDRs needs to put strong emphasis on the generation of fully described, error-characterized and consistent satellite-based ECV products (Zeng et al. in Remote Sensing 11:1–28, 2019). For example, generation of many ECVs, such as in the ESA (European Space Agency) CCI (Climate Change Initiative) projects (Plummer et al. in Remote Sens Environ 203:2–8, 2017), requires ancillary information about the state of the atmosphere, e.g., cloud screening for SST (sea surface temperature) and atmospheric correction for space-borne altimeters. As such, the consistency between the various ECV products (e.g. cloud flagged in one ECV and non-flagged in another one) extends to ensuring consistency in the approaches of CDR generation. The in-situ datasets also need to be continuously characterized in terms of their long-term accuracy, stability and homogeneity. Reanalysis results, as an alternative source of ECV, requires similar endeavors to investigate its consistency (Zeng et al. in Int J Appl Earth Obs Geoinf 42:150–161, 2015).

In this Chapter, the current practices on consistency validation will be analyzed, based on the consistency validation requirements, the validation capacities, and the current practice examples. The essentials of consistency validation will be summarized. Based on the essentials, the generic strategy for consistency validation will be proposed and discussed.

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7.1 Consistency Validation Requirements and Capacities

7.1.1 Consistency Validation Requirements

7.1.1.1 In-situ Products

For in-situ products, the scope of quality control may include [47]: (a) data validation, (b) data cleaning or remedial actions and (c) quality control monitoring. How all these aspects are in consistency shall be checked to ensure the climate quality of in-situ products.

Based on the in-situ network observations, the gridded datasets can be produced with the internationally accepted estimation methods, which include: (a) mathematical estimation methods (e.g. inverse distance weighting, spline functions); (b) estimation based on physical relationships (e.g. regression, discriminant and principal component analysis); (c) spatial estimation methods (e.g. Kriging). The combination of different methods (e.g. the use of a regression model and interpolation of residuals) is a common practice. Often, the production of gridded datasets follows a step-wise approach incorporating different estimation procedures.

The estimation method for producing gridded datasets may contain errors. This is because the spatial interpolation assumed that the climatological patterns between widely spaced stations are known and can be modeled, while in reality many factors (e.g. topography, local peculiarities or the existence of water bodies) influence the climate of a region. It is therefore essential to validate the gridded datasets to estimate such errors. The validation of gridded datasets may include: (a) split validation (testing the methodology using a smaller subset excluded in the estimation procedure); and (b) cross-validation (repeated removals of observations from the sample and analysis of residuals between observed and estimated values) [3, 4].

7.1.1.2 Satellite Products

The major challenge for climate observation is to have a consistent architecture for observations that is independent of a climate variable’s origin and observing method and principles. This requires that each key climate variable shall be measured using independent observations and examined with independent analysis. This highlights the continuing importance of single-source long-term climate datasets for climate variability and trend analysis, the uncertainty of which shall be quantified by (inter) comparing with other independent datasets [50].

The independent analysis is to verify algorithms that are used for generating climate data (e.g. intercomparison between different retrieval algorithms). It is especially crucial for satellite-based observation data where analysis systems may involve different sets of combination between algorithm theoretical basis documents (ATBDs) and instruments. For example, the independent product can be generated with 3 scenarios by: (1) using the same instrument with different sets of ATBDs; (2)

using the same ATBDs on different instruments; or (3) using different ATBDs and different instruments. It is therefore important to verify the accuracy and stability of various outputs for specific variables by thorough inter-comparison, providing insights into errors and help product users to be aware of product differences.

In addition to single-source independent datasets, integrated products are needed as well to ensure reliable conclusions on the detected variability and trends. The integrated data is produced by blending data from different sources [52, 53], or by integrating observations of variables related to one another, e.g., using data from different instruments or using other data or products to warn of potential issues [19]. For example, the estimation of soil moisture from microwave emission can benefit from analyses of precipitation (e.g. either from in-situ or satellite observation). This requires endeavor to check the physical consistency among different physical variables, apart from the inter-comparison among different independent integrated products.

Although the satellite observations play a vital role in monitoring global climate, to contribute fully and effectively to the detection of climate variability and change (thus long-term consistent climate records), the satellite observing system shall be implemented and operated in a manner to ensure that these data are sufficiently homogeneous, stable and accurate for climate purposes. To address these technical and resource challenges, the GCOS (Global Climate Observing System) Climate Monitoring Principles (GCMPs) were proposed to and extended to assist space agencies in addressing the key operational issues: (1) Continuity, consistency and overlap; (2) Orbit stability; (3) Sensor calibration; and (4) Data interpretation, sustained data products and archiving.

To follow the GCMPs and be able to address the consistency requirement, there are a few key issues that need to be reckoned: (1) Gaps in FCDRs (Fundamental Climate Data Record) must be avoided; (2) Different instruments should be well (inter) calibrated; (3) The generation of long-term ECV products shall be sustained including regular reprocessing; and (4) The optimum use of satellite data (e.g. integrated with in-situ data and model results) requires the organization of data service systems that ensure an on-going accessibility to the data in the future.

7.1.1.3 Reanalysis Products

Within the current WMO Global Framework for Climate Services (GFCS), reanalysis contributes to both components of “observation and Monitoring” and “Research, Modelling and Applications”. The reanalysis can be referred to “reanalysis products” or “reanalysis process”.

The reanalysis products (datasets) contain possibly the gridded fields of physical variables from NWP (Numerical Weather Prediction) model (e.g. including land surface and sea-state components), ocean model (e.g. including dynamic sea ice and biogeochemistry components), or atmospheric composition model (e.g. GEMS and MACC). The reanalysis products can be considered as a scientific and numerical blending of model data and observational data.

The reanalysis process refers to the activities in integrating an invariant, modern version of a data assimilation system and numerical weather prediction model, over a long time period, by assimilating a selection of observations. The reanalysis process shall also include evaluation, monitoring and quality control of reanalysis products and of observations [42, 49].

It is well acknowledged that the reanalysis products are consistent with the meteorological parameters, in the sense that they are constrained by the coupled model. On the other hand, in general, there are still significant disconnections between the various Earth system elements in the assimilation, although the models of the various elements can be as far as coupled or fully integrated.

For example, analysis updates from observations (so-called increments) are typically computed separately for each Earth system element's data assimilation, and it is only during the model integration that all states are made physically consistent between one another. This point indicates that such reanalysis results is produced by a weakly coupled data assimilation scheme, because it uses the coupled model only for generating background estimates for each analysis cycle while the analysis itself is uncoupled [11, 34]. This has consequences for the consistency validation of reanalysis production, which entails considering not only validation of the overall system/process but also the validation of the individual ECV datasets. For the consistency validation of ECV datasets, the inter-comparison of reanalysis products or with other independent datasets will be sufficient. As for the validation of reanalysis systems, it requires information for the components listed as below [49, 51]: (1) the observations input; (2) the forcing or boundary datasets input; (3) the model configuration (for the various Earth system elements); (4) the data assimilation system (in the various Earth system elements).

7.1.2 Consistency Validation Capacities

The vision of GCOS is to enable all users having access to the climate observations, data records and information that they require to address climate variability and change. GCOS strives to provide sustainably reliable physical, chemical and biological observations and data records for the total climate system—across the atmospheric, oceanic and terrestrial domains, including hydrological and carbon cycles and the cryosphere [48]. Another very important remit of GCOS is to provide the climate monitoring requirements for the observations, which can then be implemented by contributions coming from different programmes [5, 17]. To achieve this vision, both the in-situ and satellite observing systems are indispensable components for GCOS, to provide observations over the breadth of environments from ocean bottom to the upper atmosphere. The existing in-situ and satellite observing systems represent the validation capacities, which will enable the inter-comparison among independent observations and the independent analysis.

7.1.2.1 In situ-based Capacities

GCOS has coordinated three types of in-situ networks for different purposes [48]:

- To produce stable long-term series and for calibration/validation purpose, the Global Reference observing networks were built/coordinated to provide highly-detailed and accurate observations at a few locations. This includes the most advanced of the Reference networks, the GCOS Reference Upper Air Network (GRUAN). It is to note that GRUAN is not a set of identical stations, but all stations will make a core set of first priority observations. There are guidelines for setting up sites, characterizing instrument error, data quality control, and manual for the data management [37].
- The Global Baseline observing networks were built/coordinated to provide long-term high-quality data records of key global climate variables and enable calibration for the comprehensive and designated networks. It involves a limited number of selected locations that are globally distributed. For example, the GCOS Surface Network (GSN), the GCOS Upper Air Network (GUAN), the WMO Global Atmosphere Watch (GAW) and the Baseline Surface Radiation Network (BSRN) [19, 22].
- The Comprehensive Observing networks were built/coordinated to provide observations at the detailed space and time scales required to fully capture the nature, variability and change of a specific climate variable. It includes regional and national networks, for example, the GCOS-affiliated WMO GAW global Atmospheric CO_2 and CH_4 Monitoring Networks. These networks are operated primarily for non-climate monitoring but also provide important observations for climate purposes [19, 22].

The above mentioned networks are used to produce reference data for different purposes, the detailed procedures/guidelines/manuals are documented to make such selection of networks as transparent as possible [17, 18]. It serves for documenting a traceable validation process.

The difference among these three types of in-situ networks can be demonstrated by using GUAN and GRUAN. The GUAN is designed to provide evenly distributed radiosonde network over the globe, measuring temperature, pressure (geopotential height), wind, and humidity (at least to the troposphere) at least 25 days each month, although the target is the collection of twice daily radiosonde observations at the 0000 and 1200 UTC synoptic hours. The lowered observation requirement can be attributed to [37]: (1) instrumentations used in GUAN varies from country to country; (2) data collection rate is better in some areas than others; (3) lapse/inability in the acquisition of replacement radiosondes at some locations may lead to temporal gaps in the climate record; and (4) lack of sustaining resources to support existing networks, which leads to the change of instrumentation and the change in location, which will affect homogeneity of GUAN stations. It is clear that these shortfalls of GUAN can also cause inconsistency in the climate record. It is therefore needed for upper air observations meeting reference standards, which led to the establishment of GRUAN in 2004 [26].

GURAN network served as reference standards for the larger GUAN network, aiming to quantify and reduce measurement uncertainties and to make measurements in a stable way over multi-decadal time scales to achieve data homogeneity in time and spatially between measurement sites. In addition, GRUAN will provide a traceable reference standard for global satellite-based measurements of atmospheric essential climate variables and will ensure that potential gaps in satellite measurements programs do not invalidate the long-term climate record. However, it is to note that GRUAN network has its own limitations to measure all parameters with minimum systematic error [26].

Thematically, the in-situ network support different domains of ECVs, which includes 5 categories: atmosphere surface, atmosphere upper-air, atmosphere composition, oceans, and terrestrial. It is noticed that except for Terrestrial and Atmosphere-Composition categories, the observing network in the rest of domains contains both routine/baseline networks and reference networks, which indicate the relatively high capacity of the in-situ observing system for doing consistency validation. On the other hand, this indicates the relatively low capacity of the in-situ observing networks of Terrestrial and Atmosphere-Composition domains, to do consistency validation for the domain-relevant ECVs (See Table 7.1), which requires the reference in-situ observations.

7.1.2.2 Space-Based Capacities

There are 54 GCOS Essential Climate Variables (ECVs) [5, 36] required to support the work of the UNFCCC (United Nations Framework Convention on Climate Change) and the IPCC (Intergovernmental Panel on Climate Change). Table 7.2 indicates 29 of the 54 ECVs can be observed from space (noticed that the observing principles for carbon dioxide, methane and other GHGs are similar and considered as one ECV product) [20]. The space-observable ECVs are in **bold**.

To meet the requirements indicated in 1.1.2, space agencies working through the CEOS and the Coordination Group on Meteorological Satellites (CGMS) have established mechanisms to ensure coordination in agencies' operation and exploitation, for the optimum use of satellite data, by establishing Virtual Constellations on Atmospheric Composition, Precipitation, Land Surface Imaging, Ocean Surface Topography, Ocean Colour Radiometry, and Ocean Surface Vector Winds. The similar coordination mechanism was taken to avoid gaps in FCDRs, which due to missing observations or instrument changes can introduce errors in trend analyses.

The potential future gaps in the satellite ECVs have been conducted through WMO and CEOS, which has been regarded necessary to be routinely updated and acted upon [7, 46]. Developed by WMO in support of Earth Observation applications, studies and global coordination, OSCAR (Observing System Capability Analysis and Review Tool) is an online resource tool that provides the status and the planning of global observing systems as well as instrument specifications at platform level (http://www.wmo-sat.info/oscar/).

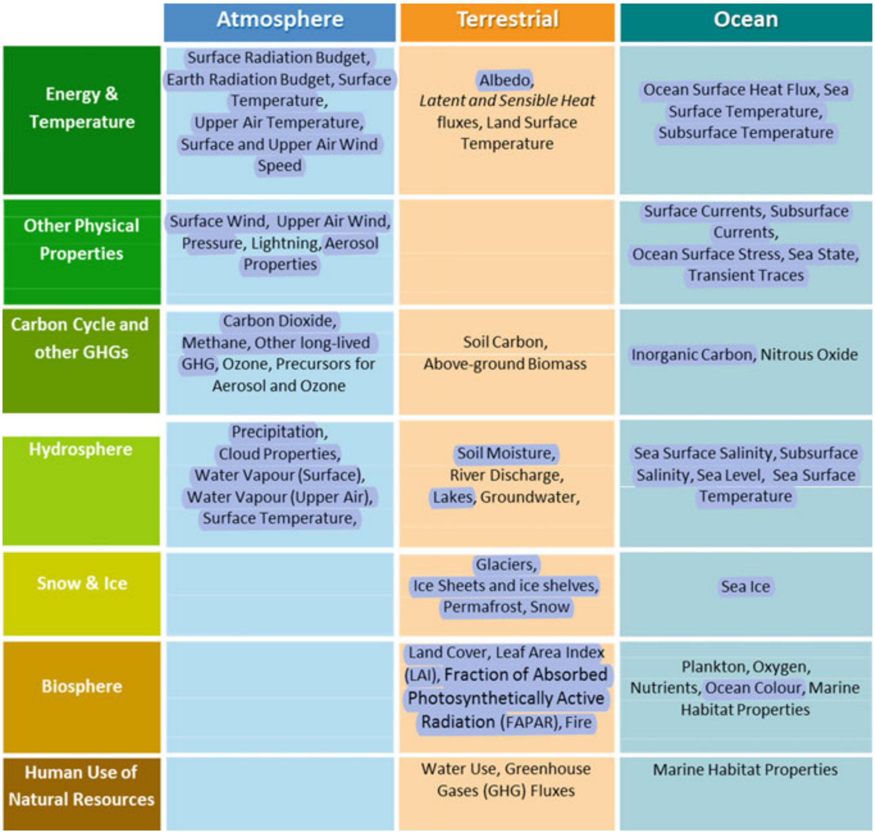
Table 7.1 Overview of all GCOS-relevant network components and systems

Atmosphere			Oceans	Terrestrial
Surface	Upper-air	Composition		
GCOS surface network (GSN)	GCOS reference upper-air network (GRUAN)	GCOS-affiliated WMO/GAW global atmospheric N2O, CO2 and CH4 monitoring networks	Global surface drifting buoy array on 5*5 degree resolution	GCOS/GTOS baseline global terrestrial network rivers (GTN-R)
Baseline surface radiation network (BSRN)	GCOS upper-air network (GUAN)	WMO/GAW GCOS global baseline total ozone network	Global tropical moored buoy network	GCOS/GTOS baseline global lake network
Full WWW & GSN	full WWW & GUAN	WMO/GAW GCOS global baseline profile ozone network	Voluntary observing ships	WWW/GOS synoptic network
Global tropical moored buoy network	Aircraft (ASDAR etc.)	WMO/GAW aerosol network	Global reference mooring network	GCOS/GTOS baseline global terrestrial network-glaciers (GTN-G)
Voluntary observing ships	Profiler (radar) network		GLOSS core sea-level network	GCOS/GTOS baseline global terrestrial network-permafrost (GTN-P)
Global reference mooring network	Ground-based GPS receiver network		Argo network	global terrestrial network hydrology (GTN-H)
GLOSS core sea-level network				
Argo network				

The inter-comparison of sensors and the (inter)calibration of instruments between satellites has received more and more attentions, which leads to the development of the Global Space-based Inter-calibration System (GSICS) jointly between the WMO Space programme, CGMS and the CEOS Working Group on Calibration and Validation (WGCV). GSICS is to ensure the generation of well-calibrated FCDRs. To focus on the sustained generation of long-term ECV products, the SCOPE-CM (The sustained coordinated processing of environmental satellite data for climate monitoring) initiative has been established with contribution from various space agencies.

The above indicates the current efforts to address the requirements for generating ECV CDR from space, and more or less represent the current capacity of satellite

Table 7.2 Overview of ECVs capable of being monitored from space grouped by measurement domain and area covered



	Atmosphere	Terrestrial	Ocean
Energy & Temperature	Surface Radiation Budget, Earth Radiation Budget, Surface Temperature, Upper Air Temperature, Surface and Upper Air Wind Speed	Albedo, *Latent and Sensible Heat* fluxes, Land Surface Temperature	Ocean Surface Heat Flux, Sea Surface Temperature, Subsurface Temperature
Other Physical Properties	Surface Wind, Upper Air Wind, Pressure, Lightning, Aerosol Properties		Surface Currents, Subsurface Currents, Ocean Surface Stress, Sea State, Transient Traces
Carbon Cycle and other GHGs	Carbon Dioxide, Methane, Other long-lived GHG, Ozone, Precursors for Aerosol and Ozone	Soil Carbon, Above-ground Biomass	Inorganic Carbon, Nitrous Oxide
Hydrosphere	Precipitation, Cloud Properties, Water Vapour (Surface), Water Vapour (Upper Air), Surface Temperature,	Soil Moisture, River Discharge, Lakes, Groundwater,	Sea Surface Salinity, Subsurface Salinity, Sea Level, Sea Surface Temperature
Snow & Ice		Glaciers, Ice Sheets and ice shelves, Permafrost, Snow	Sea Ice
Biosphere		Land Cover, Leaf Area Index (LAI), Fraction of Absorbed Photosynthetically Active Radiation (FAPAR), Fire	Plankton, Oxygen, Nutrients, Ocean Colour, Marine Habitat Properties
Human Use of Natural Resources		Water Use, Greenhouse Gases (GHG) Fluxes	Marine Habitat Properties

The highlighted ECVs are (will be) available via the Copernicus Climate Change Services (C3S) Climate Data Store (CDS) (Adopted from Table 7.2, GCOS 2016 Implementation Plan, GCOS-200)

remote sensing in contributing to GCOS ECVs. There are specific gap analysis implemented by JRC [46] and UKEOF [30], to identify how better to coordinate among the existing players to the maximum use of current resources for space-based ECVs, for Europe and UK, respectively.

The generation of many ECVs requires ancillary information about the state of the atmosphere and others. The various ECV products may use different sets of ancillary information (e.g. cloud flagged in one ECV and non-flagged in another one). This will certainly cause inconsistency among different ECV products. On the other hand, for the generation of a certain ECV, it needs different sources of data. For example, for sea surface temperature, there are different sensors observing the temperature of different “surfaces” [19, 29]: the traditional in-situ SST is taking measurement from well underneath the sea surface (e.g. near-surface and mixed-layer “bulk temperatures”); the infrared (IR) radiometer measures the ‘skin’ SST;

and, the passive microwave (MW) radiometer measures the ‘sub-skin’ SST. How to harmonize these three different observations of SST is complicated, due to different measurement depths and diurnal thermal stratification.

The similar inconsistency issue may exist in other ECV products. On the other hand, to be able to identify such inconsistency, the satellite observing system for certain ECV and the corresponding in-situ observing networks shall be maintained and collocated temporally and spatially. Nevertheless, these datasets (both satellite and in-situ) may be affected by the changes in demands on the data, observing practices and technologies. These changes can alter the characteristics of observational records (e.g. change in mean and/or variability). It is, therefore, required to follow a certain procedure to process the raw measurements before they can be used to detect climate variability and climate change. In this sense, for satellite observing systems, the mentioned GSICS and SCOPE-CM can be helpful in establishing an unbroken chain for the satellite measurements to be used/produced in a way to meet internationally recognized measurement standards, which consequently means consistent, homogeneous observational records.

7.1.2.3 Reanalysis-Based Capacities

With a sufficiently realistic global circulation model, by assimilating observational data from multiple sources into a dynamically coherent dataset, reanalysis can produce multi-decadal, gridded datasets that estimate a large variety of atmospheric, sea-state, and land surface parameters, including many that are not directly observed [13, 34, 35]. Reanalysis data can help improve the medium-range forecasts, by using them to assess the performance of operational forecast system and to evaluate the effect of new model developments and other changes [38]. This is actually corresponding to a strong feedback loop between improvements in the global observing system, advances in data assimilation methodology, and development of better forecast models through analysis [11].

The currently well-recognized need for the development of reanalysis is a more explicit representation of atmosphere–ocean interaction, which will improve surface fluxes of heat and momentum, tropical precipitation, and surface wave fields. The current reanalysis estimate of these parameters suffers from bias and drifts, due to the lack of model feedback between ocean and atmosphere and therefore the poor representation of processes that govern the near surface temperature and wind conditions [6, 11].

A similar concern holds for the representation for land surface. For example, in the current configuration of ECMWF, the 4D-Var analysis of upper-air prognostic variables is performed separately from simpler analyses of screen-level parameters (temperature, humidity) and land surface parameters (soil moisture, soil temperature, snow depth). Consequently, there is a lack of dynamic feedback in the analysis between the land surface and the atmospheric boundary layer [11, 40].

For atmospheric composition, the coupled modelling of meteorological, chemical, and aerosol variables and combined use of observations of trace species and meteorology in the 4D-Var analysis is desired. It is because these are the basic elements needed for a fully coupled data assimilation system, in which observations of atmospheric constituents lead to physically consistent adjustments to the meteorological variables, and conversely, meteorological observations can have an immediate impact on estimates of the constituent concentrations [11]. However, due to the not-yet-adequate observations (e.g. the model background is not well constrained by observations), there are large and unrealistic changes in the upper-stratospheric circulation. As a result, the current practice for atmospheric composition reanalysis does not yet allow direct adjustments to the meteorological parameters based on trace-gas observations. Instead, the observations of atmospheric constituents need to be bias-corrected (via variational bias corrections) before being assimilated into the data assimilation system for generating the coupled 4D-Var analysis of meteorological variables.

From the above, on one hand there are limits in the current reanalysis in achieving consistency among different physical parameters across domains. On the other hand, the analysis provides complete description of physically plausible atmosphere, ocean and land parameters consistent with instrumental observations. The reanalysis adds value to the instrumental record [49].

For example, by constraining the model background with the observations, reanalysis produces useful estimates for model variables that are not well observed, such as stratospheric winds, radiative fluxes, root-zone soil moisture, etc. However, due to the absence of direct observations, it is difficult to quantify the uncertainty of those model-generated variables, which depend on errors in the model as well as on the observations. Nevertheless, the reanalysis permits the budget diagnostics [2, 27, 28, 43], which are useful for demonstrating shortcomings and progress in climate reanalysis, and the examination of increments can be highly informative about shortcomings in the assimilating model [11]. It is to note that, depending on the diagnostic, the results can be different due to differences either in the observation data, the assimilation scheme or forecast model, or any combination of these.

Uncertainty characterization and consistency validation are therefore required for reanalysis (e.g. including both products and processes), to understand uncertainty that may come from insufficient observation coverage, insufficient data quality, unknown observation uncertainties or assimilating model deficiencies [21, 49].

There are currently international efforts to tackle this issue through intercomparing reanalysis, for example: the SPARC reanalysis inter-comparison project was proposed in 2012 [15], and the Reanalysis.org portal was established to provide researchers with help to obtain, read and analyze reanalysis datasets created by different organizations. The CORE-CLIMAX project has also proposed a procedure for comparing reanalysis [41], and comparing reanalysis to assimilated observations and CDRs, through inter-comparing reanalysis results. Furthermore, there are recently emerging many reanalysis inter-comparison tools [16], for example: web-based reanalysis inter-comparison tools (https://reanalyses.org/atmosphere/writ), KNMI Climate Explorer (http://climexp.knmi.nl/start.cgi? someone@somewhere), MERRA Atlas (http://gmao.gsfc.nasa.gov/ref/merra/atlas/), and the Climate Reanalyzer (http://cci-reanalyzer.org/).

7.2 Case Study: Consistency Among Hydrological Cycle Variables

Based on observation data (e.g. both in-situ and satellite), we can quantify the water cycle components in river basins and compare these to the results obtained by using reanalysis data. TWS (terrestrial water storage) are obtained by balancing precipitation, evaporation and river runoff from satellite observations and in-situ observations. The same is also obtained from Interim Reanalysis data (ERA-Interim). Upon comparing these TWS data to the GRACE (Gravity Recovery and Climate Experiment) observations of storage changes, we conclude that a method can be devised to separate the impacts on the water cycle components by climatic and human factors. Demonstration cases are presented for the Yangtze river basin (Fig. 7.1).

We start with the mass conservation equation for water, which takes the form of:

$$\frac{\partial S}{\partial t} = P_{GPCP} - E_{SEBS} - R_{Obs} \cdot f\left(P_{i,j}, E_{i,j}\right) \tag{7.1}$$

where S is the amount of water stored at surface and subsurface per unit of land surface; P_{GPCP} uses the GPCP (Global Precipitation Climatology Project) data is used; E_{SEBS} uses the SEBS (Surface Energy Balance System) [39] derived land evapotranspiration; R_{Obs} is the in-situ observed river discharge; $f\left(P_{i,j}, E_{i,j}\right) = \left(P_{i,j} - E_{i,j}\right)/(P - E)$ is a scaling factor to distribute the observed discharge to each pixel, $P_{i,j}$, $E_{i,j}$ are GPCP precipitation and SEBS ET for pixel (i, j) and P, E are the mean GPCP precipitation and SEBS ET for the catchment area of interest, all expressed in cm of water depth.

The TWS anomaly and cumulative TWS anomaly are estimated from GPCP precipitation, SEBS estimated evapotranspiration [8, 9], observed discharge as well

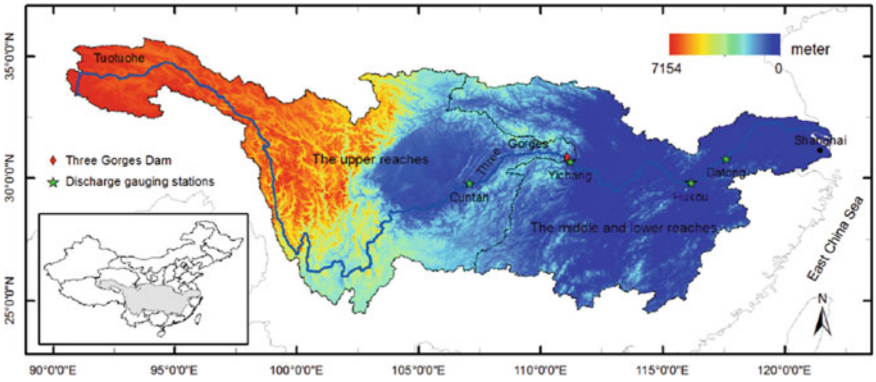


Fig. 7.1 Yangtze river basin (Upper Yangtze reach, from Tuotuohe, to Yichang; Middle reach from Yichang to Hankou; Lower reach from Hankou to the river mouth near Shanghai; Cuntan, Yichang, Hankou, and Datong are four gauging stations located along the mainstream of the Yangtze)

as from ERA-interim data, which are compared with GRACE TWS for the Upper Yangtze reach and the whole Yangtze river basin. The river discharge measurements from Yichang station for the period 2001–2010 are used for the Upper reach study. The discharge measurements from Datong for the period of 2005–2010 are used for the whole Yangtze River basin study. The GPCP precipitation data (precipitation in cm/month) was obtained at http://jisao.washington.edu/data/gpcp/; GRACE data was obtained at: http://grace.jpl.nasa.gov/ (data version: RL05.DSTvSCS1401). The GRACE monthly grid data represents the equivalent water height deviation from its average value over Jan 2004 to Dec 2009).

From the results shown in Figs. 7.2 and 7.3, it can be seen that the TWS derived from the observation data and from ERA reanalysis data are consistent with each other, indicating that both datasets capture the surface dynamics of the water cycle fluxes. However, the TWS derived from GRACE has somewhat larger amplitudes than those from observation data and reanalysis data, indicating deep groundwater contributions. From Fig. 7.3, it may be concluded that after the filling of the Three Gorges Dam reservoir (Yichang station, upper panel in Fig. 7.3) started in 2004, the storage of the upper reach increased in the following years in 2005–2007 period, but

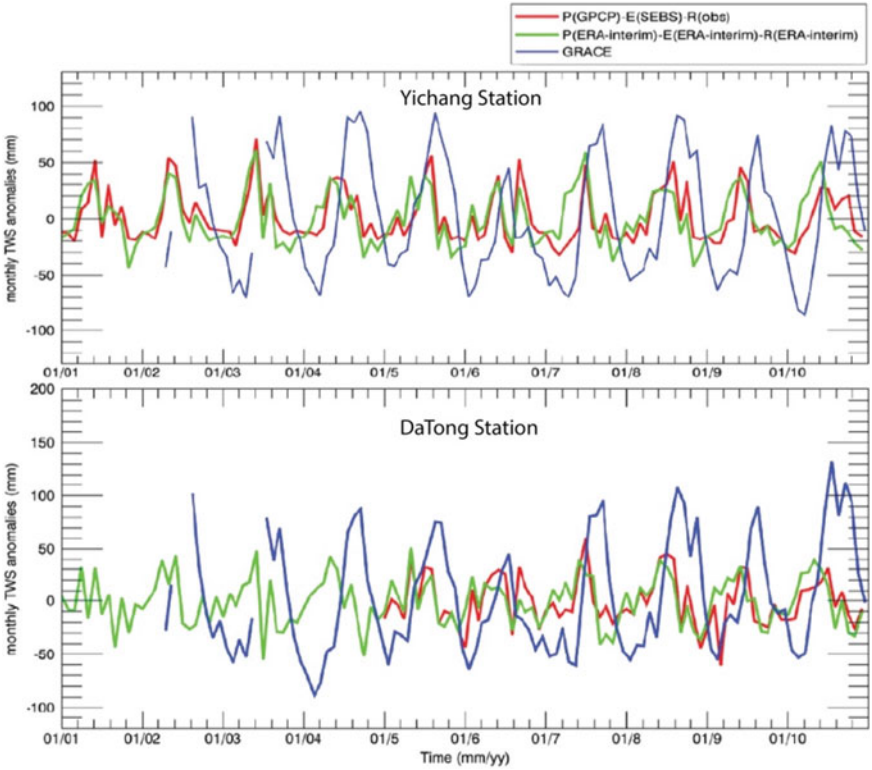


Fig. 7.2 Terrestrial water storage anomaly over (Top) Yichang Station and (bottom) Datong Station

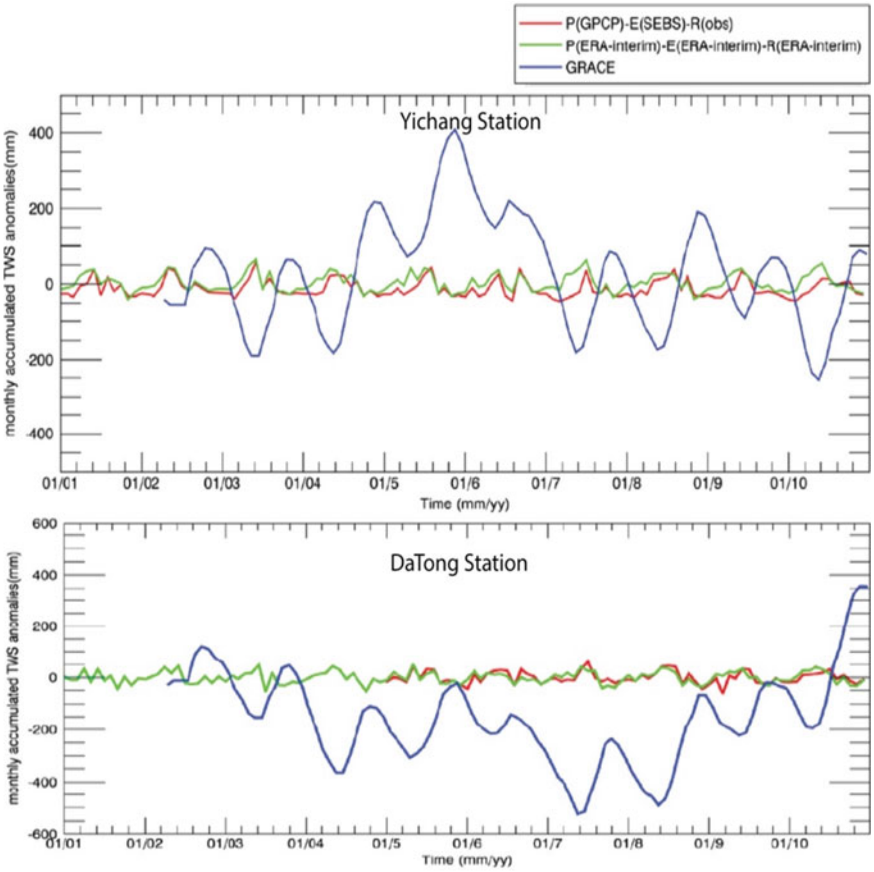


Fig. 7.3 Cumulative terrestrial water storage anomaly over *(Top) Yichang Station and (bottom) Datong Station*

returned to the average gradually afterwards. This indicates the dominant climatic control of the Yangtze River system in the upper reach. For the lower reach, it can be seen that the there was a reduced storage from 2004–2008 but it gradually returned to its pre-Three Gorges stage afterwards.

It is noted that the monthly TWS anomaly and cumulative anomaly over Yichang Station (i.e. the upper reach), calculated using an earlier version of GRACE data (RL04 ssv201008), are completely different from the results shown in Figs. 7.2and 7.3. For the TWS anomaly, the earlier version of GRACE data has a phase difference of about 10 days, when compared to the current version (results not shown). For the cumulative TWS anomaly, the earlier version does not show the increase of monthly accumulative TWS anomaly after 2004 (results not shown), which was expected due to the filling of the Three Gorges Dam reservoir (upper panel in Fig. 7.3).

The reason for the difference between the two versions of GRACE data can be very complex. Many parameter choices and solution strategies are possible for the complex inversion of relative ranging observations between the two formation-flying GRACE spacecraft, the precise orbit determination via GPS and various corrections for spacecraft accelerations not related to gravity changes. One of the most important parameters for the post-processing of GRACE observations is the land grid scaling coefficients, the use of which enables the representation of surface mass variations at small spatial scales. Without the scaling coefficients, the mass variations at small spatial scales tend to be attenuated. On the other hand, the scaling coefficients are computed by applying the same filters (e.g. de-striping, Gaussian, and degree 60 filters) applied to the GRACE data to a land-hydrology model (i.e. NCAR's CLM4), through which the gain factor is derived by minimizing the difference between the model's smoothed and unfiltered monthly water storage variations at any geographic location. With its origin, the gain factors tend to be dominated by the annual cycles of water storage variations. Meanwhile, the inter-annual trends in particular in hydrology models are very uncertain, it is therefore suggested that it may not be suitable to quantify trends. Nevertheless, within the accepted error ranges, GRACE data is still useful for detecting trends [44, 45].

From the above, it is obvious that the exact explanation for the different results over the upper Yangtze reach, calculated from the two data versions, needs intensive dedicated research. Nevertheless, it is also possible to have a quick check on the meta-information about each change made for the production of GRACE data [41]. Such meta-information can help explain if the difference between Figs. 7.2 and 7.3 could be attributed to what has been changed during the production of new version dataset. It was found that in the new version of GRACE data, July-2004, October-2004, March-2005 and February-2006 were replaced/updated, which corresponds to the dates in which the differences between the two versions of GRACE data were identified (see Figs. 7.2 and 7.3).

7.3 Essentials of Current Practices and Strategy for Future Work

7.3.1 Essentials of Consistency Validation for Current Practice Examples

According to the above, the climate monitoring needs to ensure consistency and quality of the products, the realization of which requires thorough inter-comparison on two aspects:

a. Thorough (inter)comparison among multiple independent datasets/products for a specific climate variable;

b. Thorough (inter)comparison among different climate variables, which are physically interlinked.

The first type of inter-comparison can be implemented at point or grid scales to check the product differences of a specific climate variable and the reasons for such differences, while the second type of inter-comparison will check the physical consistency from the functional point of view of different climate variables. In addition, the cross-cutting validation using data assimilating system is an alternative way to check physical consistency of ECVs across domains:

c. Cross-cutting consistency validation among different climate variables across domains, using data assimilating system.

The above three types of validation activities can be regarded as ***the quality consistency check*** on climate data products.

At the same time, it is important to recognize that different methodologies and verification approaches used for inter-comparison may lead to the same conclusion, but with different reasons behind. Other than this, the generation processes (/production chain) of different datasets and products differing from each other can complicate the analysis of the (inter)comparison results, if all the necessary information are not provided.

To facilitate the assessment on this kind (e.g. production chain), the CORE-CLIMAX project [41] proposed a System Maturity Matrix (SMM), which is adapted from Bates and Privette [1, 14]. The SMM is a tool to assess the system maturity of a CDR. SMM basically assesses whether CDR generation procedures have been compliant with best practices developed and accumulated by the scientific and engineering communities. This can be regarded as ***the process consistency check***.

It is to note that the Climate Change Initiative (CCI) of the European Space Agency (ESA) has defined three consistency levels of satellite CDRs for Earth system monitoring [36]: "(1) consistency in format and metadata to facilitate their synergetic use (technical level), (2) consistency in assumptions and auxiliary datasets to minimize incompatibilities among datasets (retrieval level); and (3) consistency between combined or multiple CDRs within their estimated uncertainties or physical constraints (scientific level)." As such, the 'process consistency check' can be mapped to the ESA-CCI's 'technical level', while the 'quality consistency check' mapped to both the 'retrieval level' and 'scientific level'.

According to ESA-CCI [36], the assessment methods for consistency on the 'retrieval level' include: visual (combined images, or homogeneity), contingency matrix, class combination maps, difference maps, and statistical comparison, the 'scientific level' includes: visual (features as expected), quantitative variability, trend analysis, difference maps, trend comparisons, and correlations & other measures of co-variability. These assessment methods are applicable to either one single ECV product (self-consistency) or those ECVs consisting of several quantities (multi-product, and mutual consistency) (e.g., the glacier ECV in ESA-CCI consists of the three products: glacier outlines, elevation change, and velocity).

Based on the definition of 'single/multi-product', [49] described an overarching structure for the assessment of quality and usability (AQUE) of ECV products, considering ‘single product assessment’, ‘multi-product intercomparison’, ‘thematic assessment’, and ‘usability assessment’. The AQUE aims to support a traceable climate service, where the uncertainty from the upstream of climate service (i.e., technical and scientific quality of ECV products) propagates into the resulting benefit (utility) for the end users.

7.3.2 Generic Strategy of Consistency Validation

For the quality consistency check, one of the first step is to understand the validation requirements (see Sect. 7.1.1). It shall be realized that for different users (therefore about different applications) the requirements will be different.

For example, there are two kinds of reanalysis (e.g. NWP-like reanalysis or reanalysis for climate change assessment), having different requirements in terms of data usage. A traditional NWP-like reanalysis (e.g. for the past 30yrs) tends to assimilate all available observations unless they are known to be unusable for certain reasons. The climate reanalysis, going further back in time (e.g. for the past 100 yrs), on the other hand, only assimilates those observations that are known to be suitable for climate applications. It implies that a climate reanalysis requires extra efforts in validating the input data than the NWP-like reanalysis.

With that in mind, it is important to implement a ***user (validation) requirement review*** as the first step, which includes (but is not limited to):

- definition of user requirements on products (e.g. coverage, vertical resolution, spatial and temporal resolution, data length etc.);
- consistency validation requirements (e.g. only inter-comparison required or the ECV consistency across domains required);
- service specification (e.g. near-real-time monitoring/forecast at European/Global Scale, value added products, satellite retrievals etc.);
- requirements for measures and metrics (e.g. root mean square error, relative frequency histograms, Pearson’s correlation coefficient etc.);
- requirements for independent reference observation data (e.g. is it traceable to in-situ measurements?);
- requirements for equivalent products (e.g. is the heuristic reference needed?).

Based on the requirement review, the dedicated ***validation plan*** can be made and may include (not limited to):

- definition of terminology (e.g. consistency, accuracy, stability etc.);
- description of data under evaluation (data processing and archiving center, model/data processor version, instrument, calibration version, log-file, input and initialization data, measured parameter, native data format, file name convention);
- reference data selection (e.g. the same as the above item, plus the information error budget of data comparison, characterization of sensitivity and information content);

- range of comparison;
- co-location criteria, conversion of units, temporal/spatial re-sampling and smoothing;
- performance and validation statistics (e.g. error budget analysis);
- description of the validation protocol;
- description of the validation process (e.g. both internal and external) [50].

It is noted that, for the description of data under evaluation and the selection of reference data, the known and relevant uncertainties shall be detailed. This will facilitate proper interpretation of the validation results and traceability of the validation process.

After implementing the validation plan, all results of validation measures shall be integrated and published as a ***validation report***. This third step needs to coordinate and harmonize all validation activities/results, available quality information, and the service endorsement information. It implies that the validation results from geophysical product and algorithm validation, through validation against service specifications and requirements, to the service endorsement by core/key users (e.g. external review) shall all be collected. Endorsement by core/key users facilitates the feedback loops of the validation process, which is the most important element of the whole validation processes. This external review element provides feedbacks from the end-users to the developers, producers and providers, i.e. the new information for improving the quality of current products.

Arguably, the three steps identified above: (1) User (Validation) Requirement Review; (2) Validation Plan; and (3) Validation Report, are general in a way to validate products corresponding to user requirements, and cannot be referred to consistency validation. On the other hand, it is needed to understand how the consistency is defined before implementing consistency validation, which can be reflected/specified in the user (validation) requirement review. And then, in the validation plan, especially for the description of the data under evaluation and the reference data selection the detailed information shall be investigated, which will help to identify the causes when inconsistency being identified. The case study shows that the cause of inconsistency can be identified from the log-files of the data production. In addition, in the validation plan, the practical aspects of consistency validation can be identified, for example: co-location criteria, conversion of units, temporal/spatial re-sampling and smoothing.

7.4 Discussion and Conclusions

The Climate Data Store (CDS) of the Copernicus Climate Change Services (C3S) envisions that it shall include essential climate variables (ECVs), uncertainty estimates, reanalysis, multi-model data (e.g. seasonal forecasts and up-to-date climate projections), and in-situ and satellite data. Furthermore, CDS should contain only 'climate compliant' data, as defined by Evaluation and Quality Control working group of C3S. This implicates that one may find certain ECV variable from different sources, and there is a need to do consistency check to determine which dataset are fit for certain particular purpose. On the other side, when there is a certain ECV variable under evaluation, one would like to collect as many as possible independent datasets, under the constraints that they are measuring the same thing, to do (inter)comparison, in order to understand comprehensively the associated uncertainty.

For the in-situ datasets, the homogeneity adjustment plays a critical role in producing long-term climate data. There are direct and indirect methodologies to do homogeneity detection and adjustment [32]. However, it is still difficult to avoid all the inhomogeneities caused by, for example, changes in instrumentation, station moves, changes in the local environment (e.g. building construction), or the introduction of different observing practices like a new formula for calculating mean daily temperature or different observation times. The existence of independent datasets and data assimilation technique provide unprecedented opportunities to spot "bugs" in the in-situ datasets [23]. The use of satellite data can also help monitoring in-situ observations, for example, by using AATSR SST data, the error characteristics of the 'bad' buoy for measuring SST can be identified [10].

For the satellite, reanalysis, and multi-model datasets, the same principle of consistency validation as discussed above (e.g. collect as many as possible available independent datasets) is applicable. On the other hand, this principle needs to be constrained with the reference data selection procedure as mentioned in Sect. 7.3. It is to note that based on the discussion in Sect. 7.3 the collection of all kinds of validation information is to identify the missing validation information and processes (e.g. validation gaps), which are necessary to set priorities for future validation reports. And, consistency validation is a key for identifying such gaps.

Through consistency validation, it is also helpful to identify gaps for the current capacities of existing networks (see Sect. 7.1.2). For example, taking water cycle closure as an example, we can thematically identify what needs to be measured. When the needed variable was compared to a dataset, one may find out that in the dataset only land fluxes were observed while soil moisture and soil temperature, or water vapor, or relative humidity were not. From this sense, one may identify the gap, the filling of which requires measurements of other relevant physical variables. This can be useful to help bring different observation networks together, which may be established from different initiatives/projects/programs. In this way, one can suggest a way to gain added-value to current existing observation entities.

In the hydrological cycle closure example implemented over Yangtze River Basin, it is assumed that the total water storage change at a scale of river basin equals to the input minus output. In this sense, the basic water balance equation (i.e. total water storage change = Precipitation—Evaporation—Runoff) can be used to identify what observations are still lacking. However, for the current case, only runoff data can be collected from in-situ observations. The precipitation data was from GPCP, the evaporation was calculated by using SEBS model. Apart from the difficulty of defining runoff data at grid scale, a harmonized approach is needed to bring different sources of data together to do consistency check. The harmonized approach can include two parts: (a) how to adjust different physical metrics to a common benchmark that enables them to be used to do consistency check; (2) the definition of a physically thematic framework to do consistency check (e.g. in this case, the water balance equation).

Nevertheless, from the Yangtze river case, the TWS anomaly signal calculated from different sources of data (e.g. GPCP precipitation, SEBS evaporation and In-situ runoff) are consistent with that calculated from reanalysis data. It seems that GPCP, SEBS evaporation, and in-situ runoff data are consistent with each other, since they are compared with model results (ERA-Interim), which can be regarded being a physically consistent system that is physically constrained by the coupled model. On the other hand, the analysis schemes for the different components are separate and use different methodologies. For example, for the atmosphere-land domains, the screen-level parameter analysis is the first to be completed and is used as input for the soil moisture and snow analysis. The analyzed surface variables generate feedback for the upper-air analysis for the next assimilation window, through their influence on the first-guess forecast that propagates information from one cycle to the next. In this sense, this can be identified as weakly coupled system. The similar weakly coupled system exists for the atmosphere–ocean domains though.

The weakly coupled data assimilation scheme is widely used in reanalysis centers. One advantage of this weakly coupled approach is that, for example, the ocean initialization, obtained by running an ocean model with surface boundary conditions from an atmospheric (re)analysis, can benefit from the wealth of atmospheric observations and sophisticated atmospheric data assimilation methods. And, such uncoupled approach also permits modularity and easy implementation. The disadvantage is that the surface properties of both atmosphere (e.g. wind conditions and near surface temperature) and oceans (e.g. sea surface temperature) cannot be consistently assimilated within the separate assimilation systems.

The efforts in developing coupled data assimilation for atmosphere and ocean have been intensively undertaking at ECMWF, e.g. with ERA-CLIM2 project, which aimed to develop a first coupled ocean–atmosphere reanalysis of the twentieth century, together with consistent estimates of carbon fluxes and stocks [6, 11]. The new data assimilation scheme has been designed in a way to allow dynamic two-way exchange of information between ocean and atmosphere within a single analysis cycle, which can accommodate observations that are sensitive to both oceanic and atmospheric variables [6, 11]. This 'strongly coupled data assimilation' technique allows feedbacks between the ocean and atmosphere models [24, 25], which facilitate the direct correction of the ocean modeling by the atmosphere observations, and vice versa.

Nevertheless, it is recognized that both the observational record and the model have inherent uncertainties that are not always quantifiable [31]. Therefore, it is important to expose all available information pertaining to these uncertainties, and make them accessible to the scientific community. It is also important to enable users to assess the observational information content of specific reanalyzed parameters as a function of space and time, depending on whether those parameters have been directly observed or indirectly constrained by observations of other parameters. All these information will allow end-users to draw meaningful inferences about the uncertainties in their own estimates, meeting the requirements for their specific applications [6, 12].

So far, there are many programmes/initiatives dedicated to the quality assurance of satellite-based ECV CDRs [49]. However, a consistent, international coordination mechanism for in-situ observations and reanalysis for climate services is not yet existing, which should be further pursued, taking the momentum generated by the Copernicus Climate Change Services. It is well recognized that understanding climate change is fully relied on the observation capacity (i.e., global satellite and conventional observational data in the atmosphere, the land, and the ocean), the development of fully coupled Earth system models, as well as data assimilation systems that can ingest these observation data. It highlights a continuous cycle of research and development in all these key activities: from in-situ data collection/rescue, satellite observation reprocessing, Earth system model advancement, to data assimilation methods for reanalysis (including its production and evaluation). Such a research cycle can, therefore, provide a continuously improving interpretation of the evolution of the Earth system.

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