System Maturity and Application Performance for Climate Data Records

Jörg Schulz

Thanks to many people that contributed over the years.

Best Practices

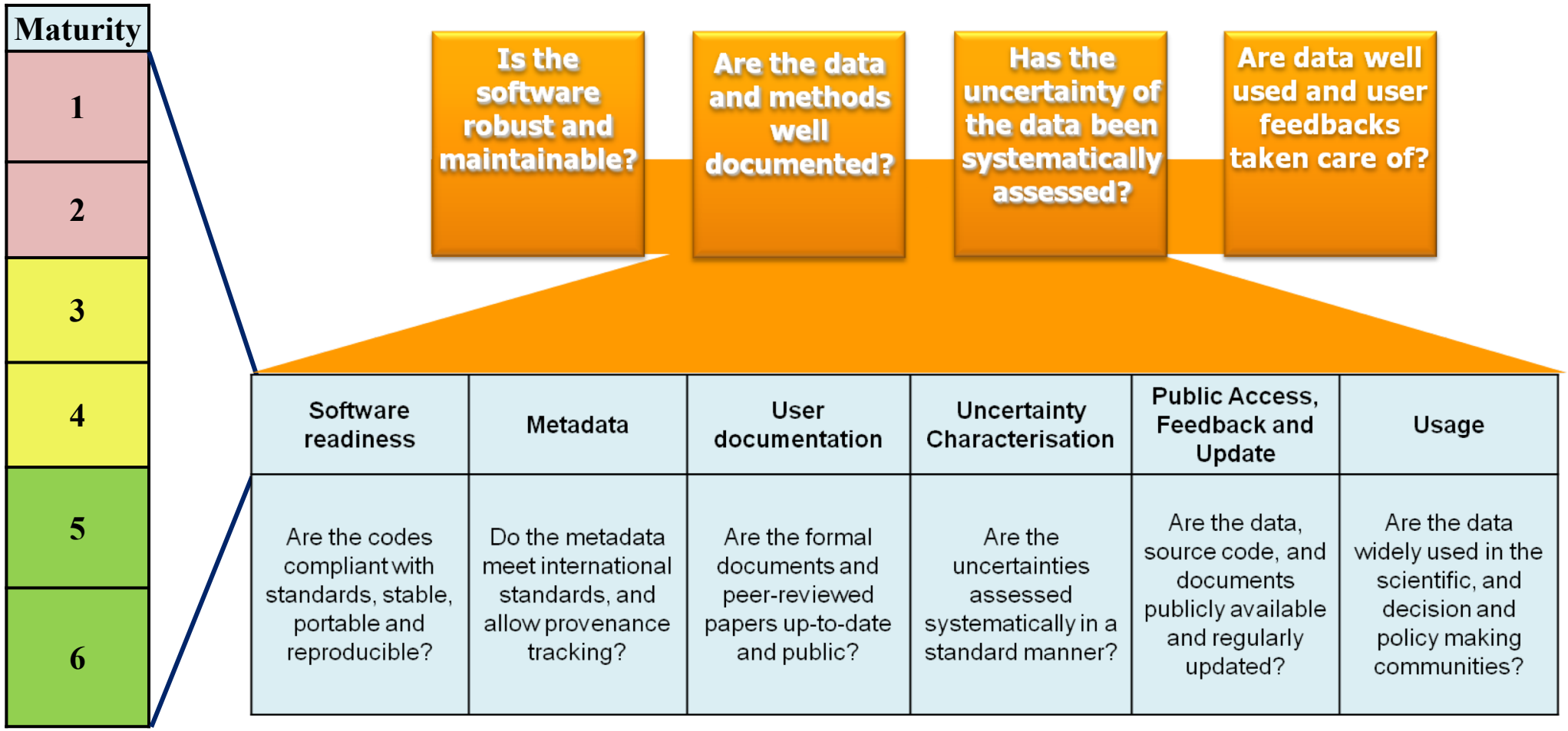
- Climate Data Record developments in the last 20-30 years have led to common elements emerging as best practices;
- How do we capture and make available these best practices and ensure their application?
- Increasingly complex observing systems and resulting data records require more process control to ensure quality, access, and preservation;
- Software Engineering is also increasingly complex and process management is required to optimise cost, schedule, productivity and quality;
- Users deserve very good documentation, openness and transparency;
- It is imperative that Climate Services respond with quantifiable metrics that inform about both the scientific quality and process maturity of CDRs.

Original CORE-CLIMAX Approach for Assessment

The capacity is assessed using three support tools developed by the project:

- **Data Record Descriptions (DRD)**
  - Contain technical specifications and links to documented information on quality;
  - Provides consistent and coherent information about CDRs produced in Europe (served as input to CMIP-6 obs4mips activities).
- **System Maturity Matrix (SMM)**
  - Evaluates if the production of a CDR follows best practices for science and engineering and is assessing if data records are used and feedback mechanisms with users are implemented;
  - The SMM can be used in self assessment mode or in an audit type assessment.
- **Application Performance Metric (APM)**
  - Evaluates the performance of a CDR with respect to a specific application;
  - Might be implemented as an interactive App that convolves user requirements with product specification information in a database.

Maturity Matrix Concept



Software readiness	Metadata	User documentation	Uncertainty Characterisation	Public Access, Feedback and Update	Usage
Are the codes compliant with standards, stable, portable and reproducible?	Do the metadata meet international standards, and allow provenance tracking?	Are the formal documents and peer-reviewed papers up-to-date and public?	Are the uncertainties assessed systematically in a standard manner?	Are the data, source code, and documents publicly available and regularly updated?	Are the data widely used in the scientific, and decision and policy making communities?

Example – DHR_FAPAR, v1.0 from QA System

Origin	JRC, http://www.qa4ecv.eu/ecvs/
Spatial Characteristics	Global
Temporal Characteristics	01 Jan 1982 - 31 Dec 2006; Daily, 10 days, monthly

Software Readiness	Metadata	User Documentation	Uncertainty Characterisation	Public access, feedback, and update	Usage
Coding Standards	Standards	Formal description of scientific methodology	Standards	Public Access/Archive	Research
Software Documentation	Collection level	Formal validation report	Validation	Version	Decision support system
Numerical Reproducibility and portability	File level	Formal product user guide	Uncertainty quantification	User feedback mechanism	
Security		Formal description of operations concept	Automated quality monitoring	Updates to record	
Legend					
1	2	3	4	5	6

Example – DHR_FAPAR, v1.0 “audit” type assessment

Origin	JRC, http://www.qa4ecv.eu/ecvs/
Spatial Characteristics	Global
Temporal Characteristics	01 Jan 1982 - 31 Dec 2006; Daily, 10 days, monthly

Software Readiness	Metadata	User Documentation	Uncertainty Characterisation	Public access, feedback, and update	Usage
Coding Standards	Standards	Formal description of scientific methodology	Standards	Public Access/Archive	Research
Software Documentation	Collection level	Formal validation report	Validation	Version	Decision support system
Numerical Reproducibility and portability	File level	Formal product user guide	Uncertainty quantification	User feedback mechanism	
Security		Formal description of operations concept	Automated quality monitoring	Updates to record	
Legend					
1	2	3	4	5	6

Fitness for Purpose?
Motivation for Application Performance Metric (APM)

- System Maturity Matrix provides assessment of whether the data set can be sustainable in terms of engineering, scientific and usage aspects;
- There is no guarantee that a data set with high System Maturity is suitable for specific applications!
- How do we assess the performance of a data set for a particular application?
- Can we develop a tool that supports the user directly by informing about available data and how good they fit to user requirements?

Support User's to Select Data

- User requirements collection exercises show a large variability in the stated requirements of users with nominally similar applications;
- But a core set of typical questions may always be isolated:

Coverage	Sampling	Uncertainty	Stability
Are the record length and spatial coverage meeting the application's requirements?	Do the spatial and temporal sampling meet the applications requirements?	Do the random and systematic uncertainties meet the requirements?	Do the temporal and spatial stability meet the requirements?

Policy maker asks “Are there trends in North Sea Temperature over last 15 years that could affect fisheries? “

Requirements

ECV Temperature	Coverage	Temporal Resolution	Horizontal Resolution	Vertical Resolution	Length of Record	Accuracy of trend / 15 yrs	Stability (K/decade)
Target	North Sea	Monthly	100 km	Any	15 yrs (2000-2014)	1.0 deg	.67
B/T	North Sea	Weekly	10 km	100 m	30 yrs (1985-2014)	.5 deg	.33
Optimal	North Sea	Daily	1 km	50 m	45 yrs (1970-2014)	.3 deg	.2

Technical Specifications

CDR Name	ECV	Coverage	Temporal Resolution	Horizontal Resolution	Vertical Resolution	Length of Record	Stability (K/decade)
HadISST1	SST (Top few meters)	Global	Monthly	80 km at 60N	Any	1870-last month	.1[1]
CCI Analysis	SST (at 20 cm)	Global	Daily	5 km at 60 N	Any	1991 - 2010	.03[2]

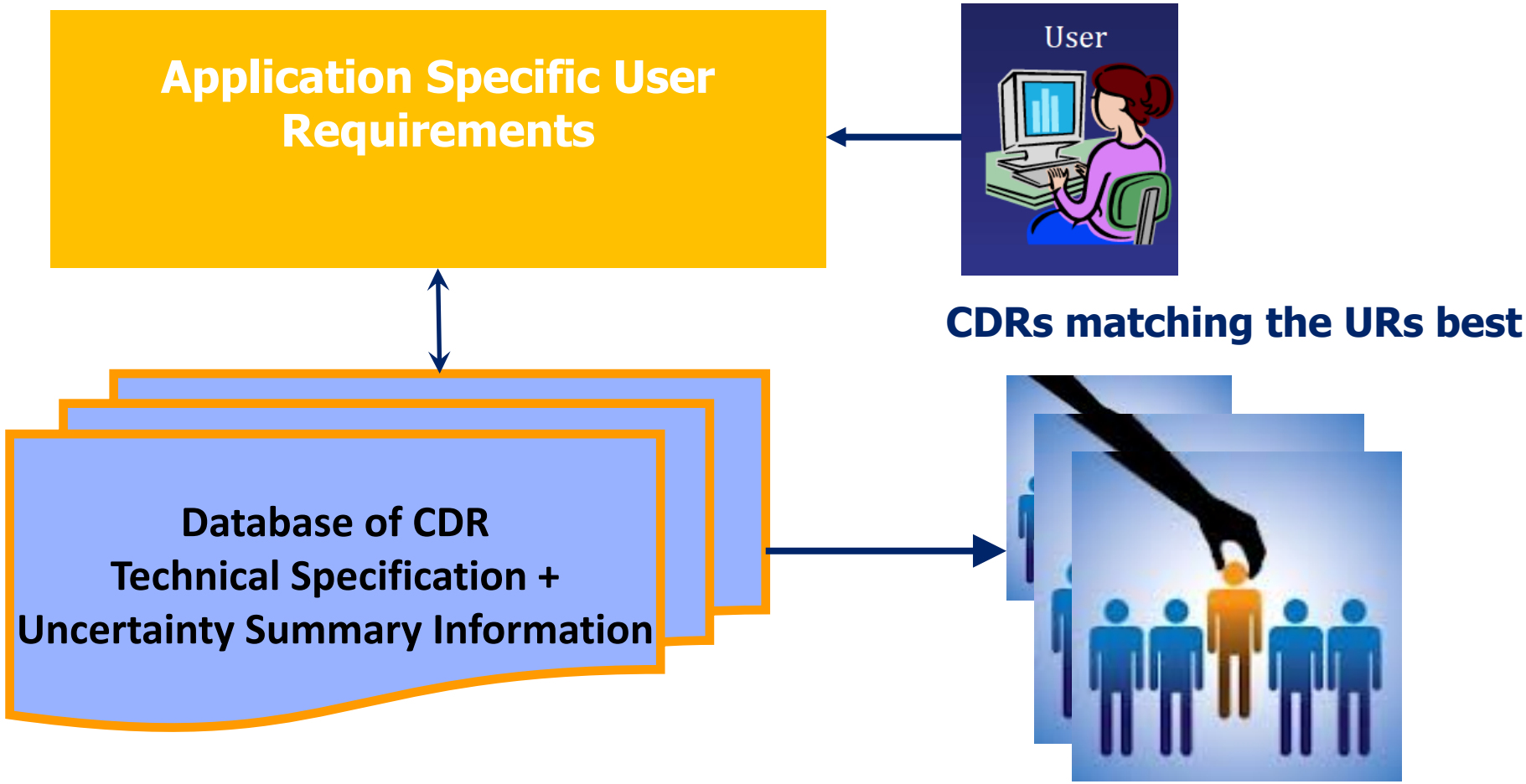
CDR Name	Coverage	Temporal Resolution	Horizontal Resolution	Vertical Resolution	Length of Record	Stability (K/decade)
HadISST1	3	1	1	1	3	3*
CCI Analysis	3	3	2	1	0/1	3*

* = treat with caution

Users “able to elucidate their requirements to a reasonable extent”, this table is actually the useful output

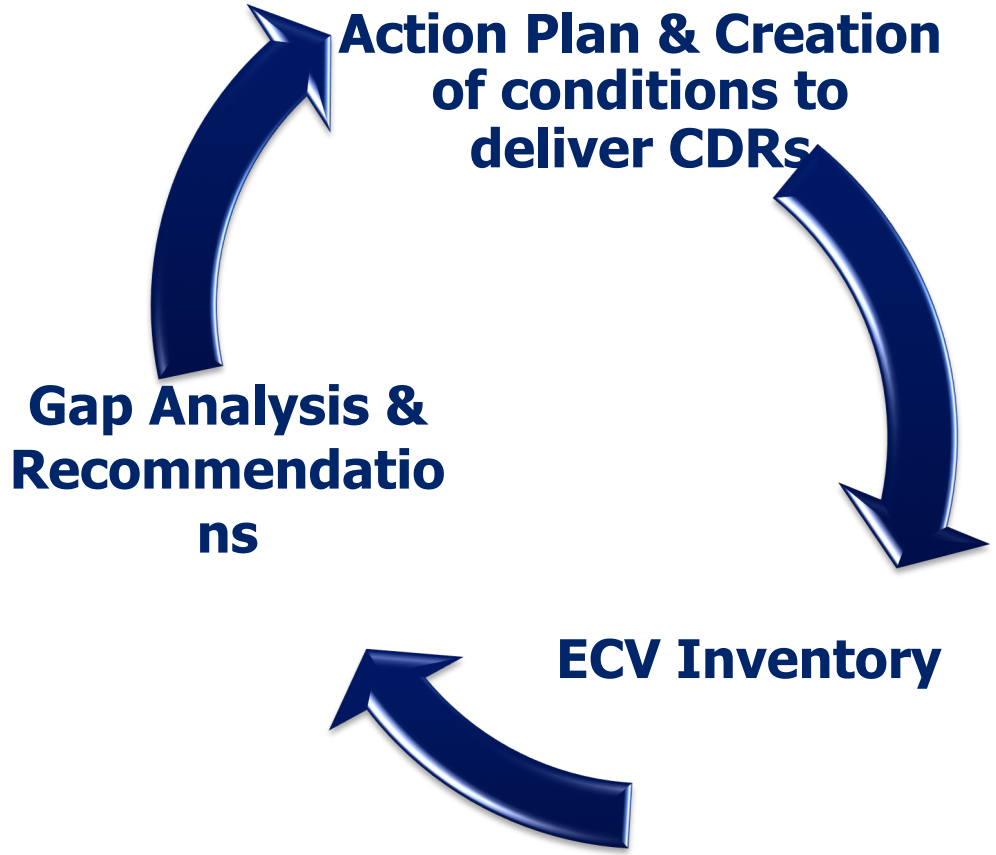
- Suggestions of datasets they can look into further
- Points them towards the trade-offs they need to think about in choosing between them

General Concept of APM



ECV Inventory - Resource for Coordinated Response to GCOS

http://climatemonitoring.info/ecvinventory



Satellite/Instrument combination		Envisat	AATSR	2002-03-01	2012-04-08	L1b
Inter-calibration Satellite/Instrument combination Comments (Optional)		Link to AATSR calibration via chains of satellite-satellite matches.				
Ground-based network calibration	Ground-based network	Calibration is not referenced to in situ networks to achieve independence				
	Link to source					
Geographical Coverage	Extent (Lat/Long)	Global				
	Domain	Ocean				
	Domain Comment (Optional)	Ice-free ocean only. Caspian Sea included.				
Horizontal resolution		0.05 degree				
Target reqs.	GCOS 154					
	GCOS 200					
Vertical resolution		0.2 cm depth SST				
Target reqs.	GCOS 154					
	GCOS 200					
Temporal resolution		Daily, spatially completed using gap filling.				
Target reqs.	GCOS 154					
	GCOS 200					
Accuracy		Standard uncertainty: estimated to be around 0.26 K.				
Target reqs.	GCOS 154					
	GCOS 200					
Stability		Only assessable for tropical regions because of lack of SI calibrated in situ data over period. 95% confidence interval (K year-1) for 1991 - 1995 -0.001 < instability < 0.022 95% confidence interval (K year-1) for 1995 - 2010 0.000 < instability < 0.003 See: http://www.esa-sst-cci.or ... sue_1-signed-accepted.pdf				
Target reqs.	GCOS 154					
	GCOS 200					

CDR Name	Coverage	Temporal Resolution	Horizontal Resolution	Vertical Resolution	Length of Record	Stability (K/decade)
HadISST1	3	1	1	1	3	3*
CCI Analysis	3	3	2	1	0/1	3*

Conclusion

- Evaluation and Quality Control needs to consider both scientific and process quality. The latter documents the application of best practices for the data record generation
- System Maturity estimates most likely differ if provided via self assessment and via “audit” type assessment. Agreement needs to be found between producer and assessor
- System Maturity estimates always need interpretation, they must not be used for a beauty contest by adding up or averaging scores or doing ranking
- Application Performance Metric approach supporting data selections by users looks promising but still needs field test
- Process maturity indicators and a tool to provide application performance metric can be added to the CEOS/CGMS WG Climate ECV Inventory (http://climatemonitoring.info/ecvinventory)

SPARES SLIDES

Sub Matrix – Software Readiness

SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARATERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE

	Coding standards	Software Documentation	Numerical Reproducibility and Portability	Security
1	No coding standard or guidance identified or defined	No documentation	Not evaluated	Not evaluated
2	Coding standard or guidance is identified or defined, but not applied	Minimal documentation	PI affirms reproducibility under identical conditions	PI affirms no security problems
3	Score 2 + standards are partially applied and some compliance results are available	Header and process description (comments) in the code, README complete	PI affirms reproducibility and portability	Submitted for data provider's security review
4	Score 3 + compliance is systematically checked in all code, but not yet compliant to the standards.	Score 3 + a draft Software Installation/User Manual	3rd party affirms reproducibility and portability	Passes data provider's security review
5	Score 4 + standards are systematically applied in all code and compliance is systematically checked in all code. Code is not fully compliant to the standards. Improvement actions to achieve full compliance are defined.	Score 4 + enhanced process descriptions throughout the code; software installation/user manual complete	Score 4 + 3rd party can install the code operationally	Continues to pass the data provider's review
6	Score 5 + code is fully compliant with standards.	As in score 5	Score 5 + Turnkey system	As in score 5

Sub Matrix – Meta Data

SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARATERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE

	Standards	Collection level	File level
1	No standard considered	None	None
2	No standard considered	Limited	Limited
3	Metadata standards identified and/or defined but not systematically applied	Sufficient to use and understand the data independent of external assistance; Sufficient for data provider to extract discovery metadata from meta data repositories	Sufficient to use and understand the data independent of external assistance
4	Score 3 + standards systematically applied at file level and collection level by data provider. Meets international standards for the dataset	Score 3 + Enhanced discovery metadata	Score 3 + Limited location (pixel, station, grid-point, etc.) level metadata
5	Score 4 + meta data standard compliance systematically checked by the data provider	Score 4 + Complete discovery metadata meets international standards	Score 4 + Complete location (pixel, station, grid-point, etc.) level metadata
6	Score 5	Score 5 + Regularly updated	Score 5

Sub Matrix – User Documentation

SOFTWARE READINESS	METADATA	**USER DOCUMENTATION**	UNCERTAINTY CHARATERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE

	Formal description of scientific methodology	Formal Validation Report	Formal Product User Guide	Formal description of operations concept
1	Limited scientific description of methodology available from PI	None	None	None
2	Comprehensive scientific description available from PI and Journal paper on methodology submitted	Report on limited validation available from PI	Limited product user guide available from PI	None
3	Score 2 + Journal paper on methodology published	Report on comprehensive validation available from PI; Paper on product validation submitted	Comprehensive User Guide available from PI	Limited description of operations concept available
4	Score 3 + Comprehensive scientific description available from Data Provider	Report on inter-comparison to other CDRs, etc. Available from PI and data Provider; Journal paper on product validation published	Score 3 + available from data provider	Comprehensive description of operations concept available
5	Score 4 + Comprehensive scientific description maintained by data provider	Score 4 + Report on data assessment results exists	Score 4 + regularly updated by data provider with product updates and/or new validation results	Operations concept and description of practical implementation available
6	Score 5 + Journal papers on product updates published	Score 5+ Journal papers more comprehensive validation, e.g., error covariance, validation of qualitative uncertainty estimates published	Score 5	Score 5 + Operations concept regularly updated

Sub-Matrix – Uncertainty Characterisation

SOFTWARE READINESS | METADATA | USER DOCUMENTATION | **UNCERTAINTY CHARATERISATION** | PUBLIC ACCESS, FEEDBACK, UPDATE | USAGE

	Standards	Validation	Uncertainty quantification	Automated Quality Monitoring
1	None	None	None	None
2	Standard uncertainty nomenclature is identified or defined	Validation using external reference data done for limited locations and times	Limited information on uncertainty arising from systematic and random effects in the measurement	None
3	Score 2 + Standard uncertainty nomenclature is applied	Validation using external reference data done for global and temporal representative locations and times	Comprehensive information on uncertainty arising from systematic and random effects in the measurement	Methods for automated quality monitoring defined
4	Score 3 + Procedures to establish SI traceability are defined	Score 3 + (Inter)comparison against corresponding CDRs (other methods, models, etc)	Score 3 + quantitative estimates of uncertainty provided within the product characterising more or less uncertain data points	Score 3 + automated monitoring partially implemented
5	Score 4 + SI traceability partly established	Score 4 + data provider participated in one inter-national data assessment	Score 4 + temporal and spatial error covariance quantified	Score 3 + monitoring fully implemented (all production levels)
6	Score 5 + SI traceability established	Score 4 + data provider participated in multiple inter-national data assessment and incorporating feedbacks into the product development cycle	Score 5 + comprehensive validation of the quantitative uncertainty estimates and error covariance	Score 5 + automated monitoring in place with results fed back to other accessible information, e.g. meta data or documentation

Sub Matrix – Public Access, Feedback and Update

SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARATERISATION	**PUBLIC ACCESS, FEEDBACK, UPDATE**	USAGE

	Public Access/Archive	Version	User Feedback Mechanism	Updates to Record
1	Data may be available through request to PI	None	None	None
2	Data available through PI	Preliminary versioning by PI	PI collects and evaluates feedback from scientific community	Irregularly by PI following scientific exchange and progress
3	Data and documentation archived and available to the public from PI	Versioning by PI	PI and Data provider collect and evaluate feedback and from scientific community	Irregularly by PI following scientific exchange and progress
4	Data and documentation archived and available to the public from Data Provider	Version control institutionalised	Data provider establishes feedback mechanism such as regular workshops, advisory groups, user help desk, etc. and utilises feedback jointly with PI	Regularly by PI utilising input from established feedback mechanism
5	Score 4 + source code archived by Data Provider	Fully established version control considering all aspects	Established feedback mechanism and international data quality assessment results are considered in periodic data record updates	Regularly operationally by data provider as dictated by availability of new input data or new methodology following user feedback
6	Score 5 + source code available to the public from Data Provider	Not used	Score 5 + Established feedback mechanism and international data quality assessment results are considered in continuous data provisions (Interim Climate Data Records)	Score 5 + capability for fast improvements in continuous data provisions established (Interim Climate Data Records)

Sub Matrix - Usage

SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARATERISATION	PUBLIC ACCESS, FEEDBACK, UPDATE	USAGE

	Research	Decision Support System
1	None	None
2	Benefits for research applications identified	Potential benefits identified
3	Benefits for research applications demonstrated by publication	Use occurring and benefits emerging
4	Score 3 + Citations on product usage occurring	Score 3 + societal and economical benefits discussed
5	Score 4 + product becomes reference for certain applications	Score 4 + societal and economical benefits demonstrated
6	Score 5 + Product and its applications becomes references in multiple research field	Score 5 + influence on decision (including policy) making demonstrated