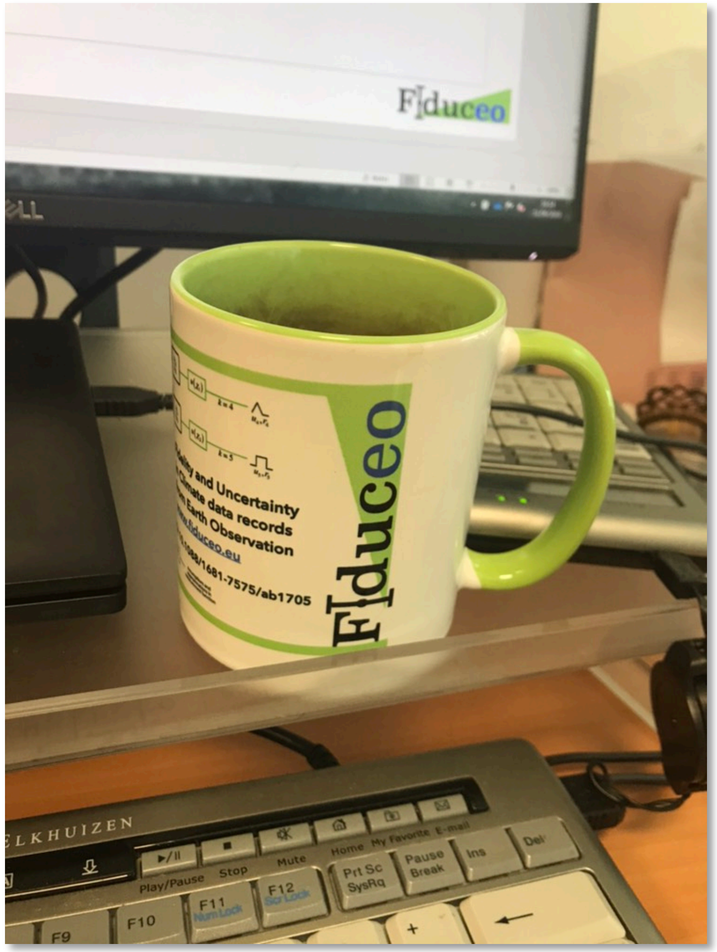
FIDUCEO has received funding from the European Union's Horizon 2020 Programme for Research and Innovation, under Grant Agreement no. 638822

Work Package 2: Metrological Methods
Final Review Meeting

Emma Woolliams[1], Jon Mittaz[1,2], Sam Hunt[1], Ralf Quast[3], Ralf Giering[3], Chris Merchant[2] and FIDUCEO partners

[1]National Physical Laboratory,
[2]University of Reading
[3]FastOpt GmbH

The Monster/Mug Paper



REVIEW • OPEN ACCESS

Applying principles of metrology to historical Earth observations from satellites

Jonathan Mittaz[1,2], Christopher J Merchant[1] and Emma R Woolliams[2]

Published 21 May 2019 • © 2019 BIPM & IOP Publishing Ltd

Metrologia, Volume 56, Number 3

Article PDF

But mostly it's about a dialogue between EO and Metrology

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Pre-FIDUCEO: Metrological Methods

CEOS QA4EO Principle (2010)

"It is critical data and derived products are easily accessible in an open manner and have associated with them an indicator of their quality traceable to reference standards (preferably SI) to enable users to assess its suitability for their application i.e. its fitness for purpose."

General Principles from the CCI Project

1. Include quantitative uncertainty information within the dataset. (Don't expect users to find uncertainty information by reading related papers.)
2. Follow metrological practice for quantifying uncertainty. The baseline good practice is to provide the total standard uncertainty for numerical variables.
3. Uncertainty estimates (or the means to calculate them) should be provided per datum in CDRs for which uncertainty varies significantly so that the uncertainty information discriminates which data are more and less certain.
4. Assuming per-datum uncertainty information is provided, avoid redundancy of this information with quality flags. Do not flag high-uncertainty data as "bad" if a valid estimate of that high uncertainty is provided; instead, use quality flags to indicate the level of confidence in the validity of the provided uncertainty and retrieval assumptions.
5. Define what uncertainty information is given in the CDR in the product documentation.
6. Describe in the product documentation the main effects causing errors, how uncertainty varies within the dataset, how errors may be correlated in time and space, and under what circumstances estimated uncertainty may be invalid (and flagged as such).
7. Use validation to evaluate both retrieved quantities and associated uncertainty estimates.
8. Propagate uncertainty appropriately (accounting for error correlation) and consistently when creating aggregated products.

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C. J. Merchant *et al.*, "Uncertainty information in climate data records from Earth observation," *Earth Syst. Sci. Data*, vol. 95194, pp. 511–527, 2017.

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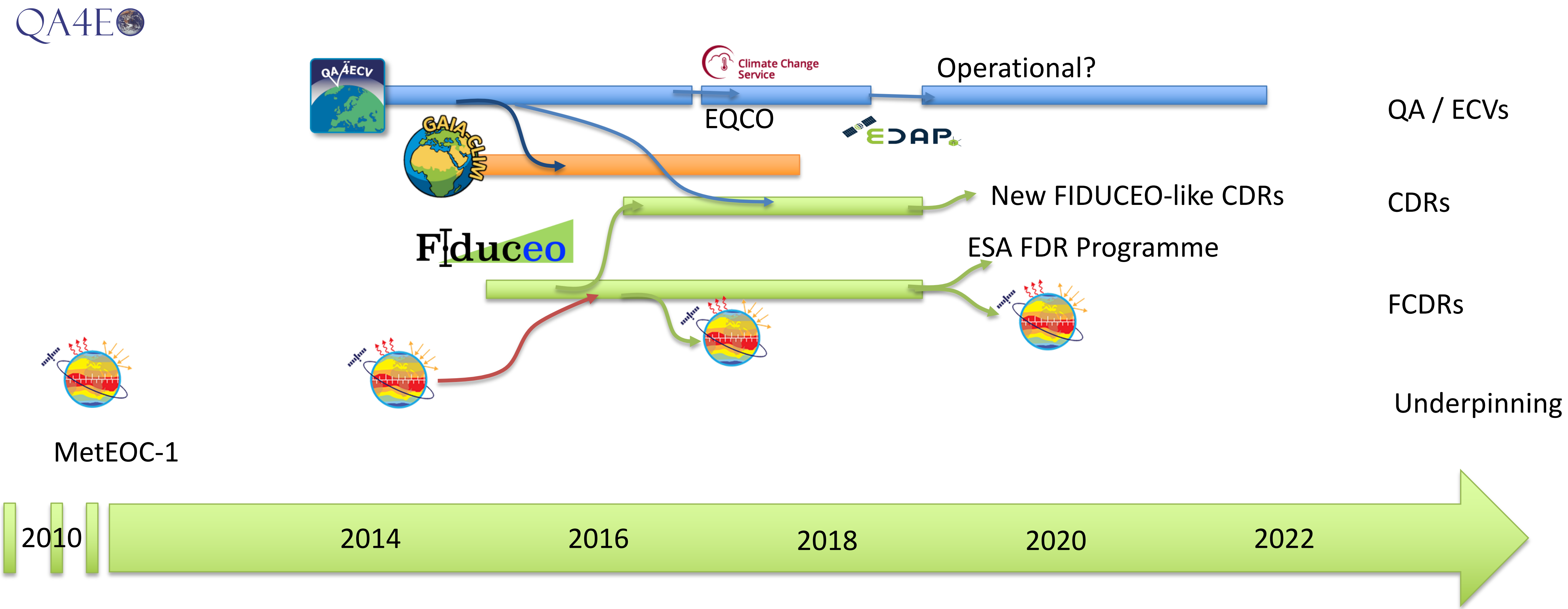
Timeline



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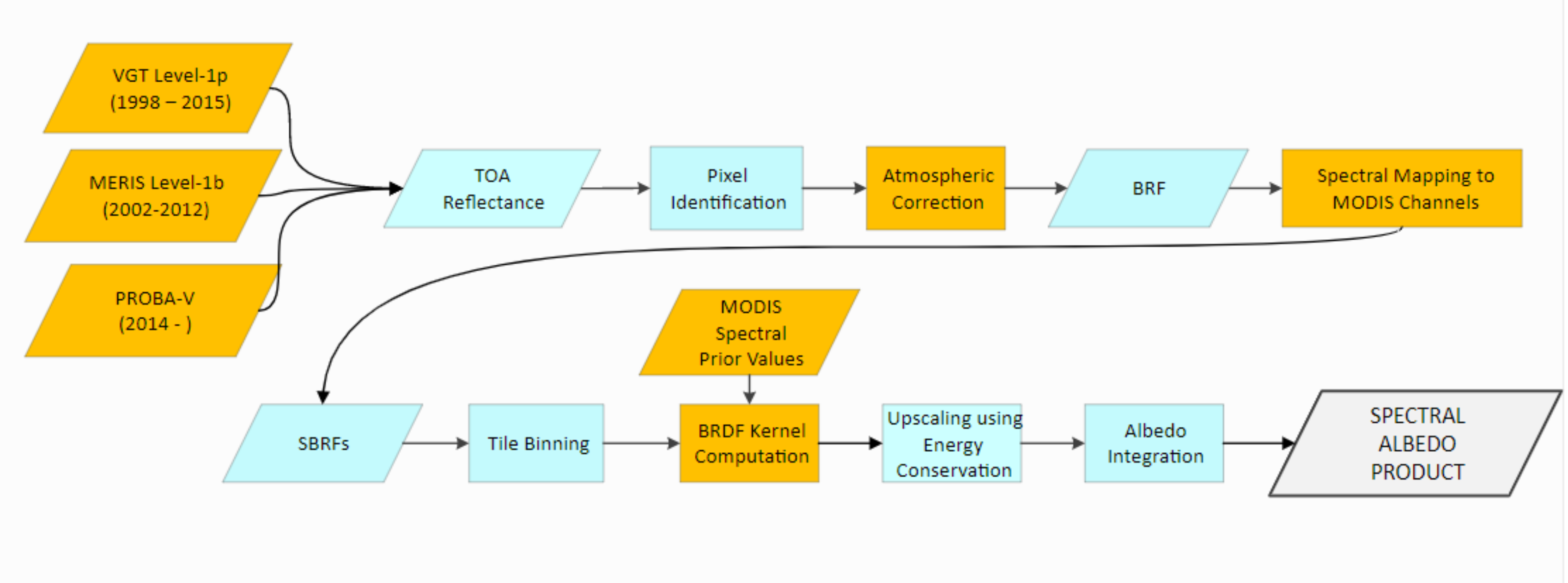
Fiduceo

DOCUMENTING FCDRS AND CDRS

Pre- Fiduceo : Metrological Methods

Traceability chains in QA4ECV (2014-2017)

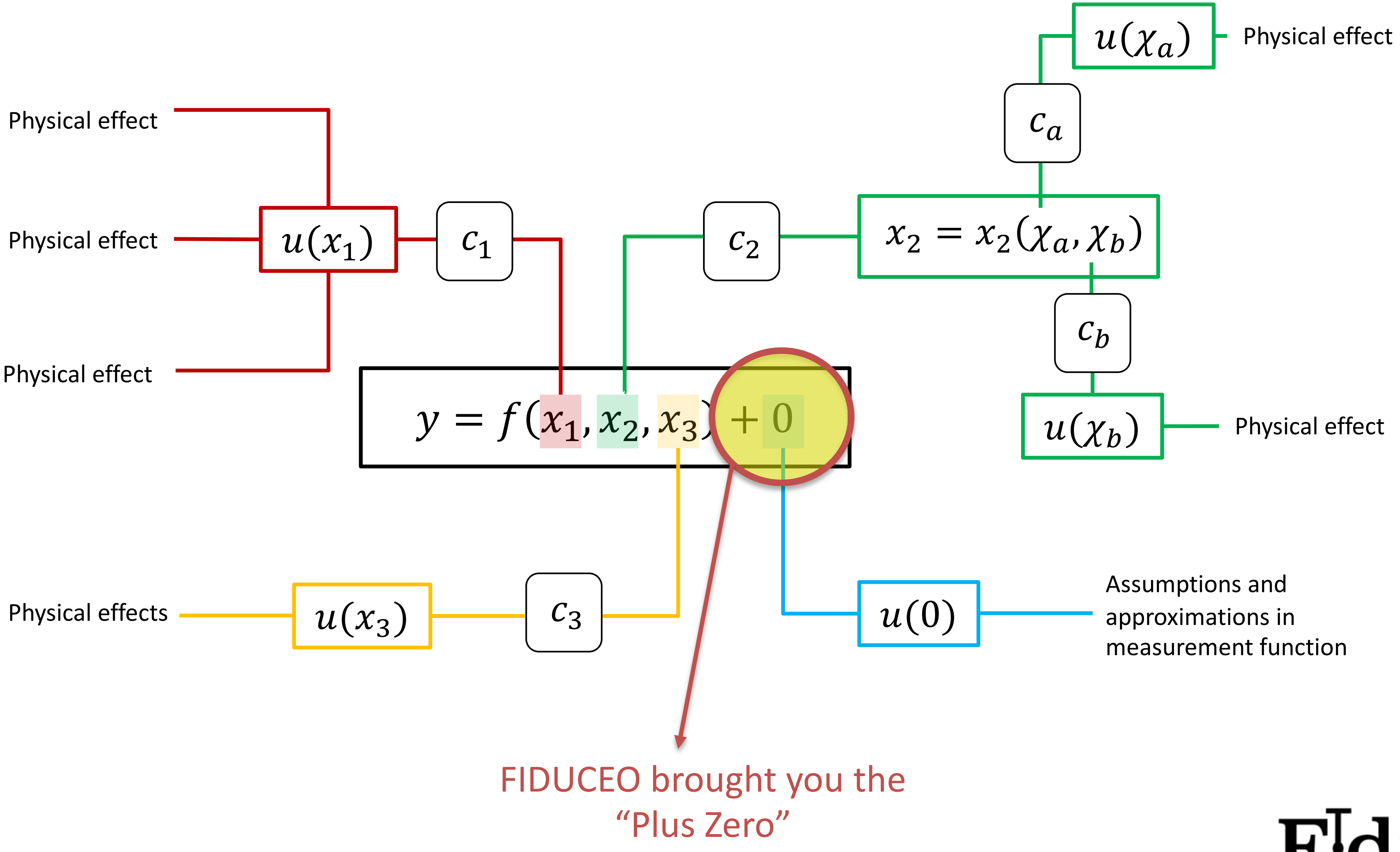


Original Concept for FIDUCEO

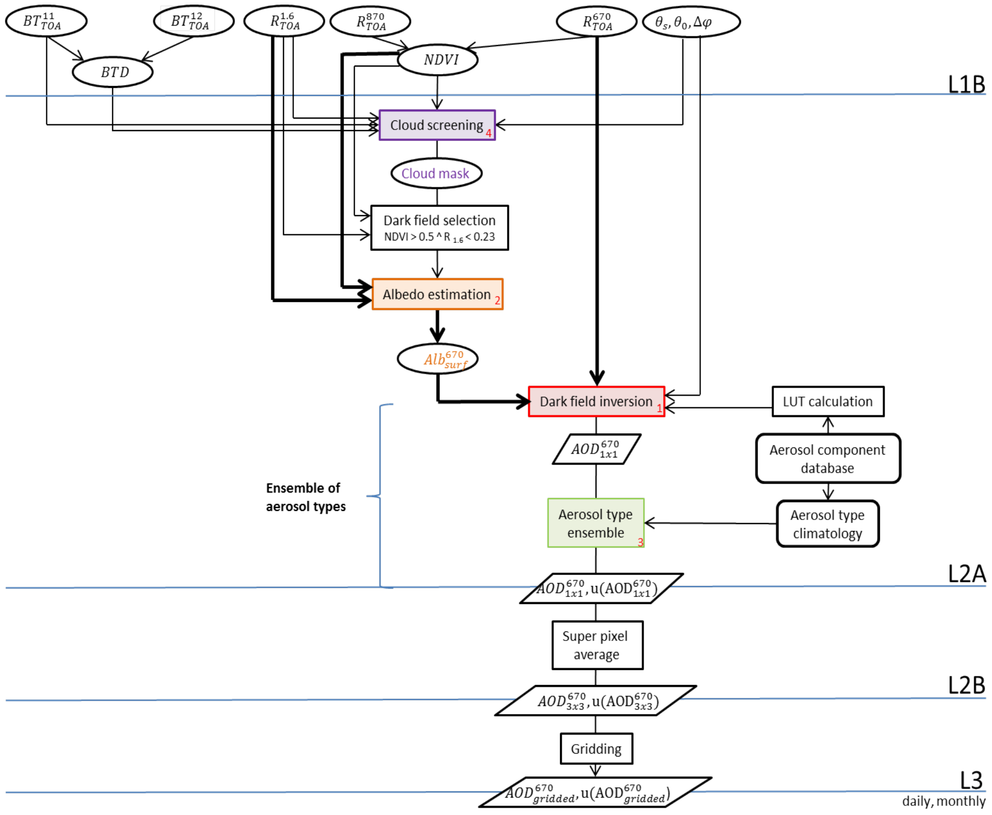
FIDUCEO Philosophy

- As simple as possible and no simpler
- All the information needed for full, open traceability
- Systematic presentation that works in documents and can be stored in NetCDF files

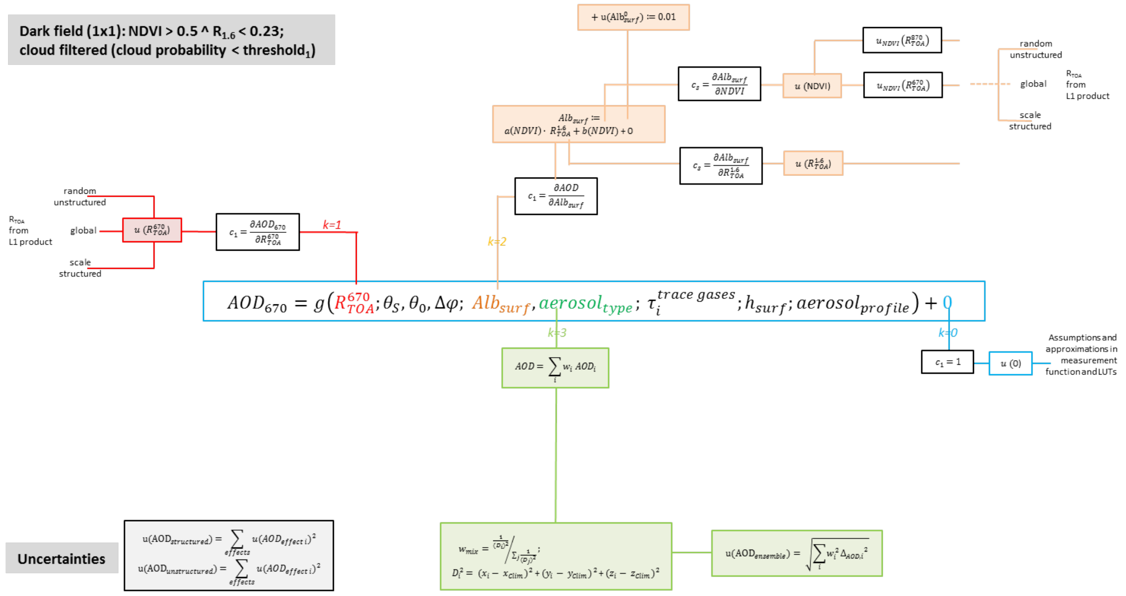
FIDUCEO Methodologies – Uncertainty Tree Diagram



CDR traceability chains and tree diagrams

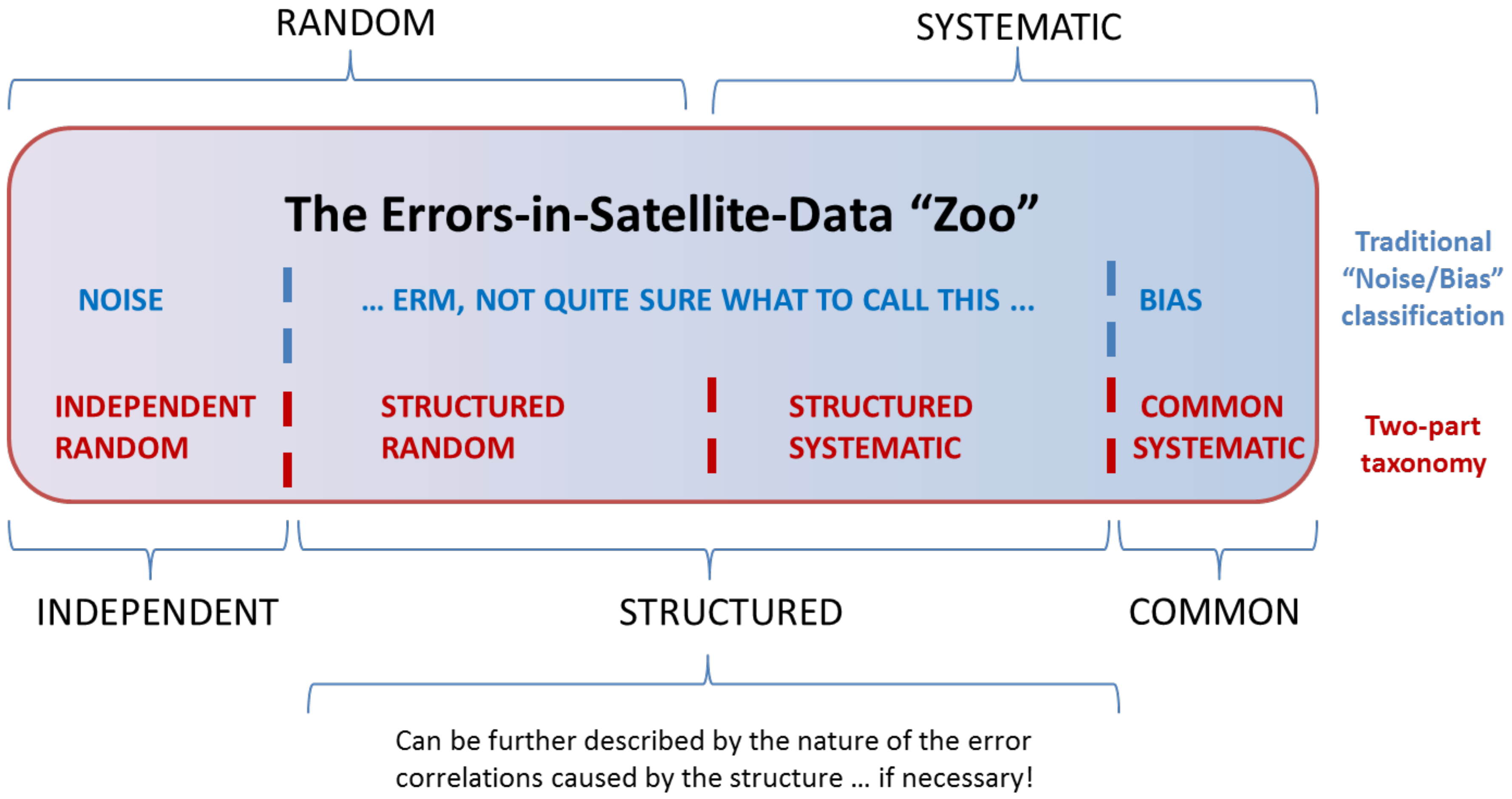


Analysis tree Level2A



Fiduceo Methodologies – Error Correlation

- Comprehensive *Effects Table* for recording error correlation information
- Define a file format that efficiently summarises this information for users



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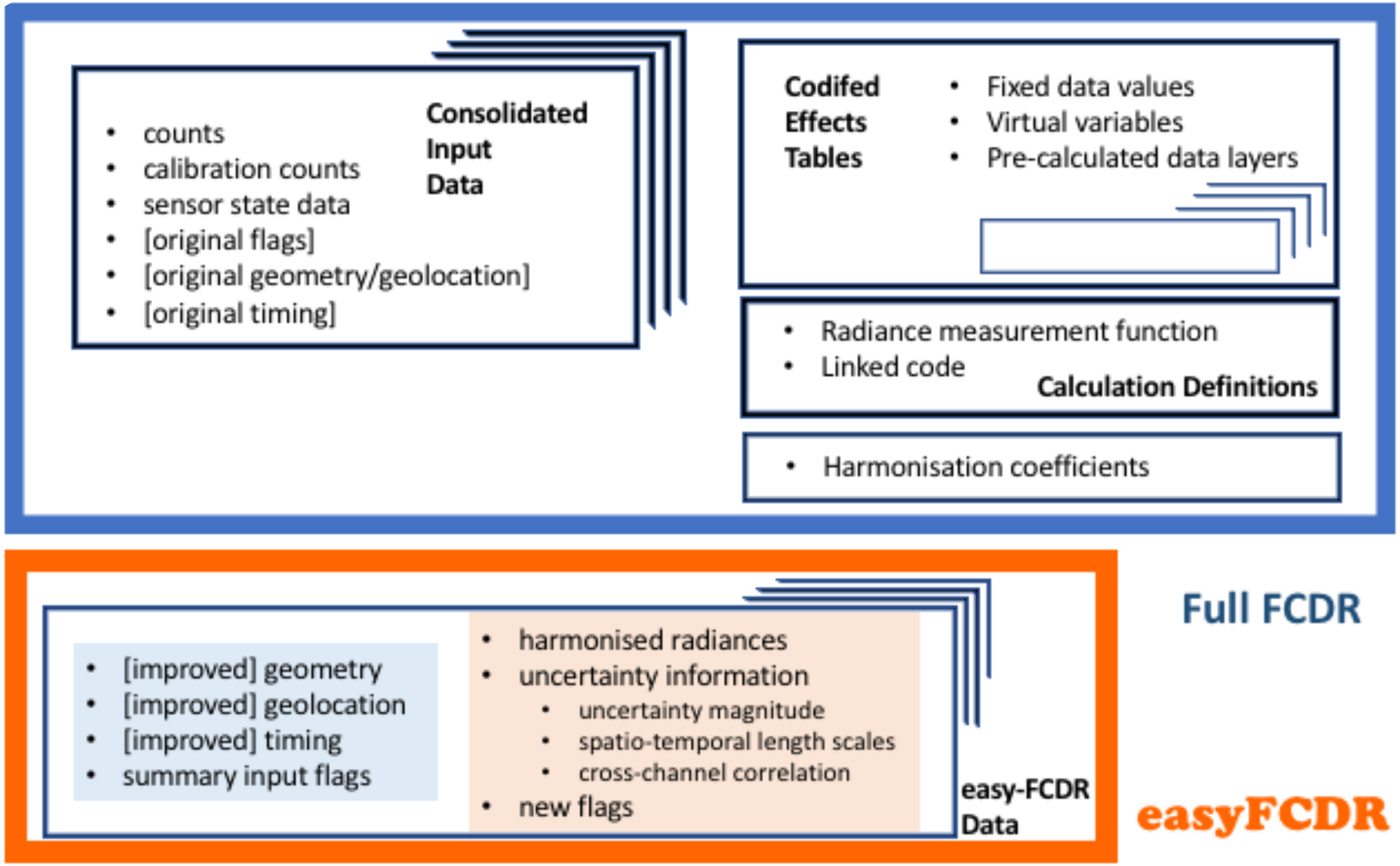
		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Correlation scale	Pixel-to-pixel [pixels]	As needed to define type
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Channels/bands	List of channels / bands affected	Channel names
	Error correlation coefficient matrix	A matrix
Uncertainty	PDF shape	Functional form
	units	Units
	magnitude	
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term

Table descriptor (k=4)		Quantity	Notes
Name of effect		Cloud mask uncertainty induced AOD uncertainty	
Affected term in measurement function			Can only be estimated on L2B superpixel level (10x10 km^2)
Maturity of analysis	Maturity of uncertainty estimate	1 – Rough estimates only	Is estimated by using 2 different thresholds for cloud probability and then calculating mean AOD with remaining selected pixels Setting of the two thresholds needs to be optimized
	Maturity of correlation scale estimate	1 - Estimated	
	If maturity of estimate is 0 or 1, how significant do you expect this effect to be?	significant	
Correlation type and form	From level 1		
	Larger scale temporal [time]	Random	
	Larger scale spatial [geospatial coordinates]	Exponential_decay	Reflecting cloud patchiness
Correlation scale	From level 1		Length scale depends on type of cloud / weather system - this information is not available routinely -> use average values of 0-10 days / 0-1000 km
	Larger scale temporal [time]	5 days	
	Larger scale spatial [geospatial coordinates]	500km	
Uncertainty	PDF shape	Random (temporal) Exponential (spatial)	
	units	Units of AOD	
	magnitude	$u(AOD_{cloud\ mask}) = AOD_{3x3}^{mean}(threshold_1) - AOD_{3x3}^{mean}(threshold_2)$	
Sensitivity coefficient		1	

Correlation form	Parameters	Description
random	none required	For fully random effects there is no correlation with any other pixel
rectangle_absolute	[-a,+b] (rectangle limits). Provide these per pixel/scanline/orbit as required. Allow for a way of representing [-∞,+∞] [rmax] States correlation coefficient for all pixel / scanline / orbit pixels. Default is rmax = 1 (fully correlated)	An effect is systematic within a range and different outside that range. For each pixel / scanline / orbit in range say number of pixels / etc either side that it shares a correlation with. For fully systematic effects notation to say "systematic with all". If rmax is defined, then the correlation coefficient is one for the pixel with itself, and is rmax with all other pixels.
triangle_relative	[n] – number of pixels/scanlines being averaged in simple rolling average (should be an odd number)	Suitable for rolling averages over a window from (–n-1)/2 to (+n-1)/2 (i.e. for n pixels/scanlines being averaged) Assumes a simple mean, not a weighted mean. No rmax is needed, since it is always 1.
bell_shaped_relative	[n] – number of pixels being averaged in a weighted rolling average, from which truncation range and standard deviation for Gaussian representation follow (truncation beyond ±n pixels) (n should be odd) OR [n,sigma] n: truncation from –n to +n, sigma: width of Gaussian representation. (n should be odd) Typically provided once per orbit file (some further consideration needed about first/last scanlines in an orbit)	Suitable for rolling averages over a window from (–n-1)/2 to (+n-1)/2 (i.e. for n pixels/scanlines being averaged). Assumes a weighted mean, for any weights (and thus also includes things like spline fitting). Also suitable for anything else where the assumption is that "closer pixels/scanlines are more correlated than further pixels". This can use two terms – n gives the truncation range outside which the assumption is there is no (or negligible) correlation, and sigma gives how fast the correlation drops off. The derivation of the width sigma to use for a weighted rolling average is given in Appendix B.4.4.
Stepped_triangle_absolute	[-a,+b,n] per pixel/scanline/orbit etc (n will be same for different pixels)	The step is a rectangular absolute from –a to +b with a correlation coefficient of one, after which the correlation coefficients drops for another a+b+1 lines, and then again. n is the number of calibration windows averaged. See Appendix B.4.5

FCDR Full & Easy Overview



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TOOLS FOR FCDRS AND CDRS

Error correlation in uncertainty propagation

$$u_c^2(y) = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$$

$$u_c^2(y) = \boldsymbol{c}_y \boldsymbol{V}_x \boldsymbol{c}_y^{\mathrm{T}}$$

For a single output quantity – not an image

$$\boldsymbol{c}_y = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n} \end{pmatrix}^{\mathrm{T}}$$

$$\boldsymbol{V}_x = \begin{pmatrix} u^2(x_1) & u(x_1, x_2) & \cdots & u(x_1, x_n) \\ u(x_2, x_1) & u^2(x_2) & \cdots & u(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ u(x_n, x_1) & u(x_n, x_2) & \cdots & u^2(x_n) \end{pmatrix}$$

But how do you work out the covariance matrix?

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Introducing $\boldsymbol{CURU^{\mathrm{T}}C^{\mathrm{T}}}$

$$V_{\mathrm{LE},T} = \begin{pmatrix} c_{\mathrm{LA},T} & 0 & 0 \\ 0 & c_{\mathrm{LB},T} & 0 \\ 0 & 0 & c_{\mathrm{LC},T} \end{pmatrix} \begin{pmatrix} u_T & 0 & 0 \\ 0 & u_T & 0 \\ 0 & 0 & u_T \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} u_T & 0 & 0 \\ 0 & u_T & 0 \\ 0 & 0 & u_T \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} c_{\mathrm{LA},T} & 0 & 0 \\ 0 & c_{\mathrm{LB},T} & 0 \\ 0 & 0 & c_{\mathrm{LC},T} \end{pmatrix}^{\mathrm{T}}$$

Covariance matrix for Earth Radiances in different channels due to common temperature error

$u(T)$

Temperature uncertainty in K

The same throughout by definition

Full correlation

$$c_{\mathrm{LA},T} = \frac{\partial L_{\mathrm{E,A}}}{\partial L_{\mathrm{ICT,A}}} \frac{\partial L_{\mathrm{ICT,A}}}{\partial T}$$

Sensitivity coefficient to convert from temperature to Earth radiance uncertainty

THIS is how you work out the covariance matrix

Maths tools methodology

Journal Publications

remote sensing

Article

Radiance Uncertainty Characterisation to Facilitate Climate Data Record Creation

Christopher J. Merchant [1,*], Gerrit Holl [2], Jonathan P. D. Mittaz [2] and Emma R. Woolliams [3]

[1] National Centre for Earth Observation and Department of Meteorology, University of Reading, Reading RG6 6AL, UK

REVIEW • OPEN ACCESS

Applying principles of metrology to historical Earth observations from satellites

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Article PDF

FIDUCEO documents

- D2-2 and D2-4 reports
- FIDUCEO Notation document

FIDUCEO Tools

- Uncertainty propagation at FCDR tool
- Regridding iPython notebook
- Uncertainty propagation iPython notebook

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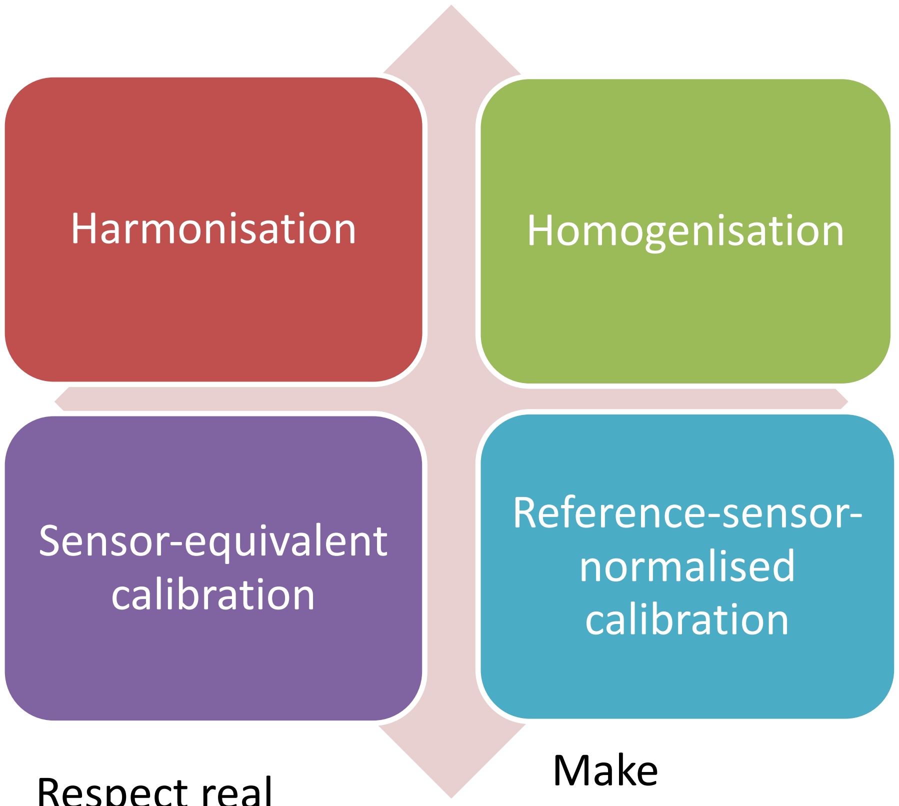
Fiduceo

Harmonisation definition

Recalibration

Bias Correction



Respect real differences

Make sensors look the same

- Definition being used by ESA
- GSICS newsletter publication

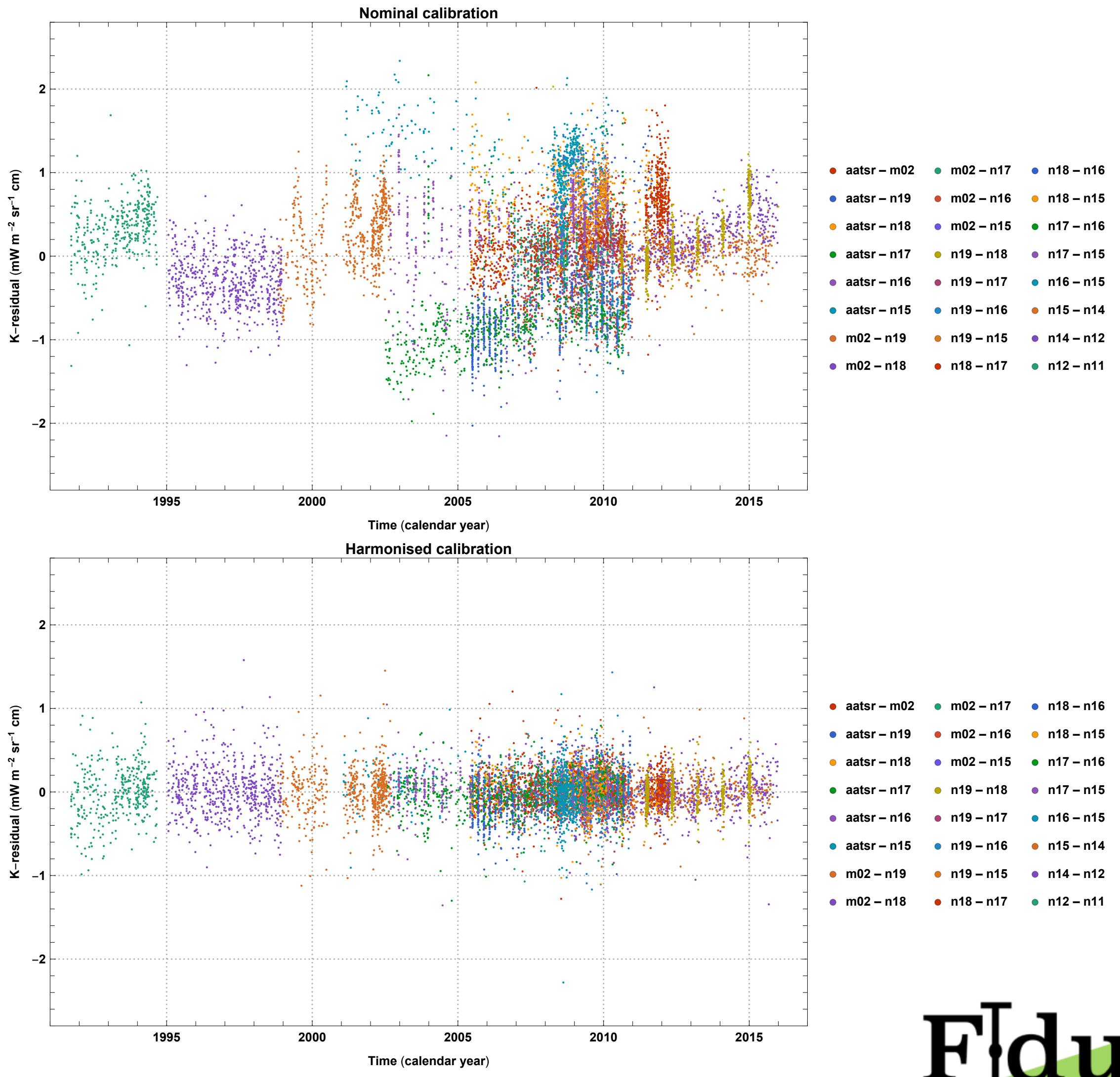
After Fiduceo : Harmonisation

- Developed concept for harmonisation – to solve the full harmonisation problem taking into account full error correlation information

(Prior to FIDUCEO – could only cope with data volumes if error correlation was ignored)

- Developed two code sets – EIV (NPL) and mEIV (FastOpt). EIV on Github.
- Both methods use same (defined) input format and produce same output format
- Code to analyse and interpret harmonisation output on Github

- Methods cross compared



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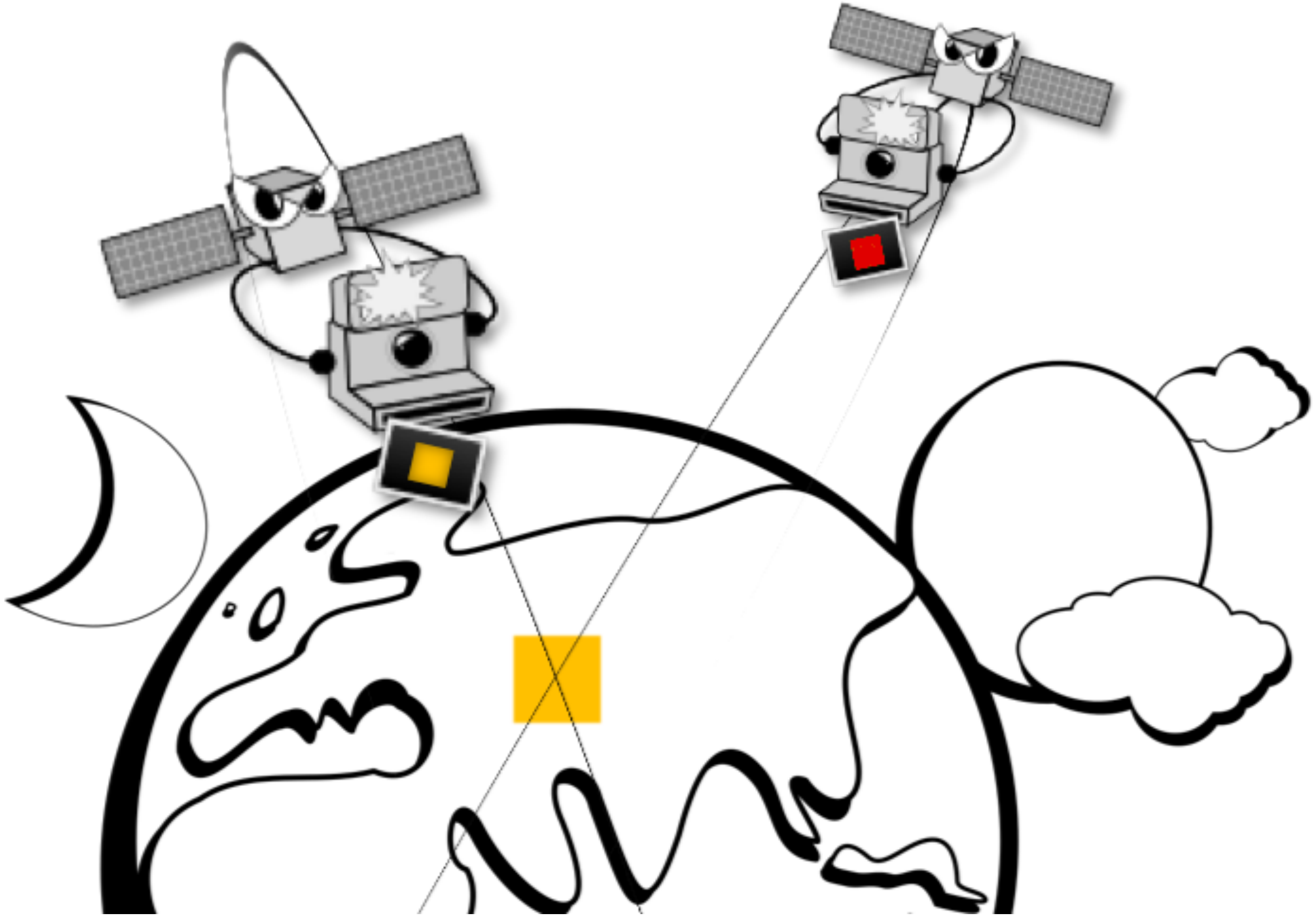
$$L(\boldsymbol{x}, \boldsymbol{\alpha}) = \alpha_1 + (\epsilon + \alpha_2)\, L_{\mathrm{ICT}}\, \frac{C_{\mathrm{E}} - \bar{C}_{\mathrm{S}}}{\bar{C}_{\mathrm{ICT}} - \bar{C}_{\mathrm{S}}} + \alpha_3 (C_{\mathrm{E}} - \bar{C}_{\mathrm{S}})(\bar{C}_{\mathrm{ICT}} - \bar{C}_{\mathrm{S}}) + \alpha_4 \frac{T - 295\ \mathrm{K}}{10\ \mathrm{K}}$$

Dual-sensor matchups for relative calibration

$$L^i - L^j = K^{ij}$$



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Harmonisation - methodology

remote sensing

MDPI

Article

A Novel Framework to Harmonise Satellite Data Series for Climate Applications

Ralf Giering [1,*], Ralf Quast [1], Jonathan P. D. Mittaz [2], Samuel E. Hunt [3], Peter M. Harris [3], Emma R. Woolliams [3] and Christopher J. Merchant [2]

1 FastOpt GmbH, 22767 Hamburg, Germany; ralf.quast@fastopt.de
2 Department of Meteorology, University of Reading, Reading RG6 6AL, UK; j.mittaz@reading.ac.uk (J.P.D.M.); c.j.merchant@reading.ac.uk (C.J.M.)

IGARSS 2019 Conference

A Metrological Approach to Producing Harmonised Fundamental Climate Data Records from Long-Term Sensor Series Data

Publisher: IEEE

8 Author(s) Samuel E. Hunt ; Ralf Quast ; Peter M. Harris ; Jonathan P.D. Mittaz ; Emma R. Woolliams ; Ralf Giering ; ... View All Authors

- EIV method, examples and data formats described on Github
- Training material on legacy website

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In hindsight, we should have…

Use simple ODR method to test your measurement equation

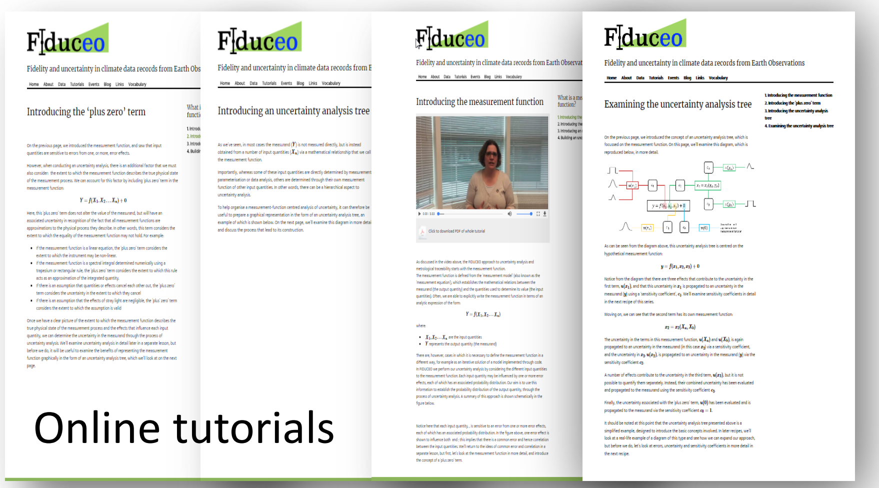
Review results and improve the measurement equation

Use full EIV / m-EIV method to obtain harmonisation coefficients

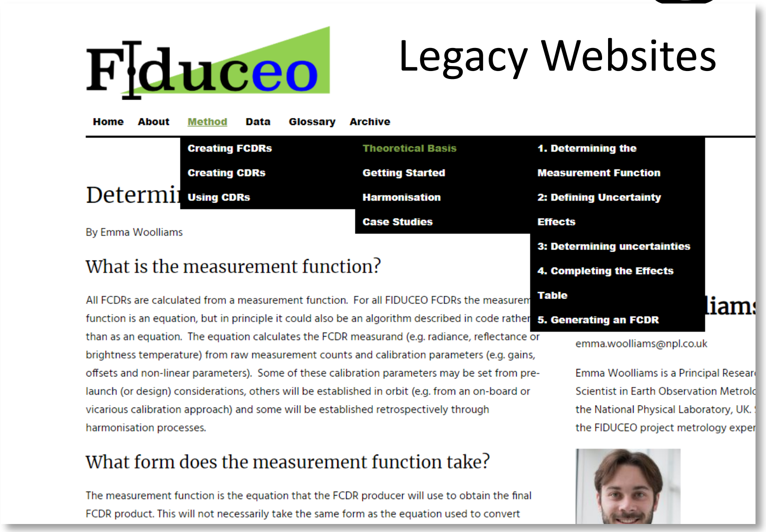
and dedicated much greater resource to design of the K inputs

TRAINING AND LEGACY

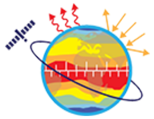
FIDUCEO Training



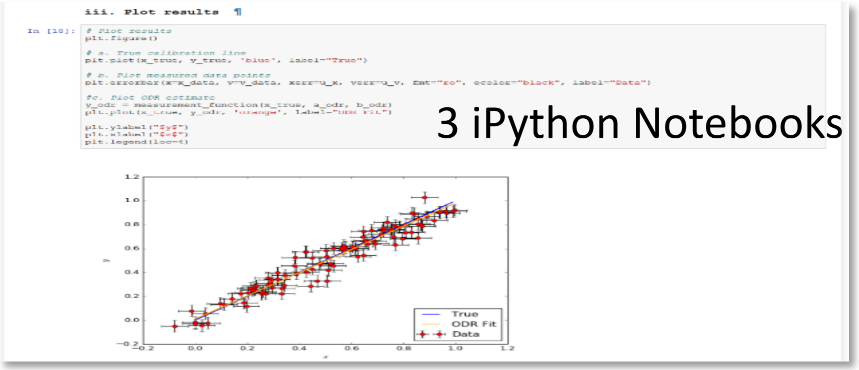
Online tutorials



Legacy Websites



Material being developed into an e-Course by NPL (MetEOC funding – will acknowledge FIDUCEO)



3 iPython Notebooks

- 2 Workshops in Lisbon
- D2-2 and D2-4 report templates and guidance documents
- Workshops with ESA

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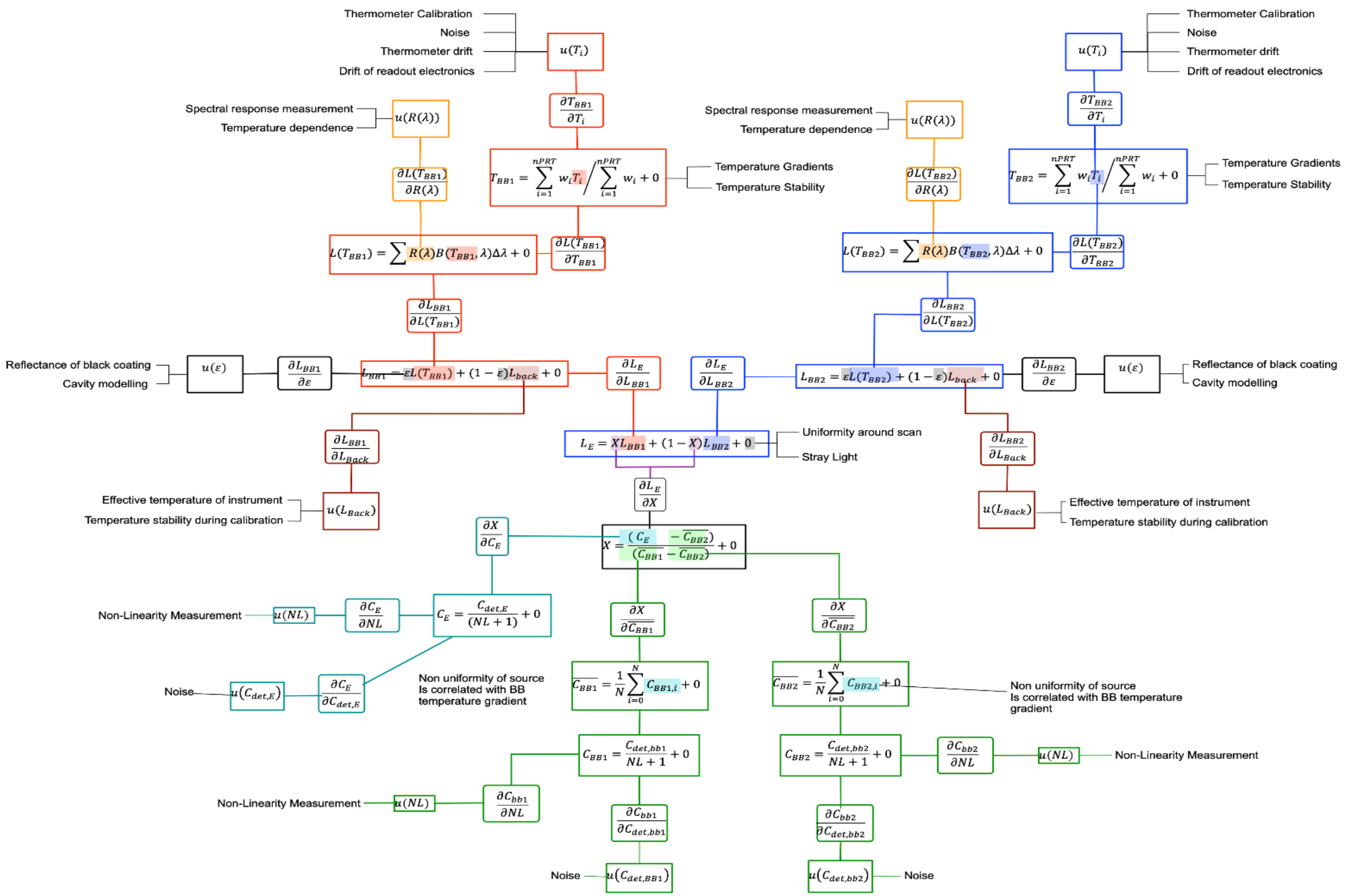
Fiduceo

Legacy



- SLSTR on Sentinel 3 (MetEOC project)
- Other presentations at FIDUCEO Workshop
- Other applications

Legacy

- FDR4ALT ITT from ESA

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Methodologies developed within the FIDUCEO project shall be also evaluated and possibly taken into account; in particular the approach based on the use of the measurement equation, the harmonisation of the sensor series, and the creation of an Uncertainty Tree Diagram which properly accounts for, and visualises, all possible sources of uncertainty (effects) and gaps in knowledge. Appropriate methods for propagating the observational uncertainty estimates when averaging or accumulating a variable shall be adopted (if necessary) in order to consider different temporal and spatial scales.

IN SUMMARY

Pre-Fiduceo: Metrological Methods

- No uncertainty propagation from L0 → L1
- Desire for "metrological methods" but implementation examples limited
- Error-correlation seen as an advanced "extra" topic
- Traceability chains – but not uncertainty diagrams

Post-FIDUCEO: Metrological Methods

- Tree diagrams
- Effects tables
- CURUC
- Training Material
- Harmonisation concepts

- New metrology
- New Earth Observation
- New terminology
- New philosophy

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FIDUCEO

A metrologist's observation

- Before FIDUCEO people said …
  - Metrology is alright for the lab but it doesn't really work for satellite data which is "special"
- Before the FDR4ALT kick off meeting on Monday people said …
  - Metrology is alright for FIDUCEO-like radiometric instruments, but it doesn't really work for active sensors, which are "special"