CURRENT STATUS OF FLEX LEVEL-2 DATA PROCESSING CHAIN

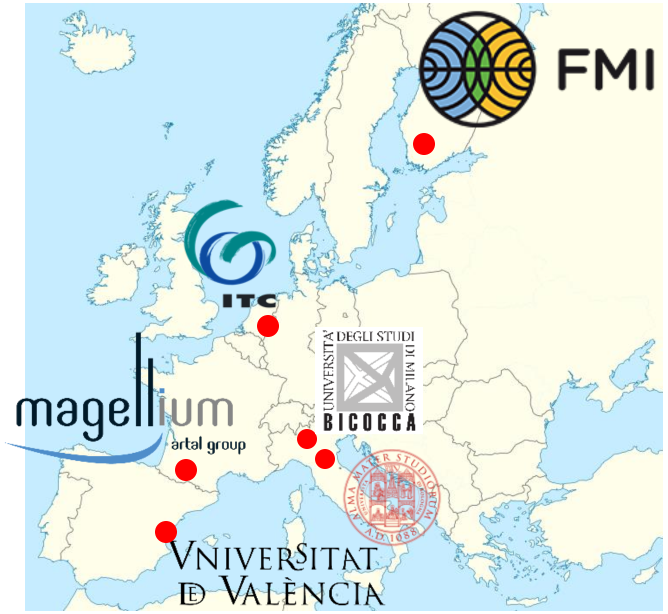
Jorge Vicent Servera, G. Matot, N. Sabater, P. Kolmonen, S. Cogliati, S. Van Wittenberghe, J. Moreno
M. Ferrato, R. Santer, F. Magnani, C. van der Tol and M. Drusch

jorge.vicent-servera@magellium.fr earthobservation.magellium.com

THE FLEX L2 STUDY: PROJECT OVERVIEW

Main objectives

- **Document** FLEX L2 algorithms for future implementation in Ground Segment
- **Develop** a pre-operational processing chain from L1B to L2
- **Validate** algorithms with synthetic FLEX data (from **E2ES**)
- Others: contribute to the definition of FLEX L2 products, quality check of L1B,...



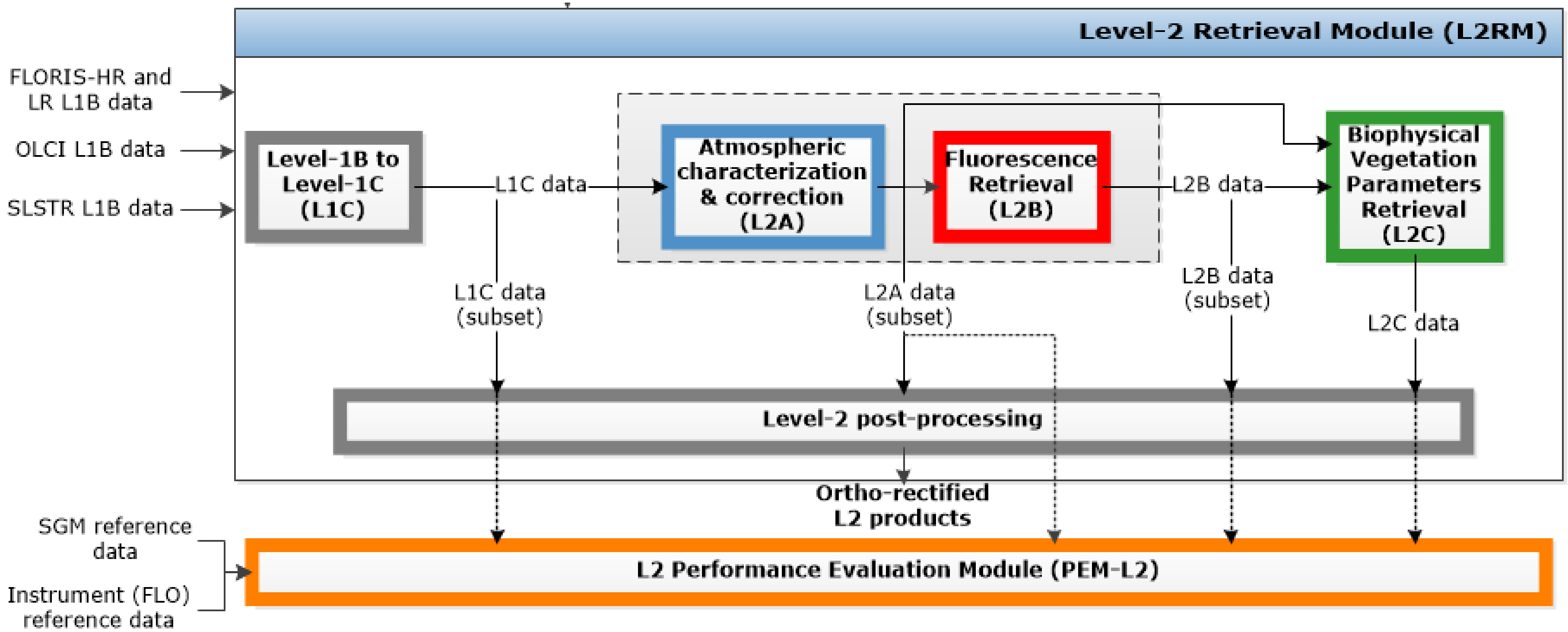
Project phases

- **Main phase** (2 yr): set-up, definition of architecture & interfaces, 1st implementation of L2 processing chain
- **CCN3** (2 yr): consolidation of algorithms
- **CCN4** (6 months): preparation for M-CDR and future Ground Segment project

KO — 11/2017
KO (CCN3) — 07/2020
FR (CCN3) — 07/2022
FR (CCN4) — 01/2023

High-level architecture and interfaces

- Four main modules: from TOA radiances (L1C) to photosynthesis products (L2C)
- Post-processing: orthoprojection of final L2 products in Sentinel-2 UTM tiles
- Inputs and auxiliary data:
  - FLEX, OLCI and SLSTR L1B products (radiances and metadata)
  - Atmospheric LUTs, retrieval coefficients, DEM, spectral responses...



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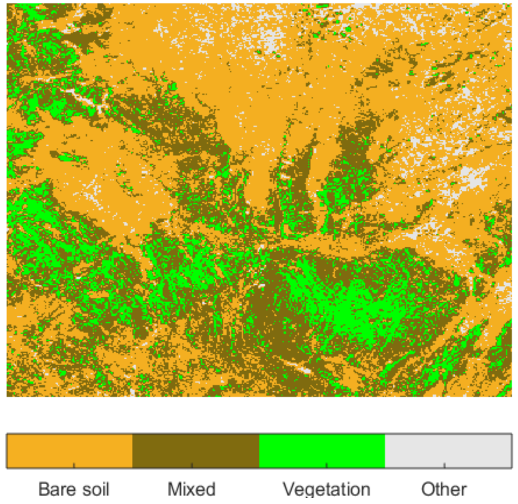
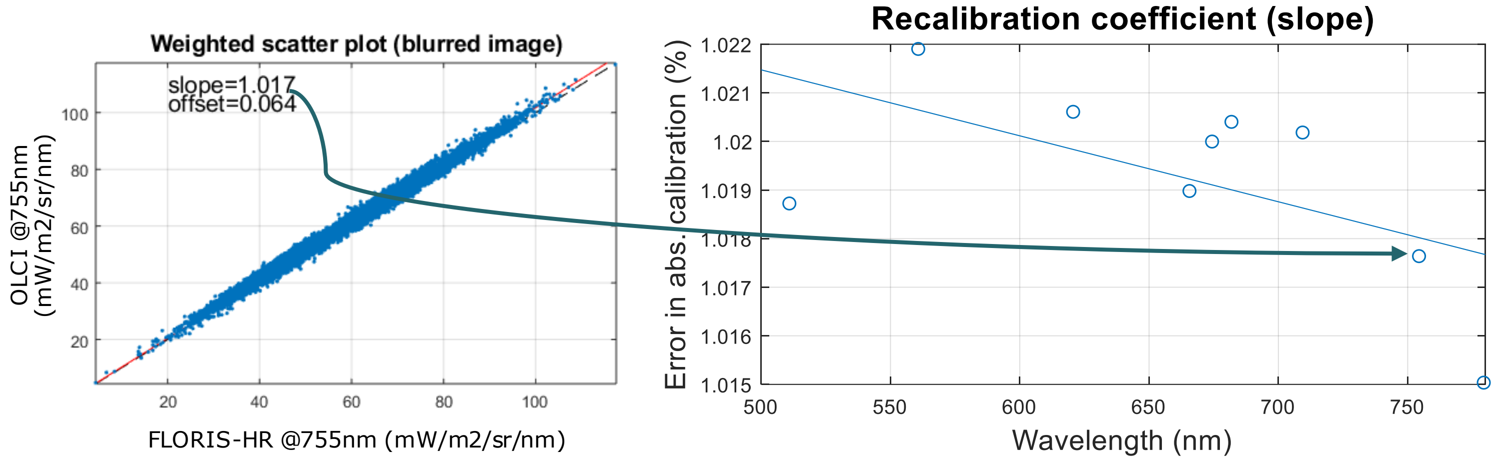
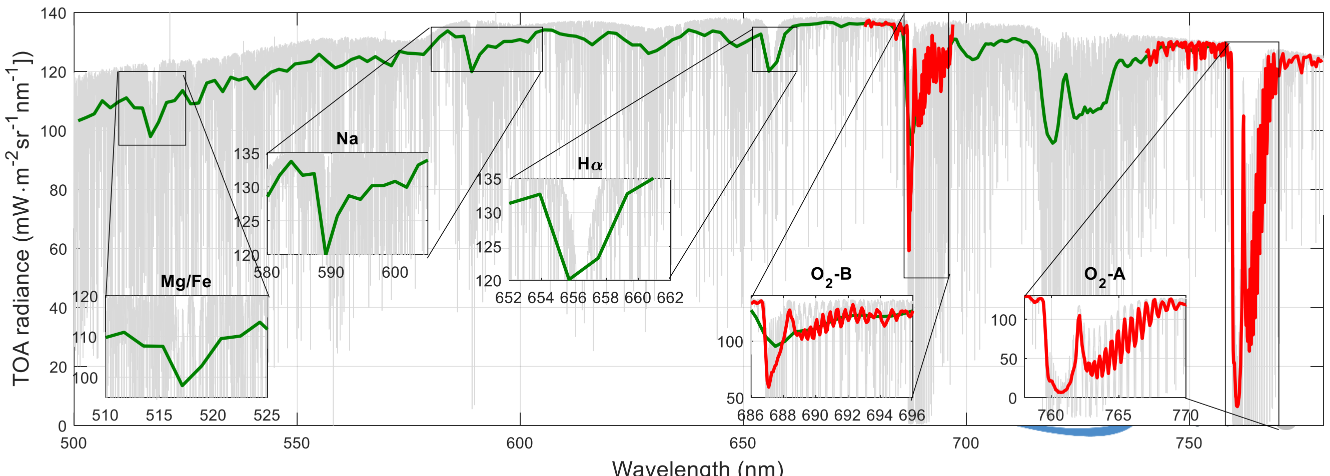
L1C MODULE: PRE-PROCESSING

- Pixel classification (bare-soil, sparse/dense veg.) based on spectral indices
- Cloud shadow detection from geometric and radiometric information
- Consistency check between FLORIS and OLCI radiometry



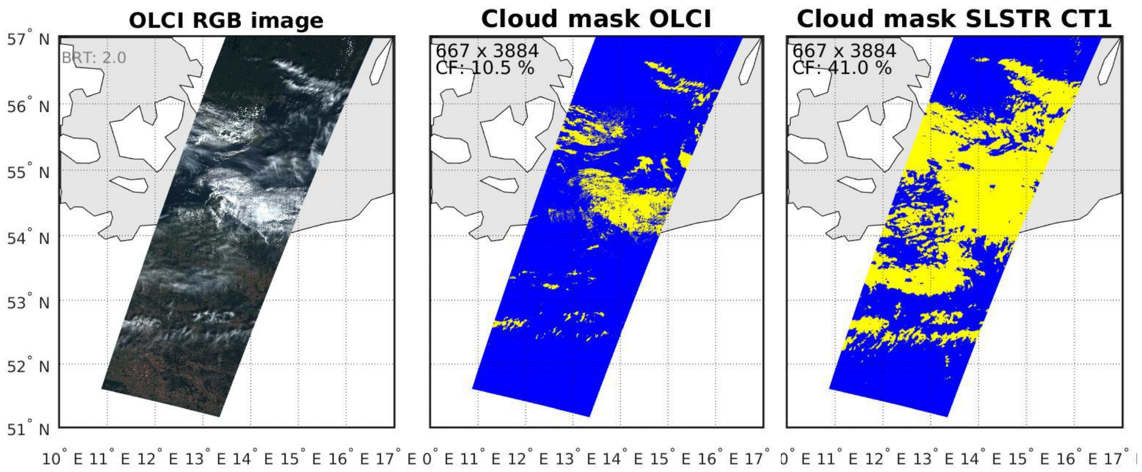


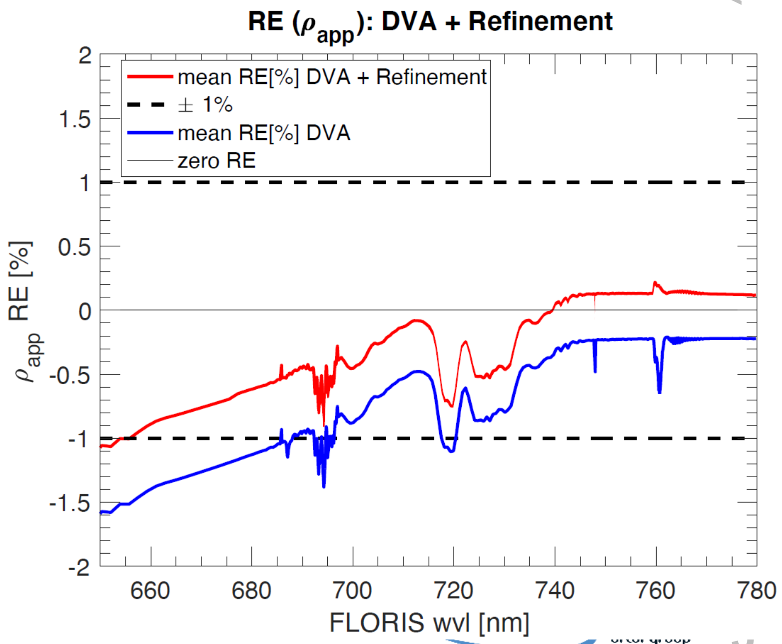
- Spectral calibration against reference (MODTRAN) spectra (Meroni et al. 2010)
  - Across-track characterization (smile)
  - Fourier analysis for first guess of FWHM
  - Spectrum normalization (Felde et al. 2003)

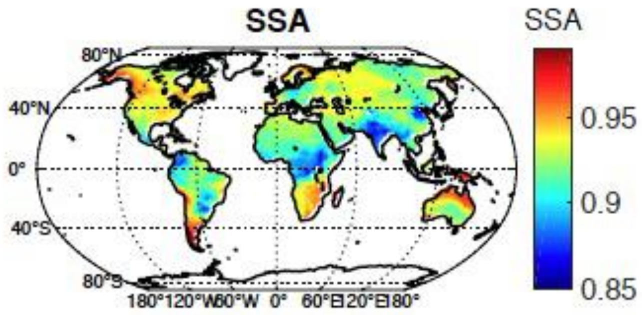


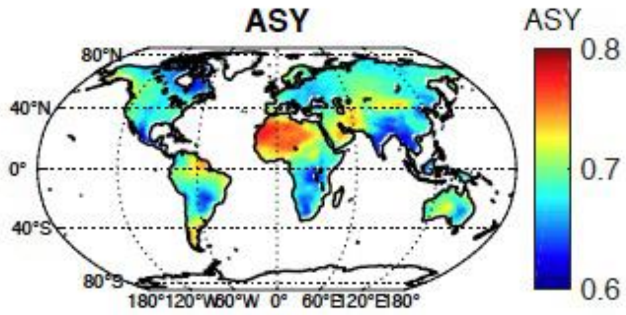
L2A MODULE: ATMOSPHERIC CORRECTION

- **Cloud screening**: based on dynamic thresholds from OLCI+SLSTR radiances
- **Aerosol retrieval**:
  1. SLSTR dual-viewing algorithm (DVA):
     - $\rho_{(Ob)} = k\rho_{(N)}$ where k is assumed spectrally constant and retrieved from SWIR channels
  2. Refinement using FLORIS data at O2A band
     - Shape of O2A absorption sensitive to aerosol opt. properties
     - Difference measured and simulated (w/ DVA results) radiance allows disentangling SIF contribution from aerosol scattering
     - Use of climatology to constrain retrieval









L2B MODULE: FLUORESCENCE RETRIEVAL

Fluorescence/Reflectance spectra retrieval (670-780 nm)

Retrieval cost function

$$J(x) = [y - F(x,b)]^T S_\epsilon^{-1} [y - F(x,b)] + \Lambda\,(\mathbf{x} - \mathbf{x_a})^{\mathrm{T}} \mathbf{S_a}^{-1} (\mathbf{x} - \mathbf{x_a})$$

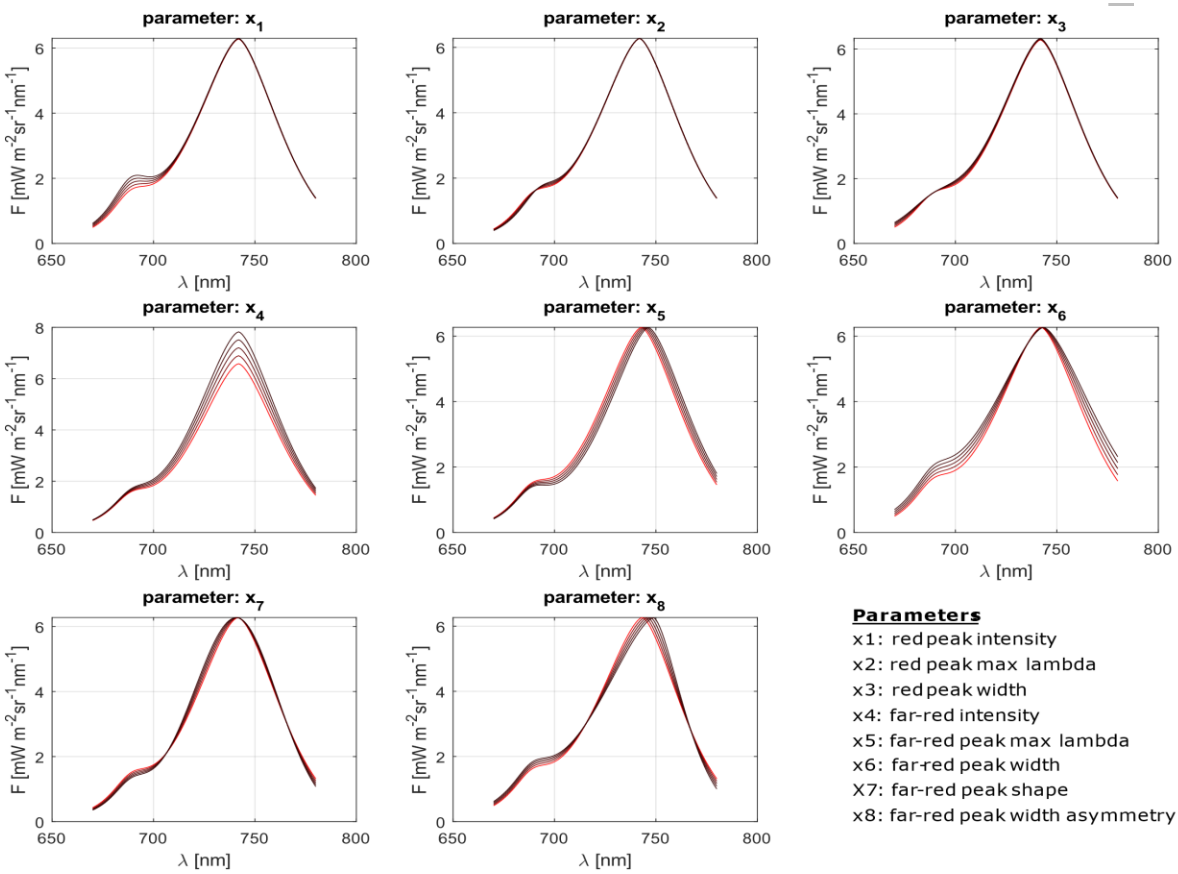
free parameters (a-priori) probability cov. matrix

a-priori

measurement uncertainty cov. matrix

scaling parameter

Constant parameters (geometry, ISRF...)



Forward model

$$y = F(x,b) + \epsilon \qquad x = [x_F, x_R]$$

- Fluorescence (x_F): 2 peaks function
- Reflectance (x_R): piece-wise cubic spline

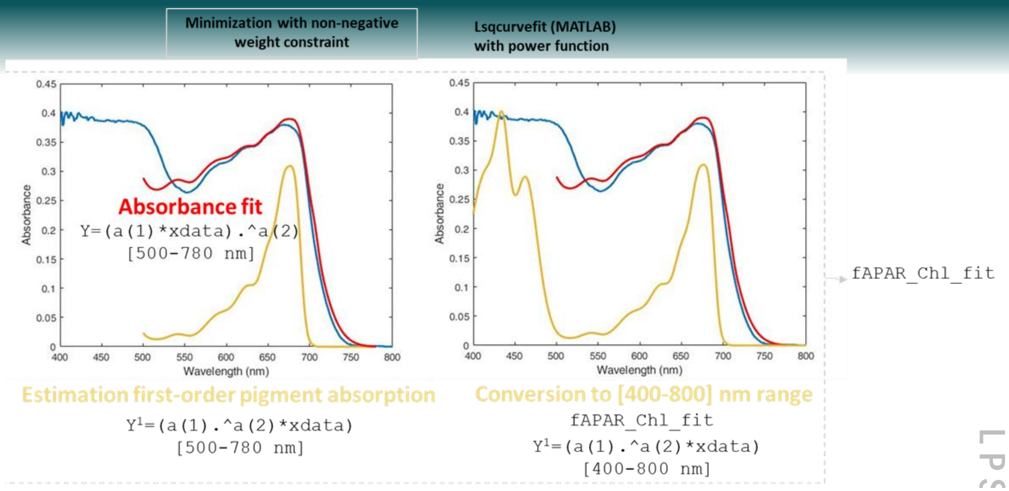
Minimization method: Levenberg-Marquardt

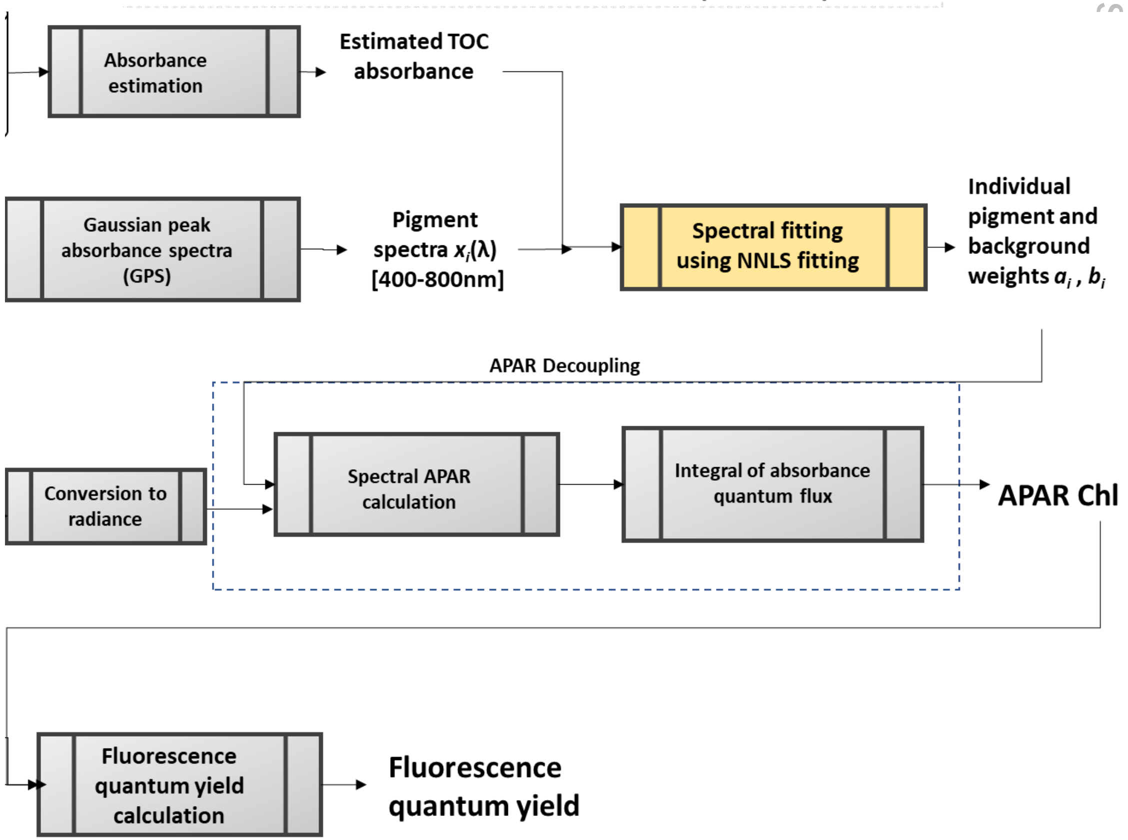
L2C MODULE: FROM BIOPHYSICAL PARAMETERS TO PHOTOSYNTHESIS

L2C Algorithms for delivery of FQE

- APAR Chlorophyll product based on spectral fitting of real reflectance FLORIS-LR (500-780 nm)
- L2B SIF spectrum and APAR Chl: conversion to [µmol m^{-2} s^{-1}]
- Fluorescence quantum efficiency (FQE): ratio emitted to absorbed photons by Chl

- Poster session **A4.01 no.65107**: fluorescence quantum efficiency

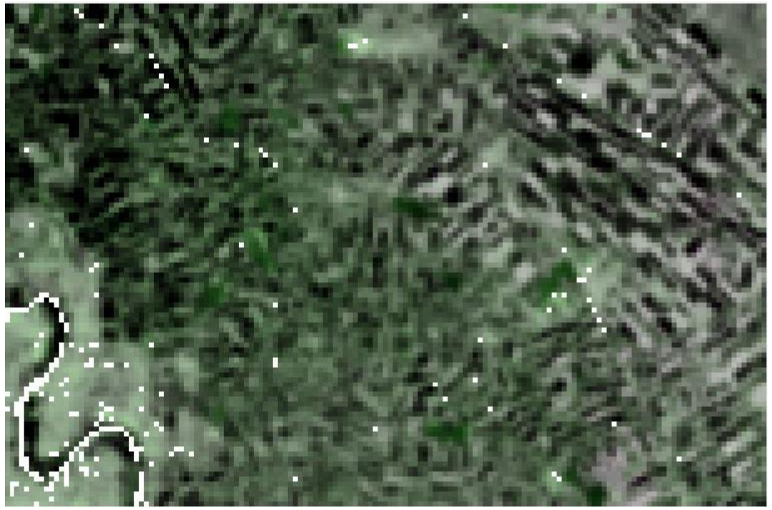


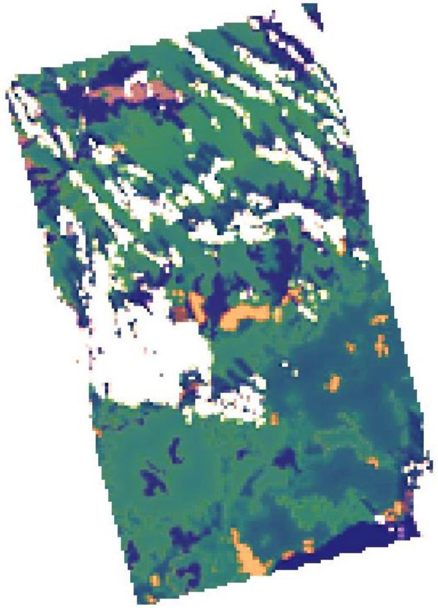


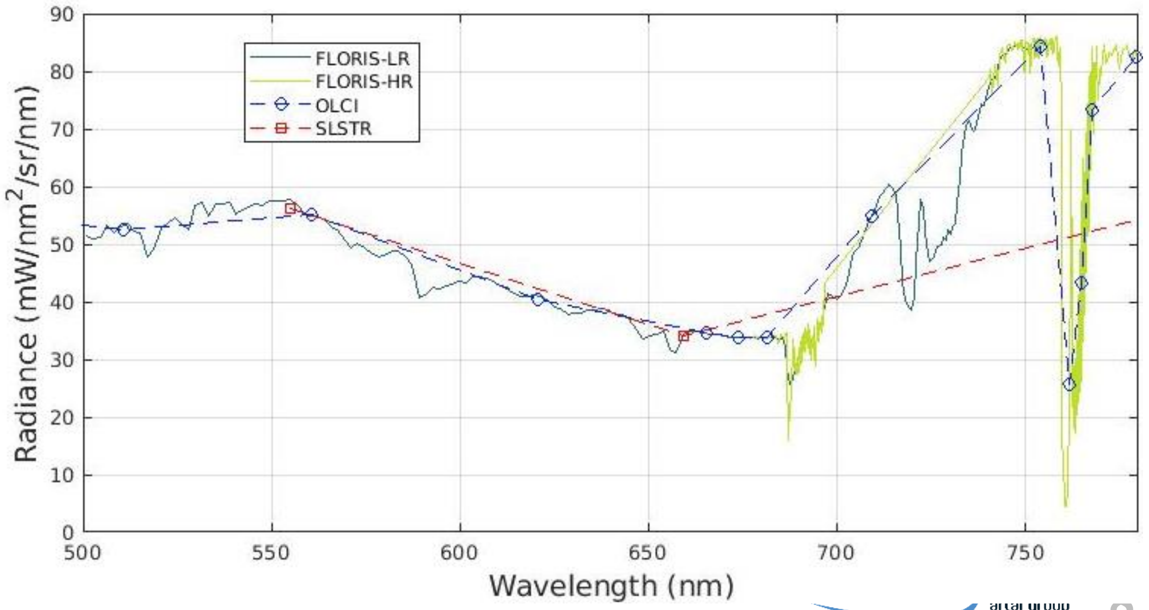
VALIDATION RESULTS (L2RM V3.2)

Validation test scenarios

- In-house simulated FLEX-like L1B products: from Sentinel-2 L1C product (resampled to 300m), SCOPE+MODTRAN simulations, instrument characteristics (from E2ES), noise and calibration errors included
- FLEX E2ES (FIPS/GPP v2.1) simulated scenarios: noisy data, various atmospheric conditions, BRDF effects







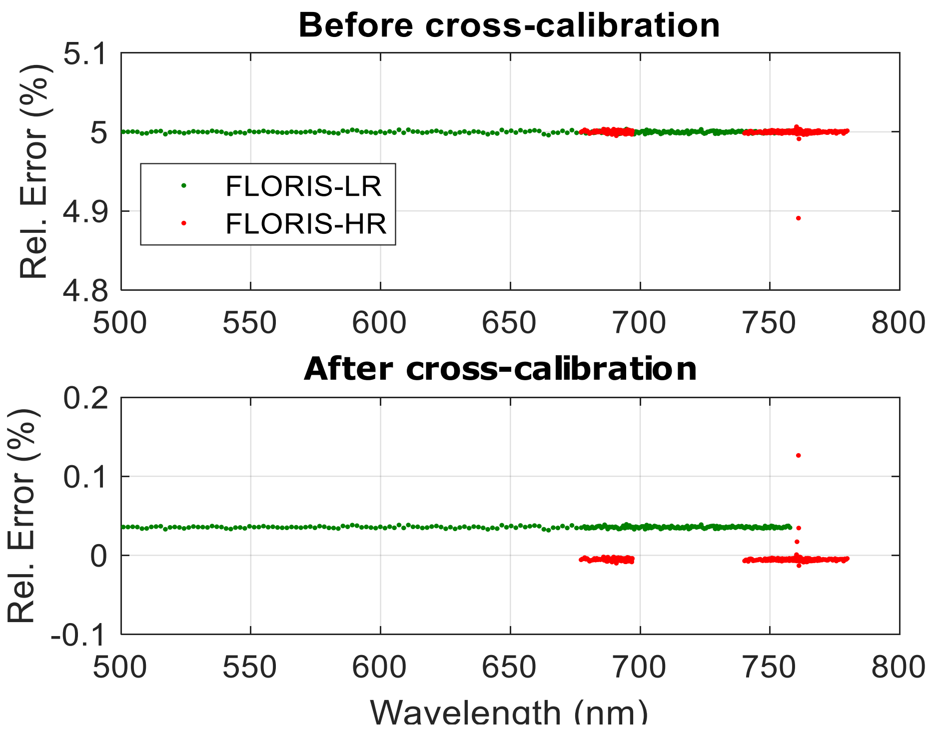
(Vicent et al. 2016, Tenjo et al. 2018, Verhoef et al. 2017)

Validation results: L1C algorithms

- Spectral calibration within requirements
- Smile effect taken into account in both FLORIS spectrometers
- Robust against noises, calibration errors and atmospheric conditions

Band	Average error in barycenter (nm)	Avg. error in FWHM (nm)
O2 bands (HR)	0.004	<0.004
H2O (LR)	0.06	0.19
Others (LR)	0.14	0.37

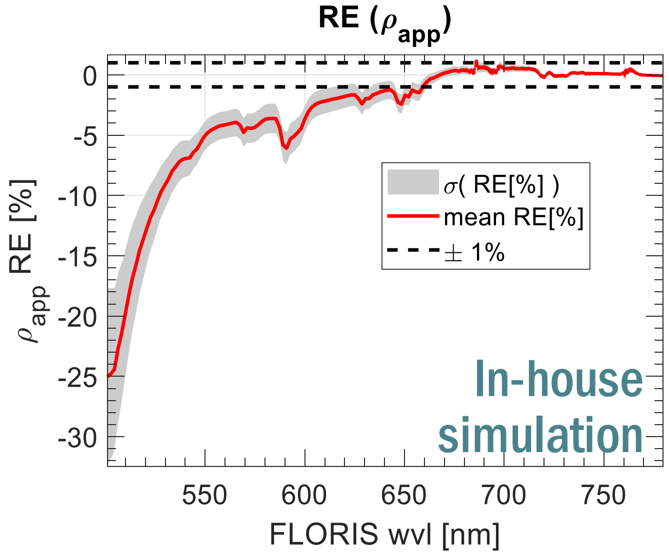
- Abs./rel. radiometric cross-calibration errors: 0.05±0.3% (abs.), <0.13% (rel. for HR)
- Algorithm can be adapted based on the expected performance of L1B radiometric calibration

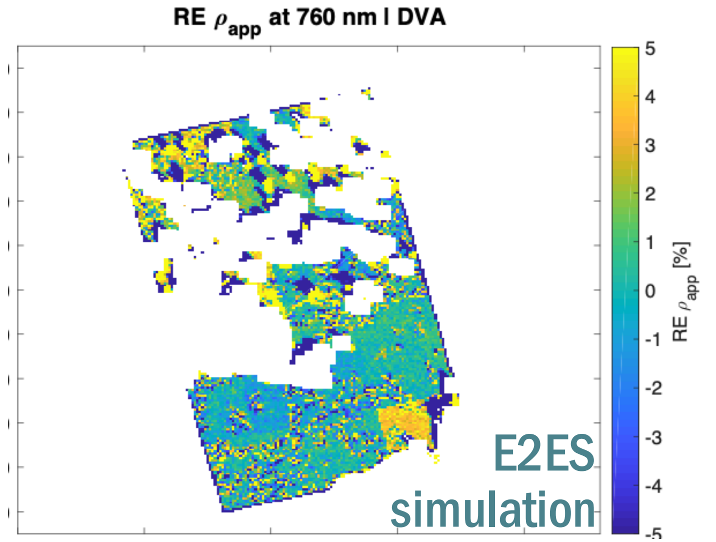


Validation results: L2A algorithms

- Errors in atmosphere characterization ➔ 1-2% in surface reflectance (in 650-780 nm)

Parameter	Error
AOT	<0.05
Angstrom	0.7
Asymmetry	0.05-0.1
CWV	$<0.1\ g{\cdot}cm^{-2}$





Assumptions, challenges and ideas

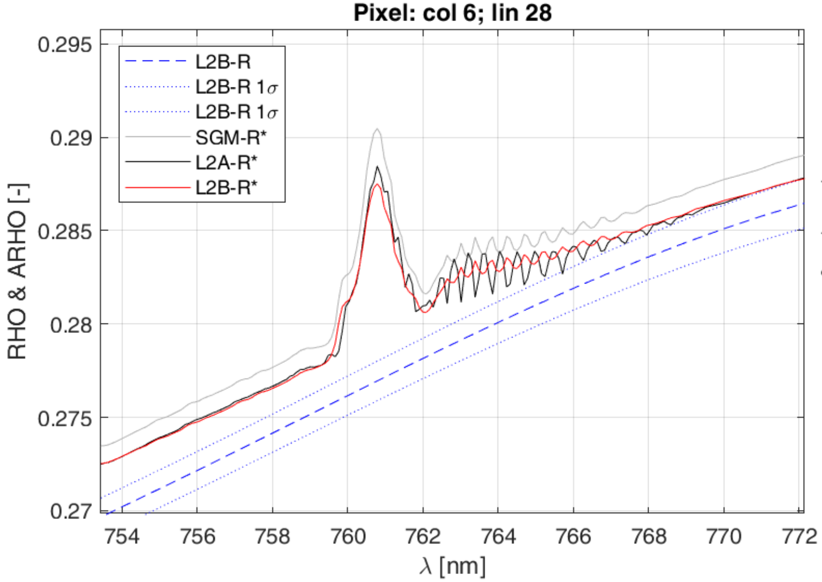
- Spectrally-constant aerosol optical properties
- Phase function (Henyey-Greenstein)
- Constrain aerosols from climatology (correlations)

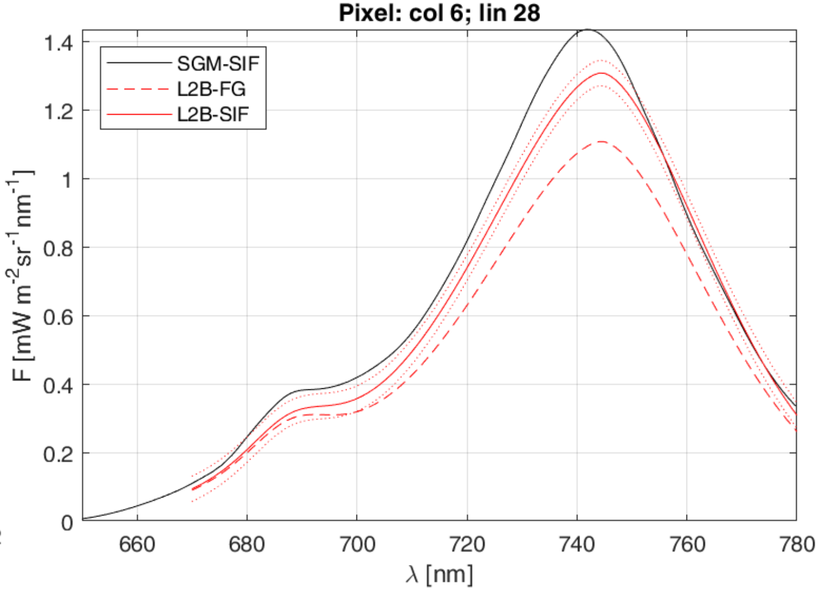
VALIDATION RESULTS (L2RM V3.2)

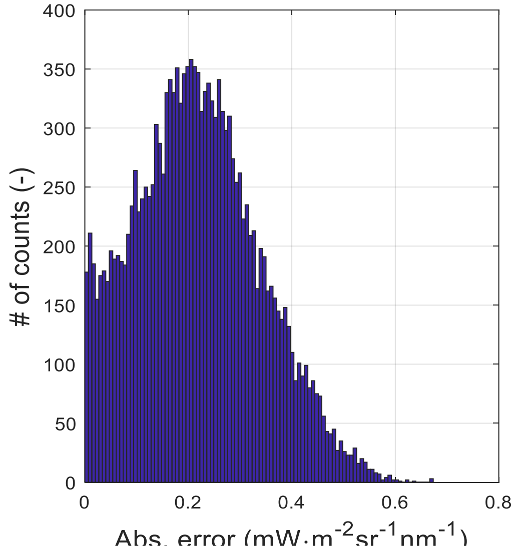
Validation results: L2B algorithms

- Errors within requirements except for far-red peak and red-edge
- Curve fitting compensates random error from previous modules
- O2B values close to the first-guess. Far-red peak values sensitive to errors in atmospheric correction

SIF param.	Avg. error in SIF (mW·m^{-2}sr^{-1}nm^{-1})
O2B	<0.2
Red peak	<0.2
O2A	<0.15
Far-red peak	<0.4







2022

CURRENT CHALLENGES

- FLORIS spectral response ➔ impact in surface reflectance and SIF retrieval
  - Increase robustness of L2 algorithms
- Retrieval of aerosol asymmetry still a challenge
- Compensation of radiometric effects due to pressure-temperature profile (actual vs "standard" profiles)
- Sensitivity of SIF retrieval to errors in atmospheric correction
- Atmospheric LUT size: computation time, handling data volume

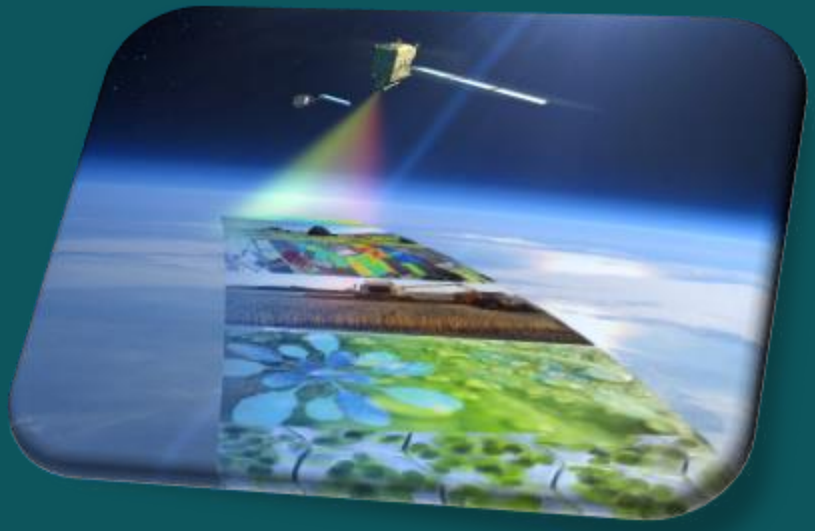
FLORIS				
	Variable	N grid points	Values	Units
ATM	MODEL	5	MLS, MLW, SAS, SAW, Tropical	-
AER	AOD	7	0.03, 0.05, 0.15, 0.25, 0.36, 0.48, 0.60	-
	α	2	0.02, 2	-
	SSA	2	0.8, 1	-
	ASY(g)	2	0.55, 0.8	-
GAS	H_2O	6	0.50, 1.12, 1.90, 2.83, 3.91, and 5.00	g/cm^2
	O_3	2	0.17, 0.38	atm-cm
GEO	Elevation	5	0, 0.72, 1.55, 2.38, 3.00	Km
	VZA	2	0,6	deg
	SZA	12	20.00 , 29.47, 38.95, 51.58, 57.90, 61.05, 64.21, 67.37, 70.53, 73.68, 76.84, and 80.00	deg
	RAA	4	0, 40, 140, 180	deg

Reduced LUT (L2RM v3.2)

- Nearly 24'000 points (out of 3.6 million)
- 3 min/simu. (12 cores) ➔ Total time: 5 days
- File size (double precision) ➔ 26 Gb

SUMMARY & FUTURE DEVELOPMENTS (CCN4)

- **L1C module**:
  - Main features: Fusion of 4 instrument with radiometric, spectral and geometric harmonization
  - Future developments: (1) L1B quality check, (2) adapt L1C, (3) pixel classification
- **L2A module**:
  - Main features: 3 atm. corr. methods (SLSTR: DVA; FLORIS: O2 absorption; OLCI: spectral matching)
  - Future developments: (1) contingency plan for absence of S3 data, (2) updates in FLORIS refinement method (robustness to noises, include O2B), (3) use ECMWF temperature profile
- **L2B module**:
  - Main features: State-of-the-art SIF retrieval based on optimal estimation theory
  - Future developments: (1) Fine-tuning of Optimal Estimation parameters, (2) multi-criteria weighting scheme for curve fitting, (3) stratification of covariance matrix
- **L2C module**:
  - Main features: L2C processing from biophysical parameters to photosynthesis
  - Future developments: (1) Revision of absorbance fitting for APAR retrieval, (2) correction of SIF shape distortions (reabsorption, PSI/PSII,…)



Thank you for your attention.

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jorge.vicent-servera@magellium.fr

BACK-UP

Other main features

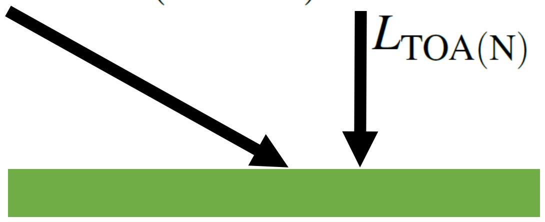
- Error propagation from L1B to L2C products
- Robustness against noises and errors in the L1B data
- Although focus is scientific development, many routines have been optimized
- Design of atmospheric LUTs for global processing

L2A module: DVA algorithm

- Ratio between reflectance in nadir and oblique spectrally constant (k) and obtained from SWIR channels
- Rearanging the equations ➔ cost function involving nadir and oblique views

$$L_{\mathrm{TOA(Ob)}} = L_{0\mathrm{(Ob)}} + \frac{E_{\mathrm{TOC}} T^{\uparrow}_{\mathrm{(Ob)}} \rho_{\mathrm{(Ob)}}}{\pi(1 - SA)}$$

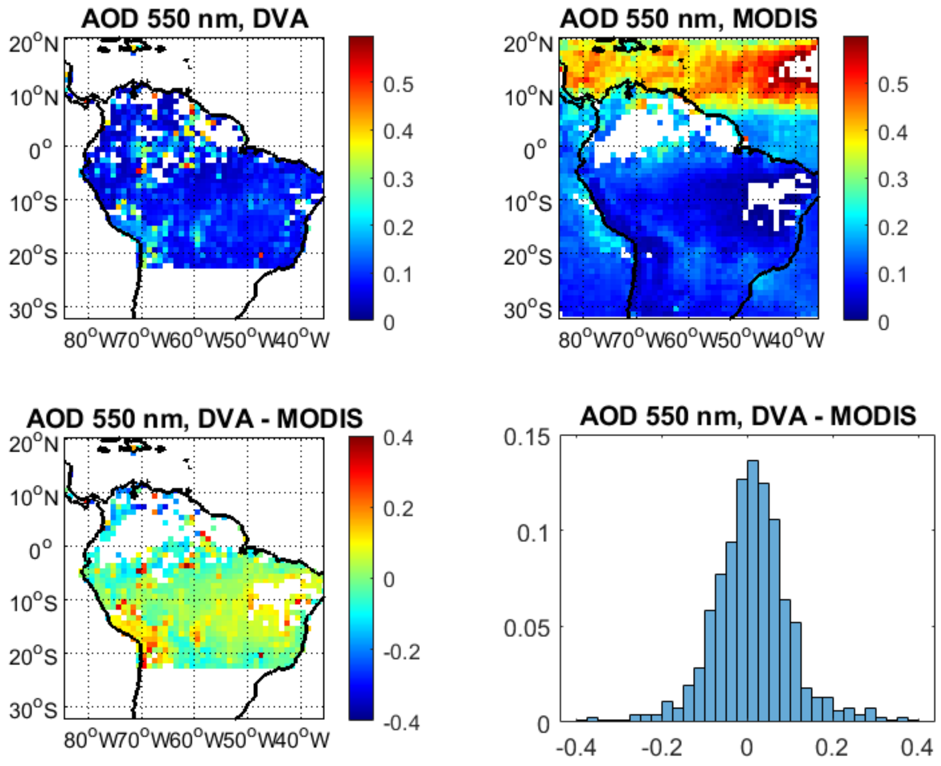
$$L_{\mathrm{TOA(N)}} = L_{0\mathrm{(N)}} + \frac{E_{\mathrm{TOC}} T^{\uparrow}_{\mathrm{(N)}} \rho_{\mathrm{(N)}}}{\pi(1 - SA)}$$



$$\arg_{\mathrm{AOT},\alpha,g} \min \sum_{i=1}^{N_\lambda} \left[\frac{L_{\mathrm{TOA(N)}} - L_{0\mathrm{(N)}}(\mathrm{AOT},\alpha,g)}{E_{\mathrm{TOC}}(\mathrm{AOT},\alpha,g) T^{\uparrow}_{\mathrm{(N)}}(\mathrm{AOT},\alpha,g)} - \frac{L_{\mathrm{TOA(Ob)}} - L_{0\mathrm{(Ob)}}(\mathrm{AOT},\alpha,g)}{k E_{\mathrm{TOC}}(\mathrm{AOT},\alpha,g) T^{\uparrow}_{\mathrm{(Ob)}}(\mathrm{AOT},\alpha,g)} \right]^2$$

L2A validation

- DVA method validated with real S3 products (920 scenes)
- Aerosol retrieval compared with MODIS products
  - MODIS extensively validated against AERONET
  - Comparison DVA vs MODIS allows visualization of spatial distributions (not sparse w/ AERONET)



- Validation with E2ES datasets provide accuracies in-line with estimates from real S3:
  - Errors in AOD: <0.08

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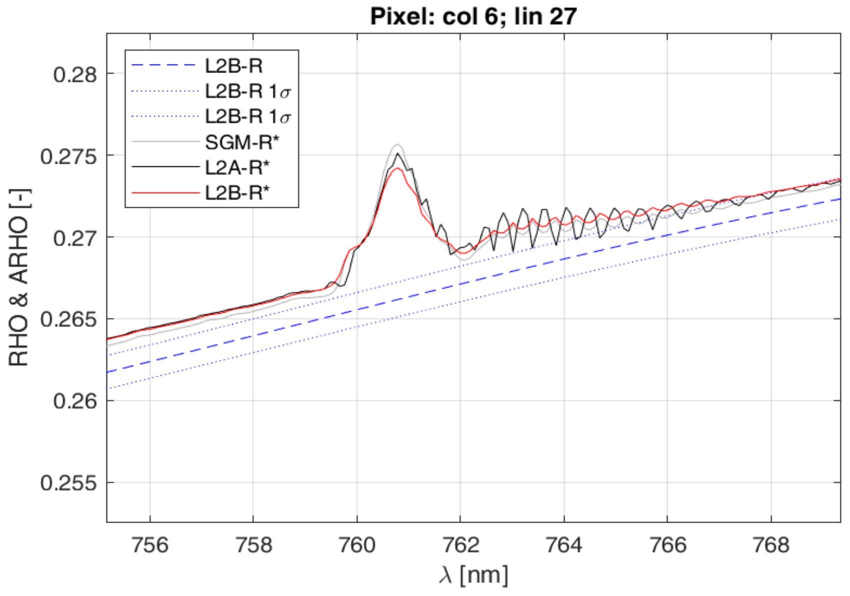
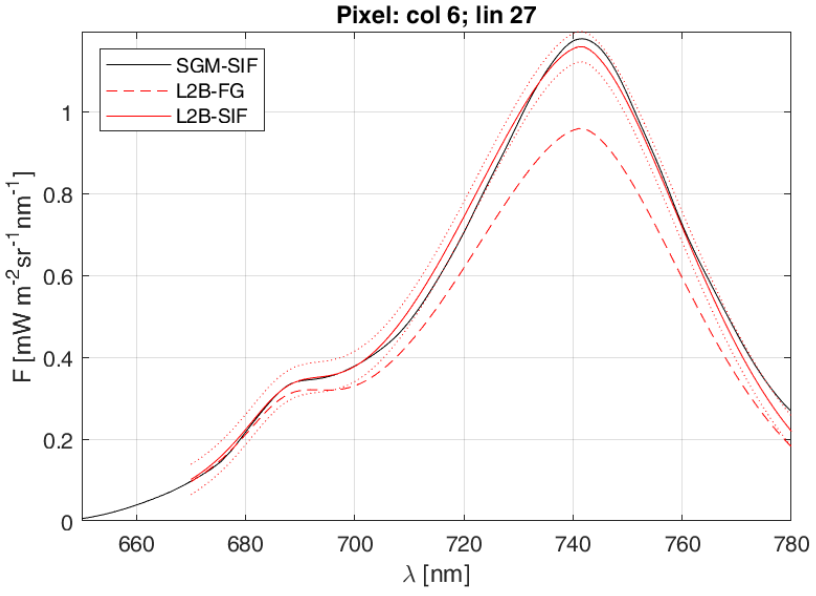
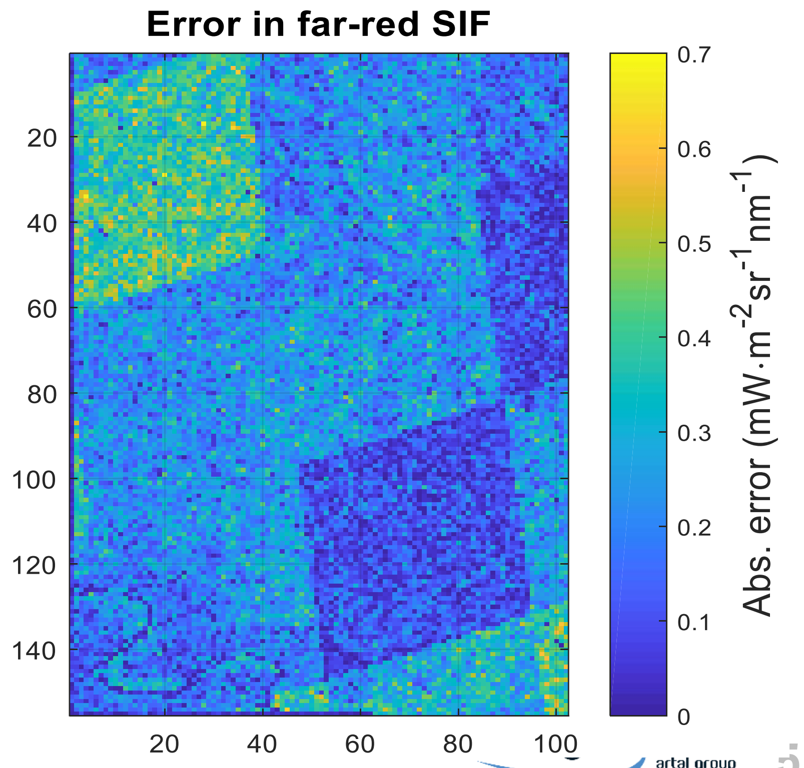
L2B module: SIF retrieval

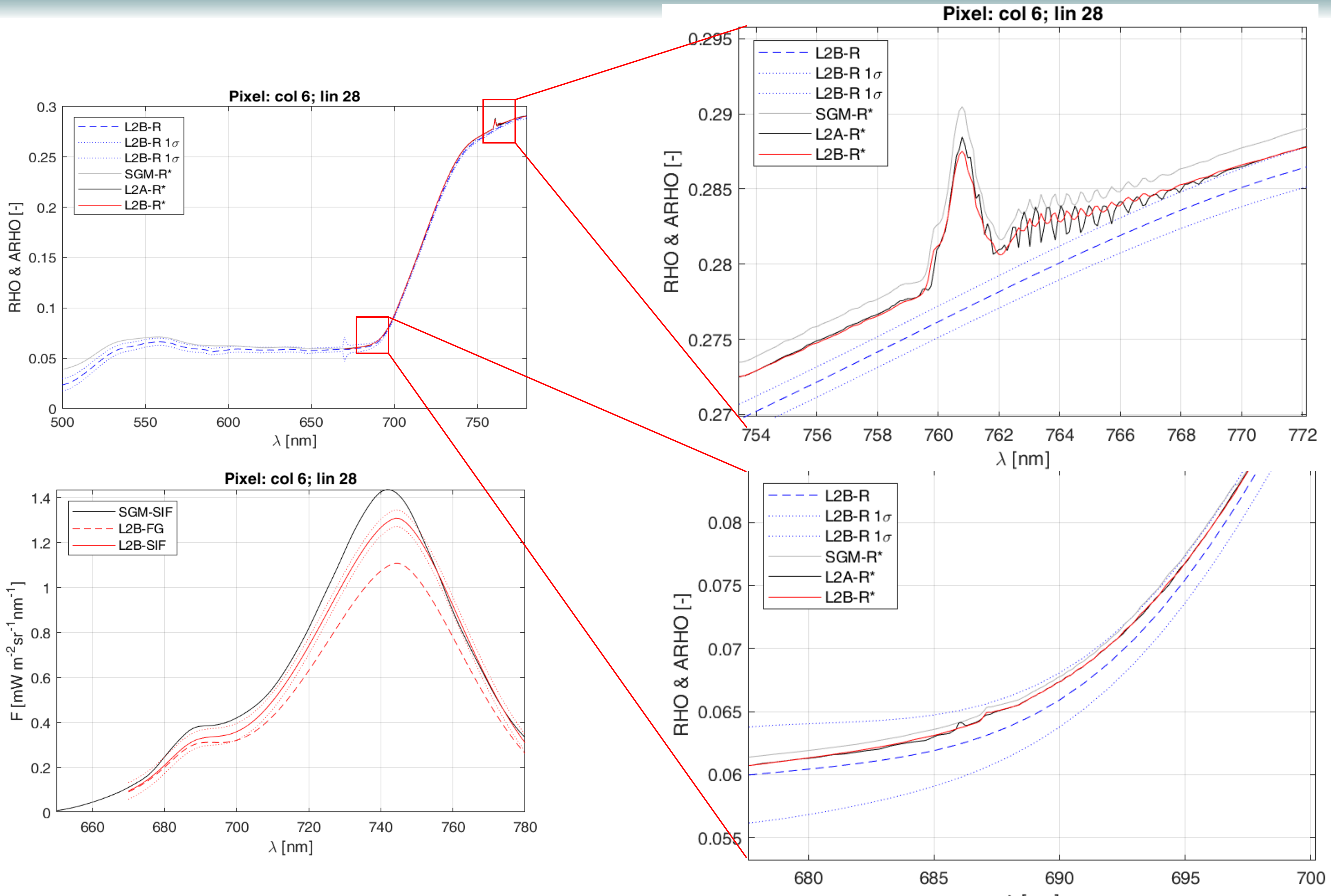
- Example of “good” retrieval
- Error map for the far-red SIF ➔ dependency of aerosol retrieval (macro-pixels)







BACK-UP



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