ITINERIS

Data inversion techniques

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  ISMAR-CNR

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Ministero dell'Università e della Ricerca

Italiadomani

Data Inversion Tecniques: Outline

- Information ‘Space’ dimensions
- Inversion Approaches

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- **Information ‘Space’ dimensions**
- Inversion Approaches

INVERSION OF THE REMOTELY SENSED SIGNAL

The measured radiation *L* can be considered as a vector in a multidimensional space:

$$L = f\left[\lambda, s_{x,y,z}, t, (\theta_s, \theta_v, \varphi), (I, Q, U, V)\right]$$

where

λ = wavelength

$s_{x,y,z}$ = *x, y, z* position in the space (e.g. in the image)

t = time

$\theta_s,\theta_v,\varphi$ = set of angles that define the observation-illumination geometry (i.e the path: radiation source-observed object-instrument)

I,Q,U,V = Polarization of the measured radiation

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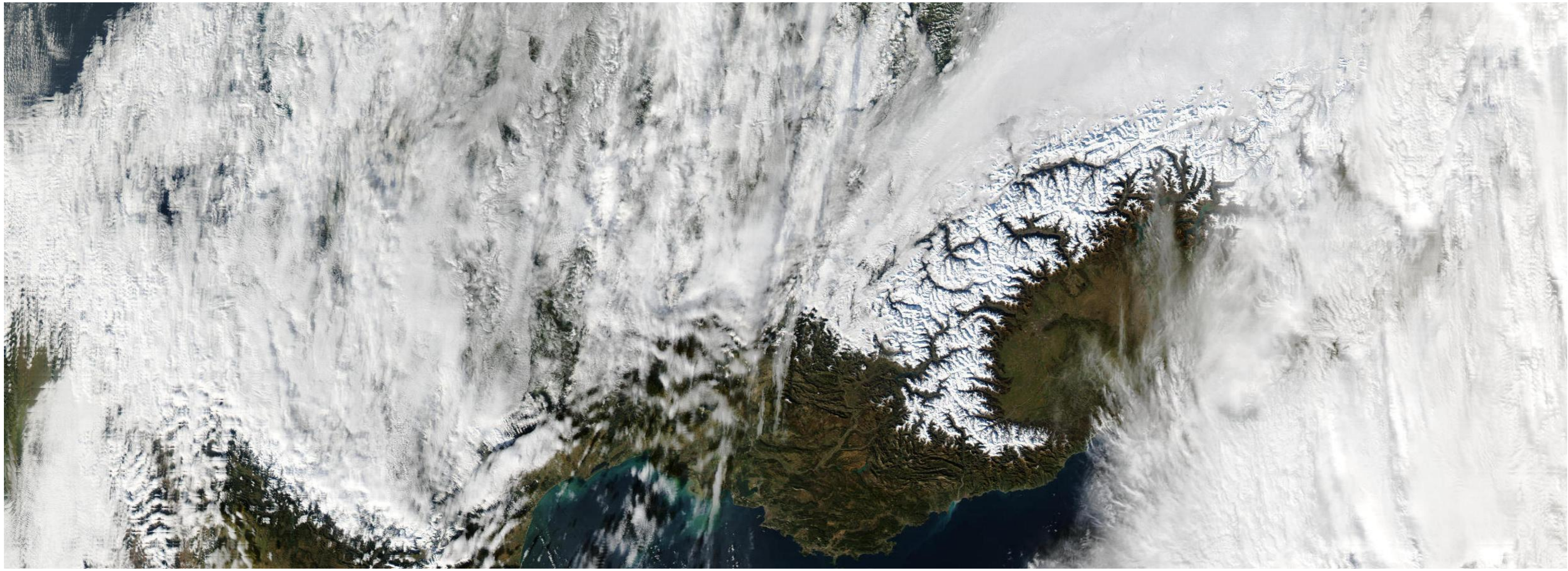
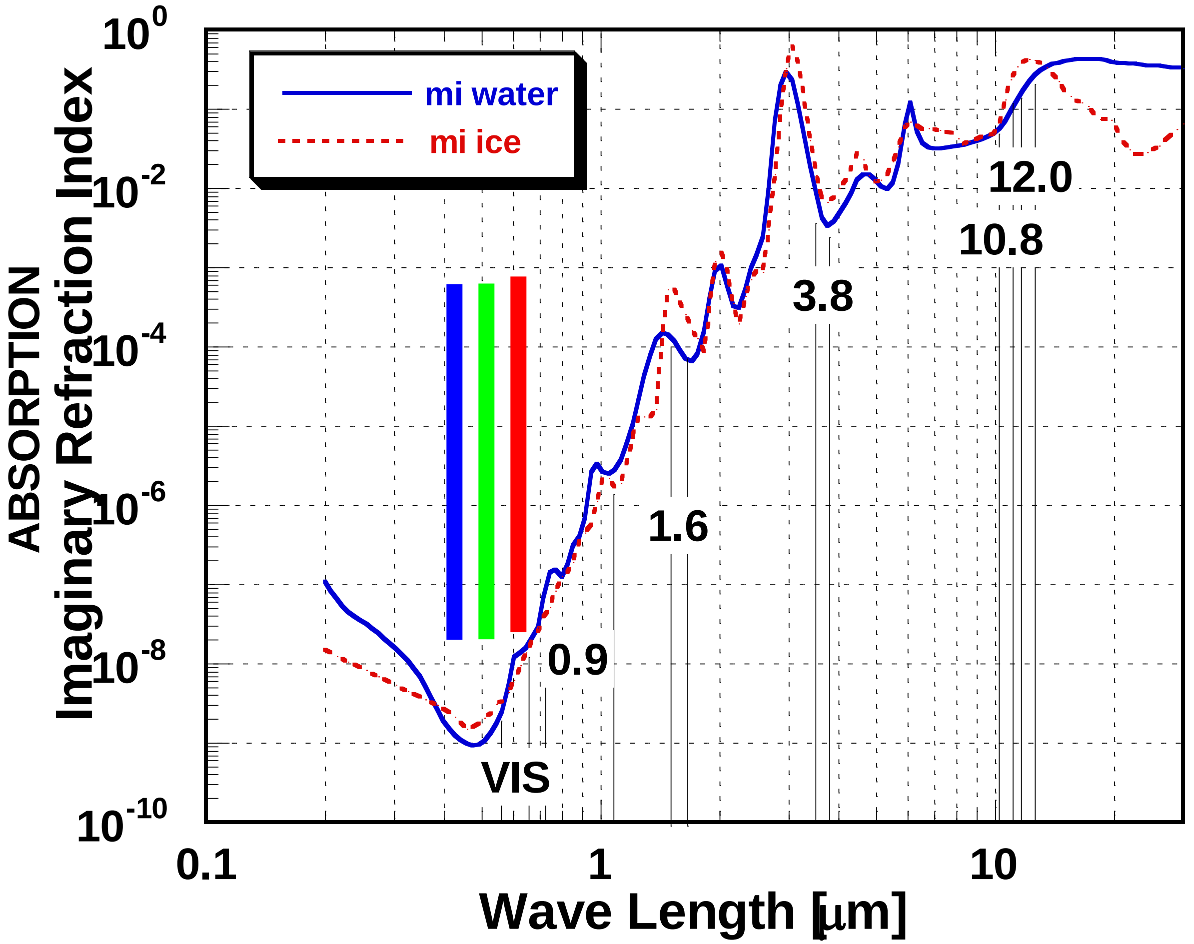
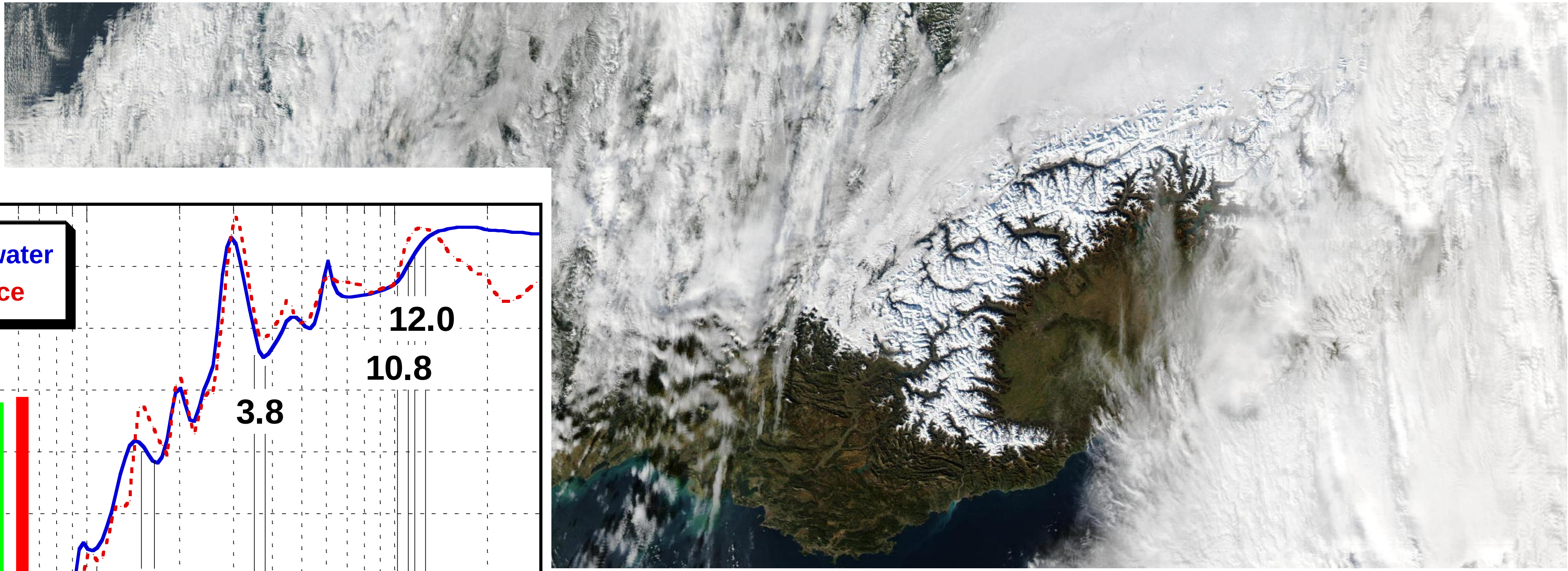
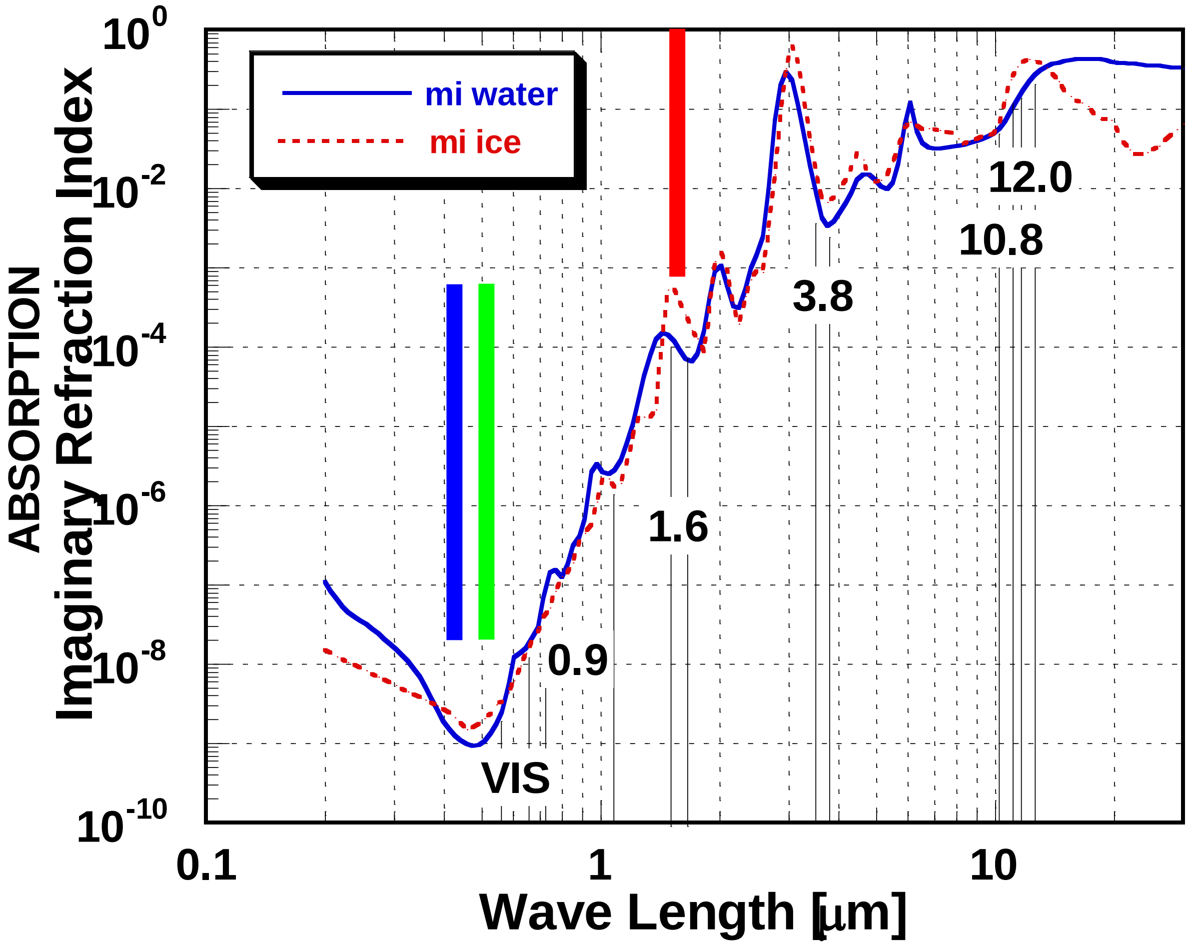



mi water
mi ice
ABSORPTION
Imaginary Refraction Index
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
12.0
10.8
3.8
1.6
0.9
VIS
0.1
1
10
Wave Length [μm]





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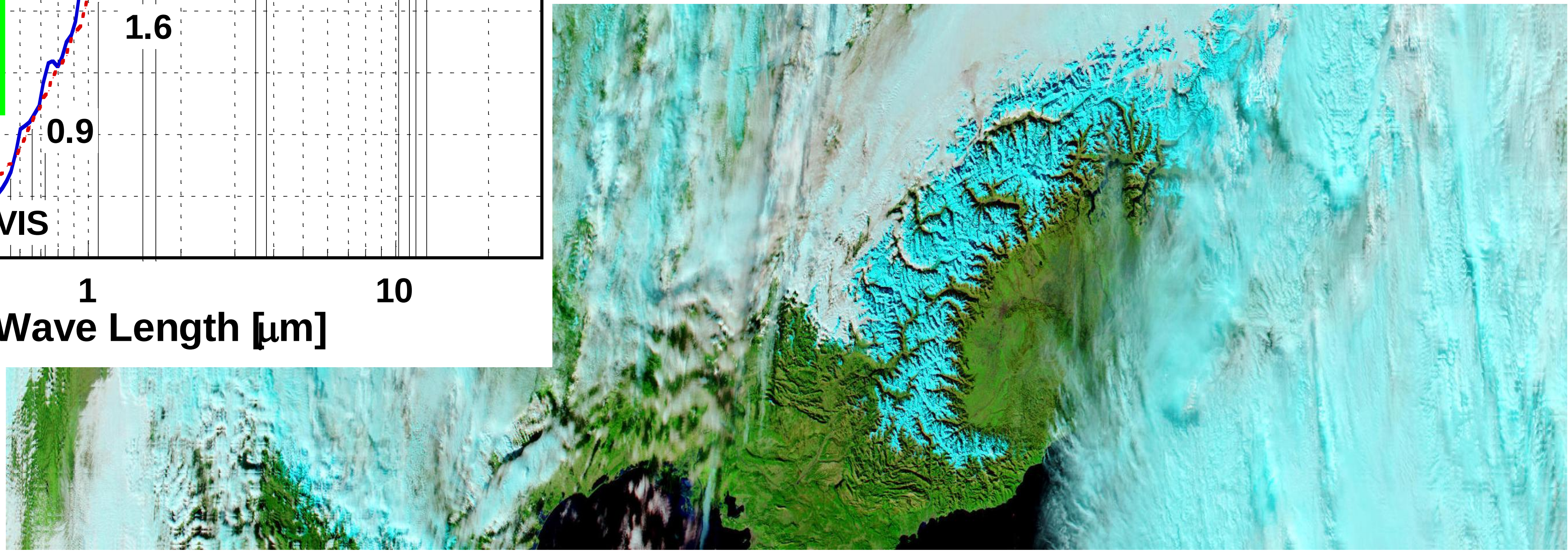

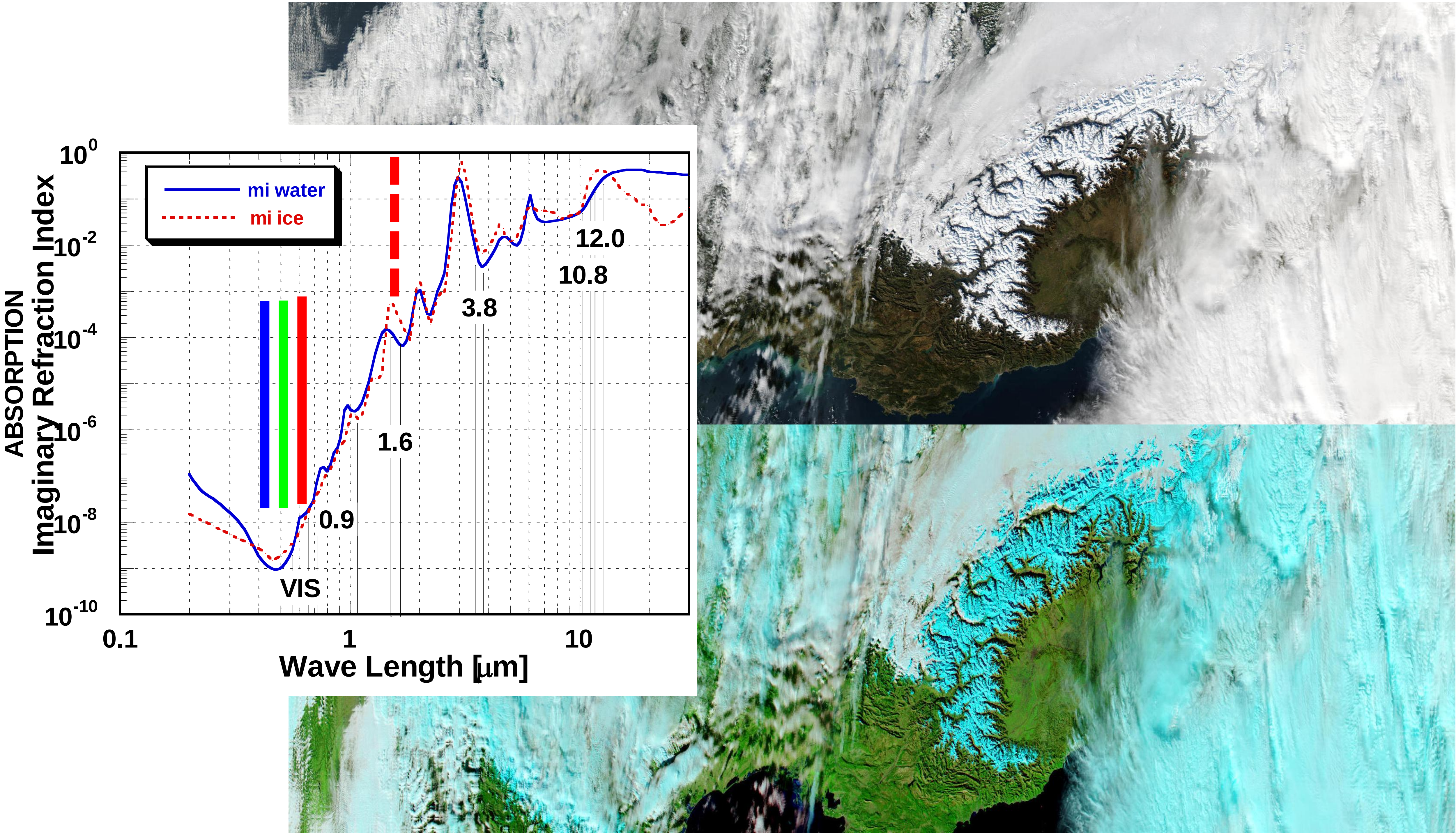

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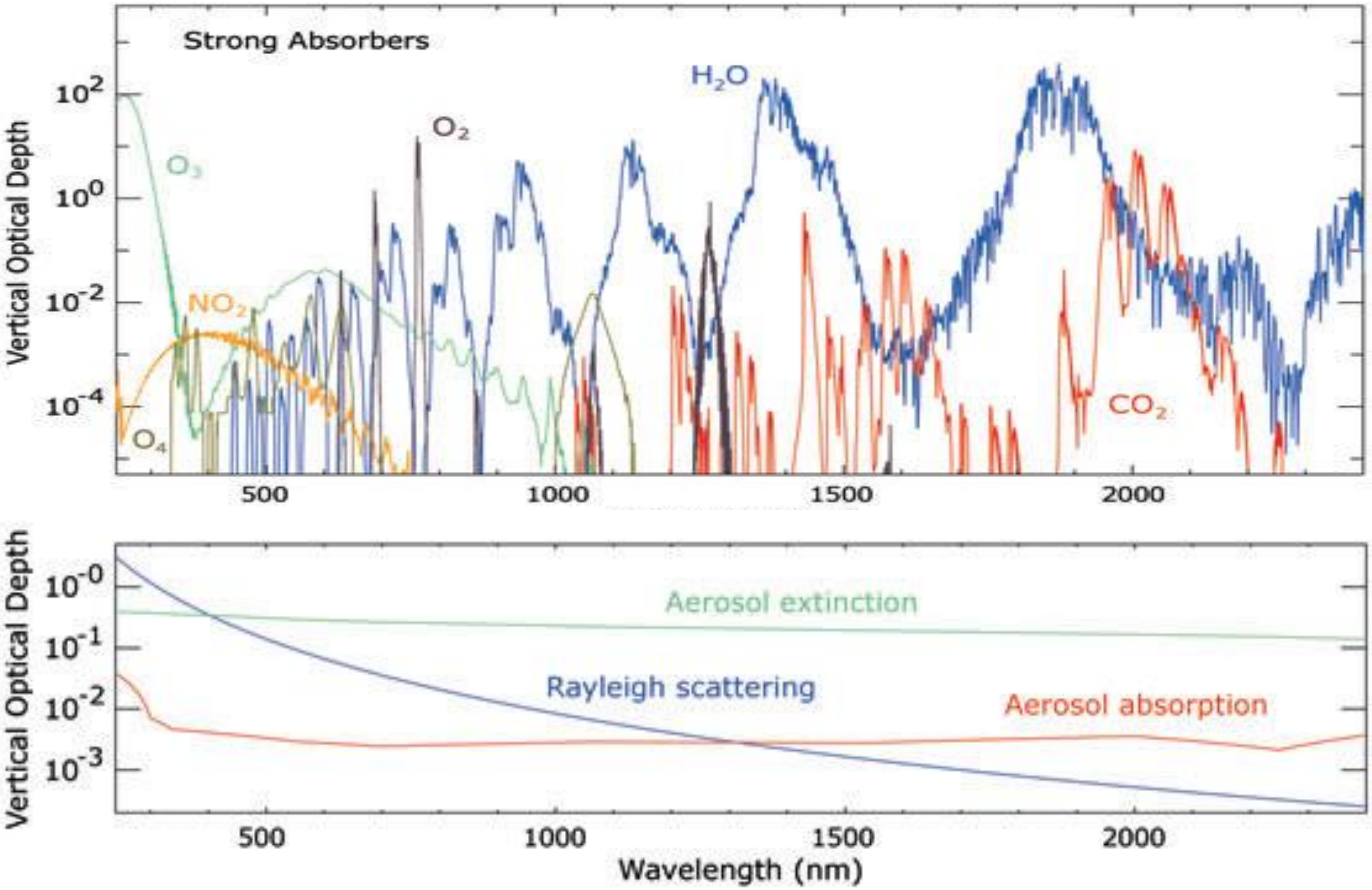

Examples of gas absorption spectra (upper panel) and scattering extinction (lower panel) in the solar (UV/VIS/SWIR) range: **scattering spectral dependence smoother than gas absorption one**

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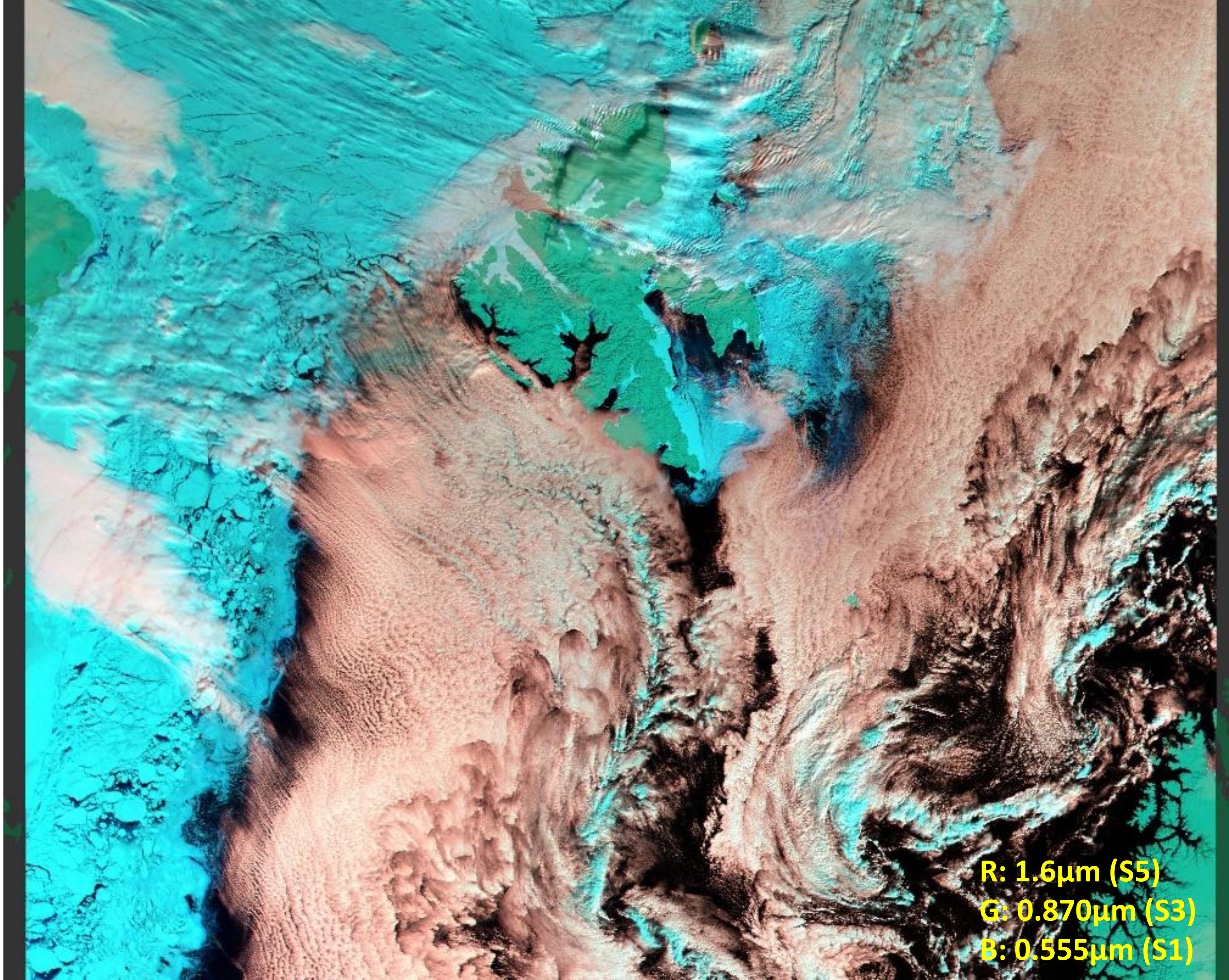
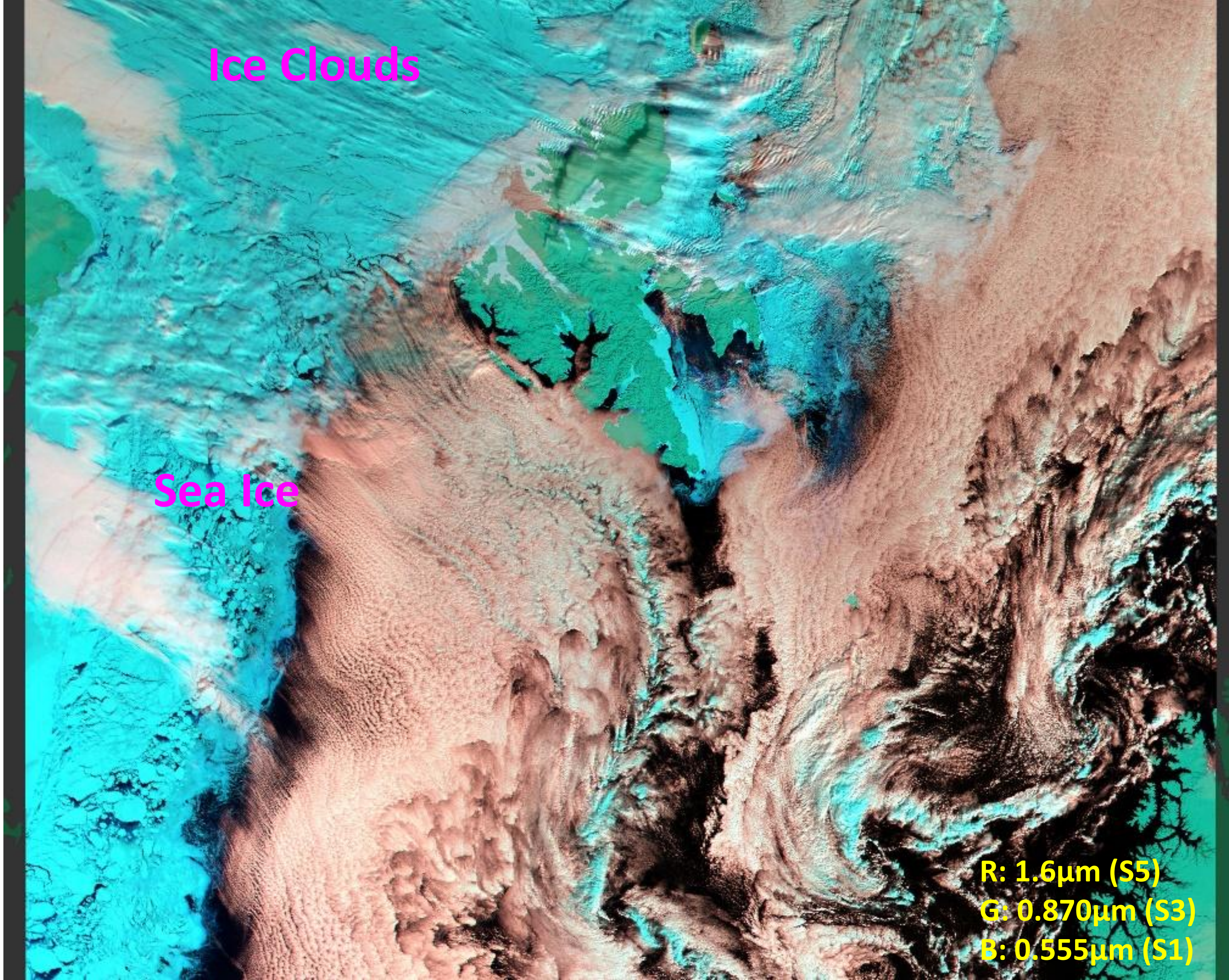
Can you distinguish Sea Ice from Ice Clouds?




Ice Clouds
Sea Ice
R: 1.6µm (S5)
G: 0.870µm (S3)
B: 0.555µm (S1)

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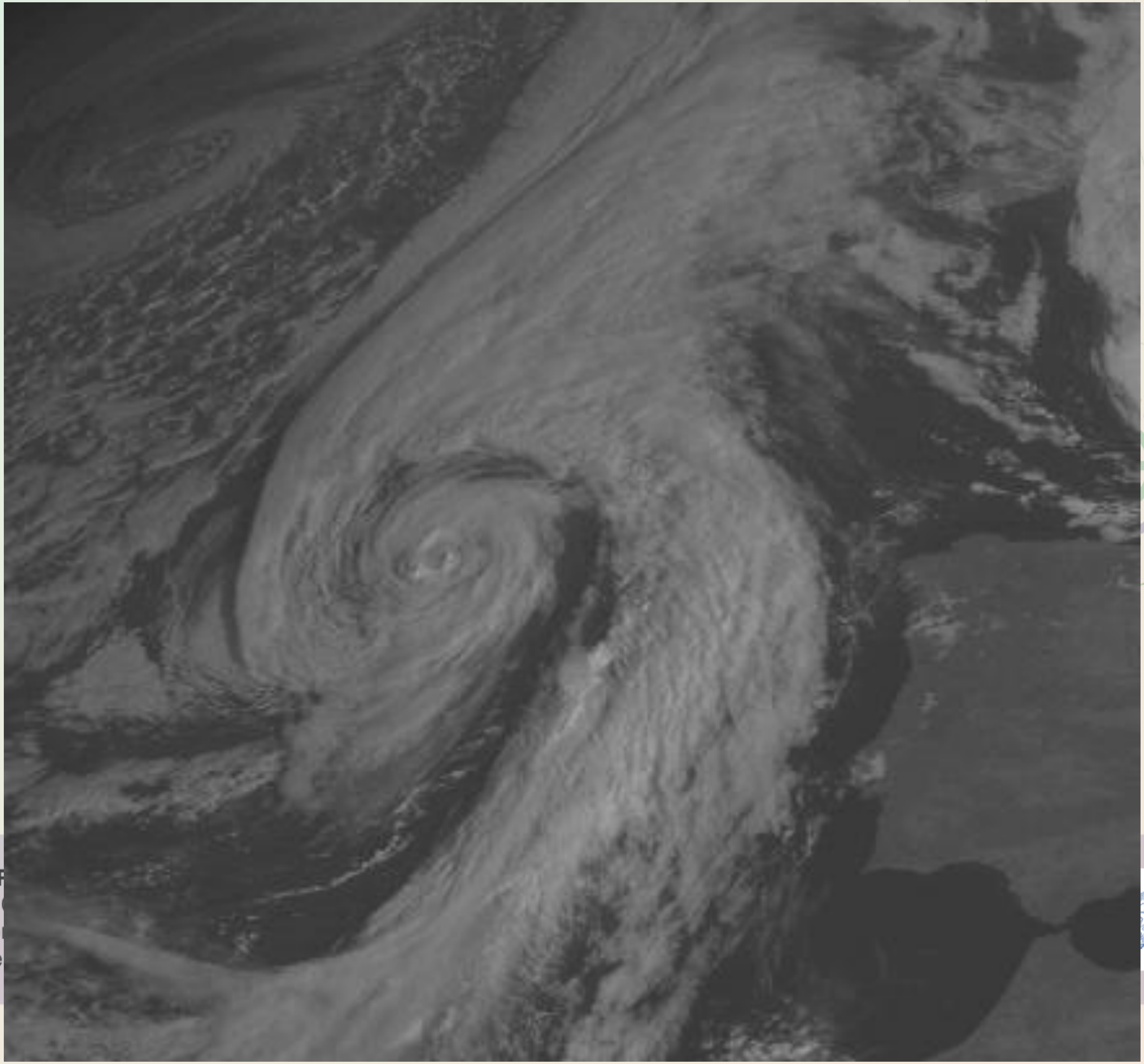

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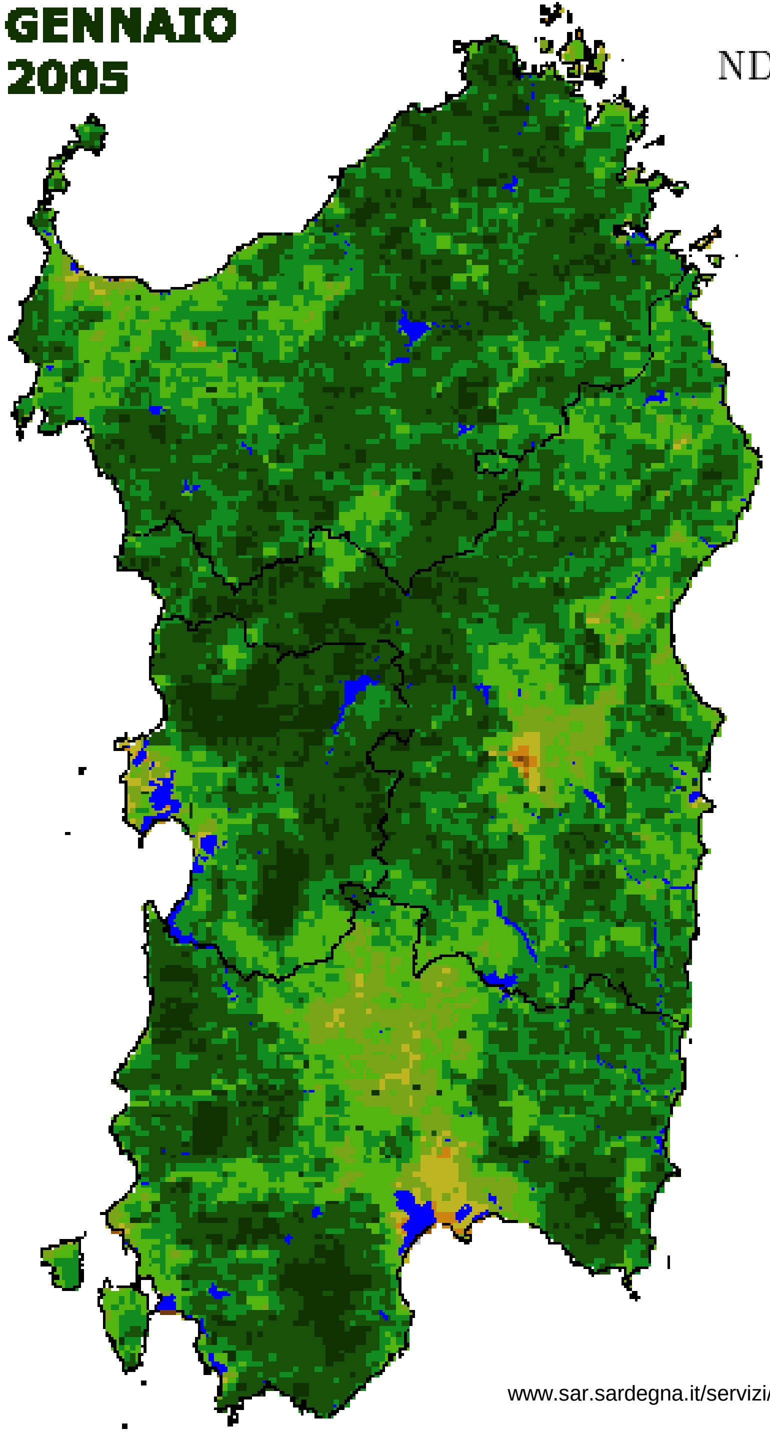
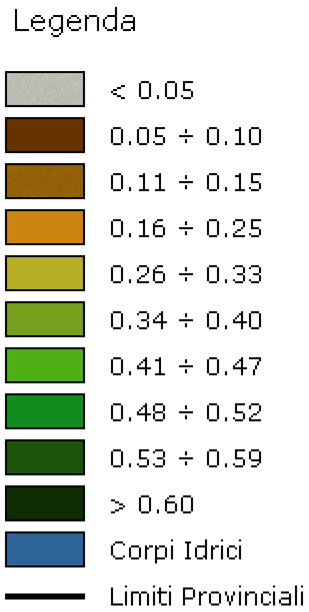
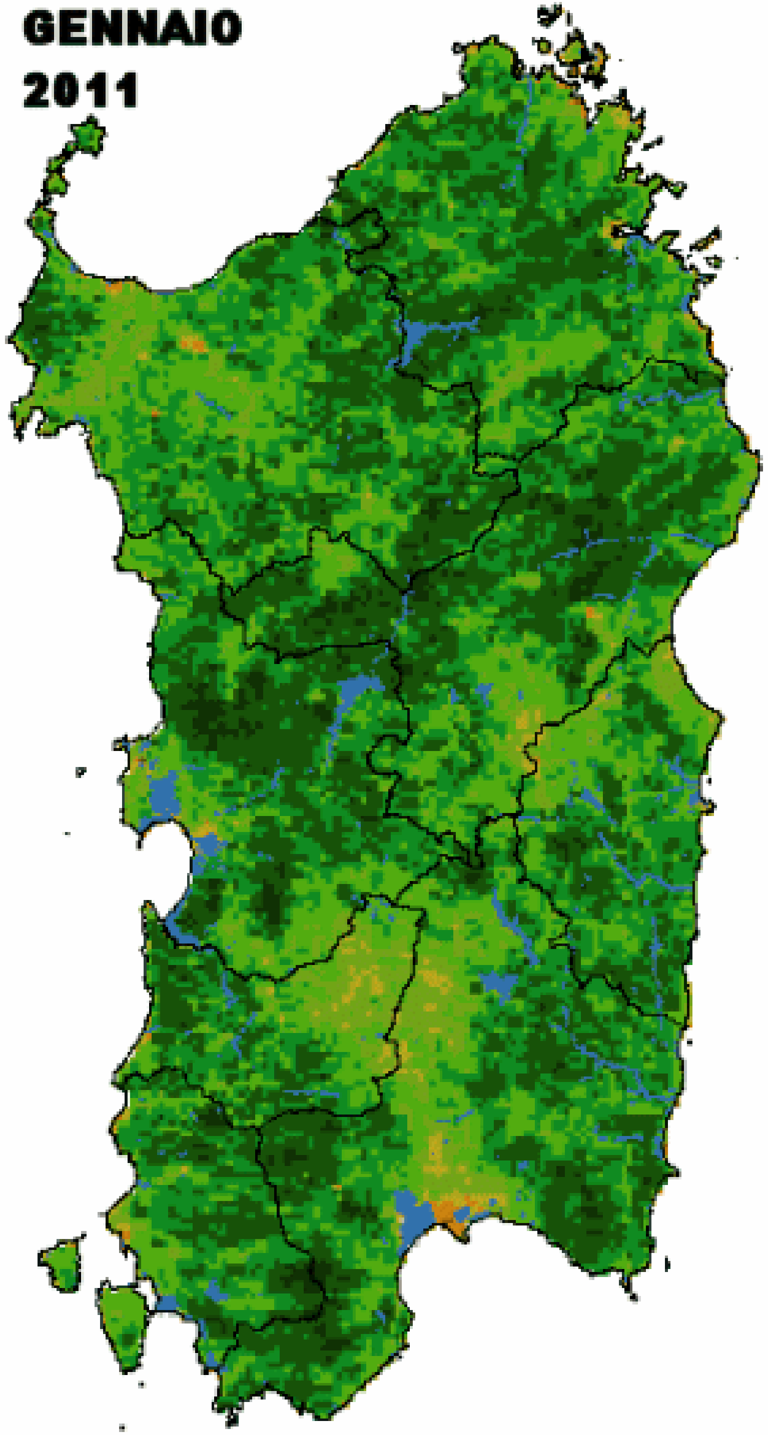
$$\text{NDVI} = \frac{(\text{NIR} - \text{VIS})}{(\text{NIR} + \text{VIS})}$$







www.sar.sardegna.it/servizi/sit/vegetazione.

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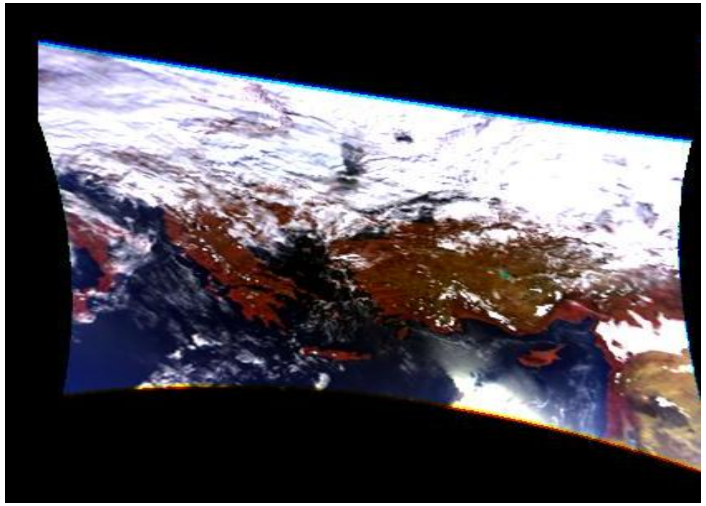
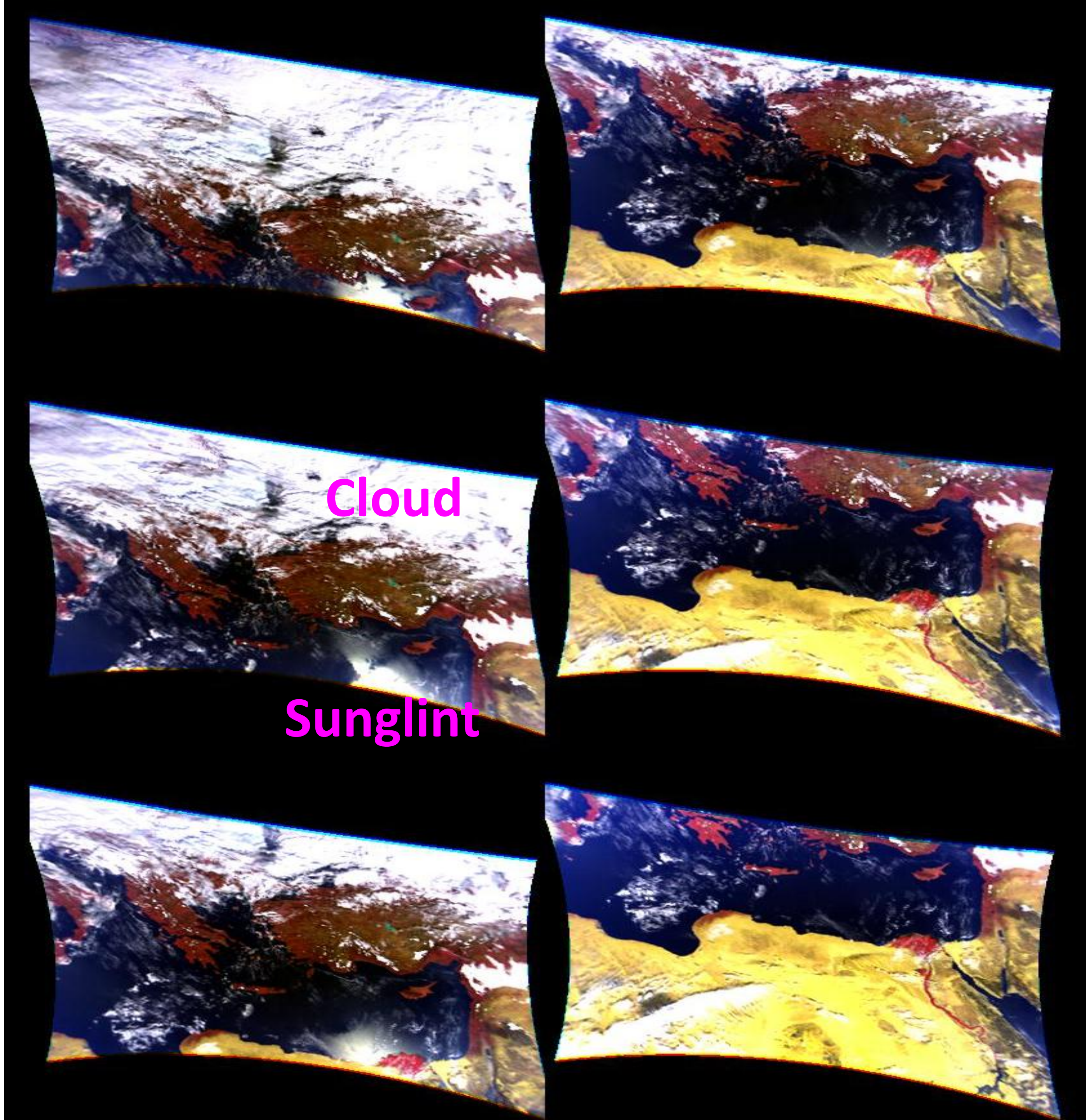
White=Cloud




Cloud
Sunglint

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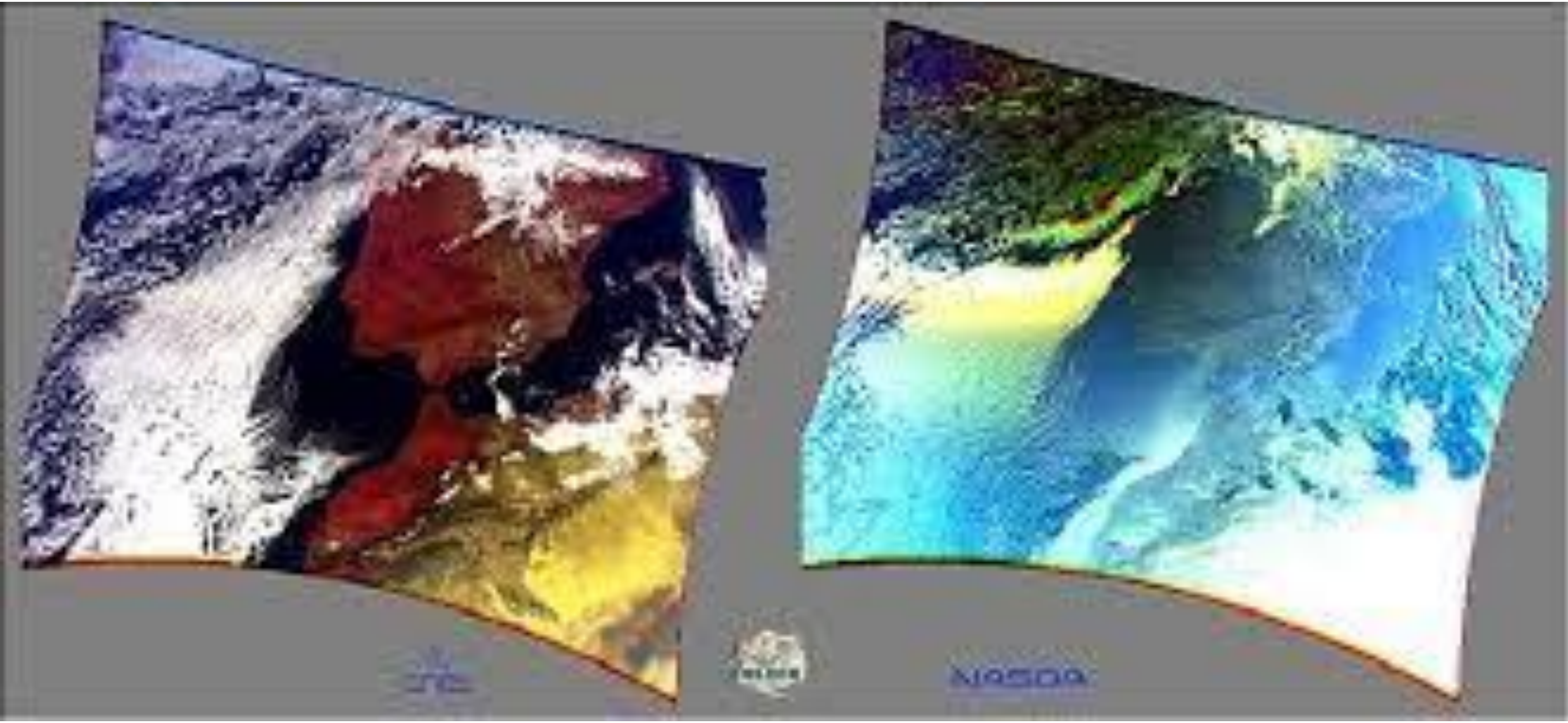
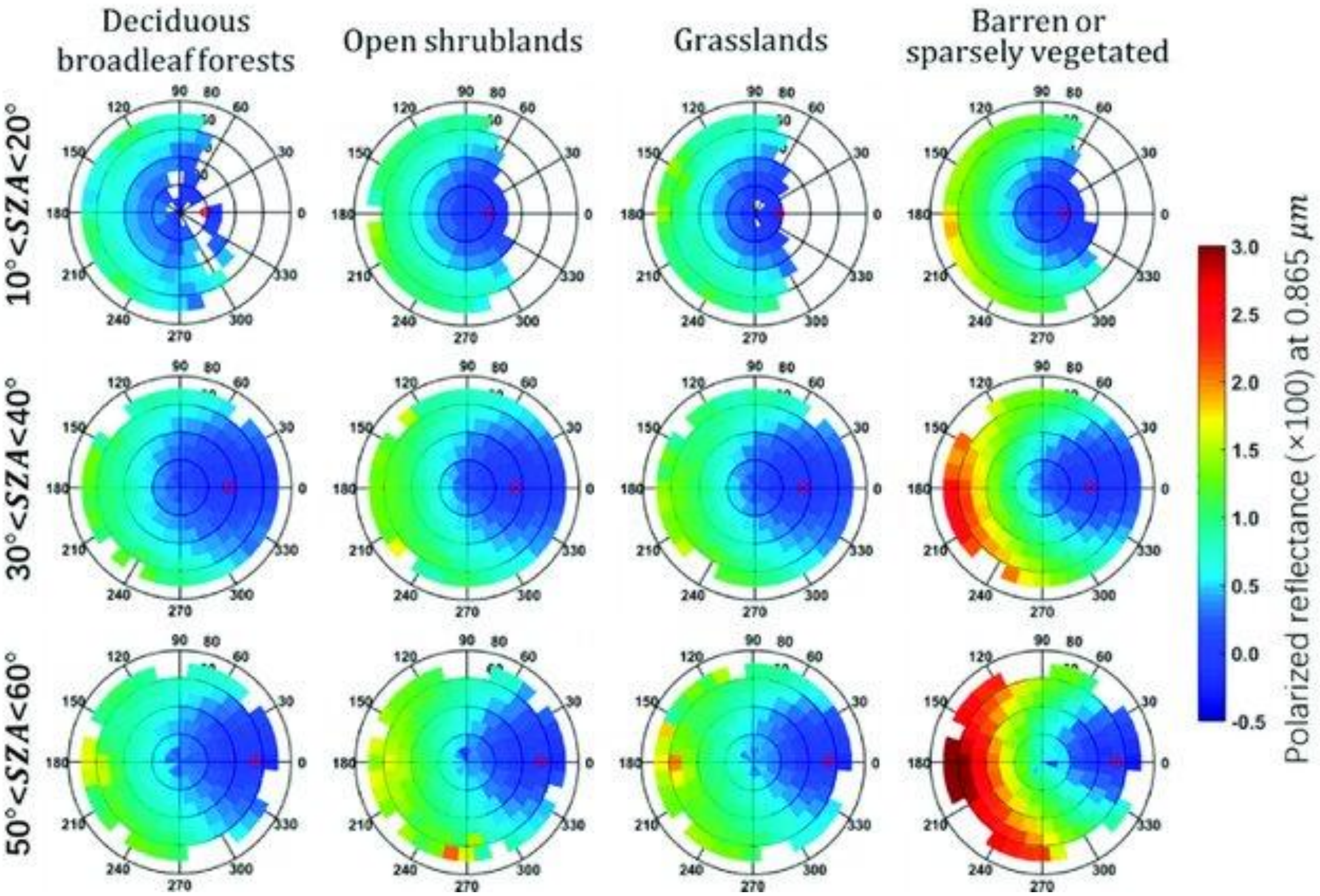
Example of POLDER RGB composites

Intensity Polarization



Example of polarized reflectance directional distribution as a function of vegetation type



https://www.mdpi.com/2072-4292/12/2/248

Data Inversion Tecniques: Outline

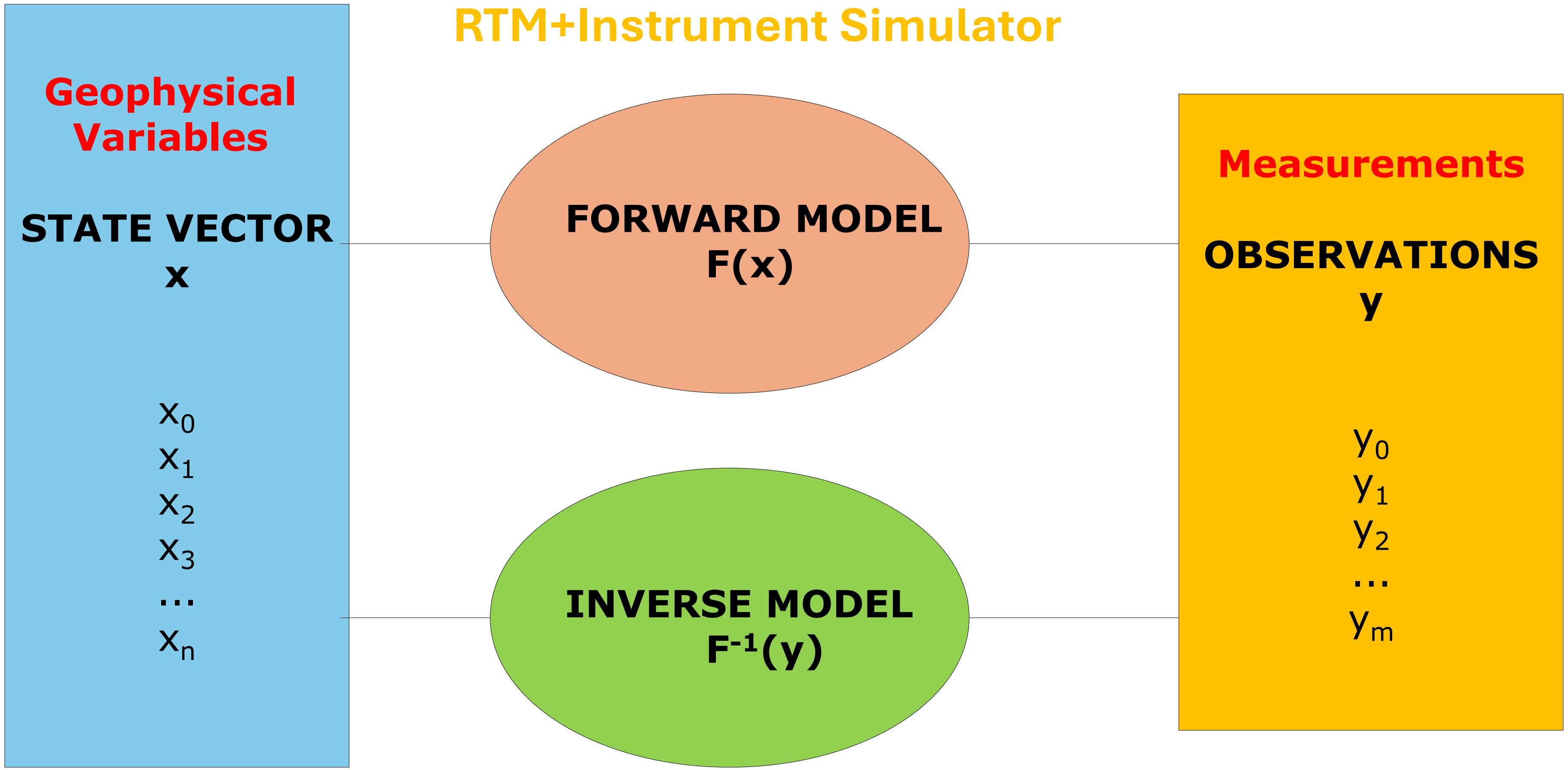
- Information ‘Space’ dimensions
- **Inversion Approaches**

Inversion Approaches: Ingredients

- **X**: *State Vector*: vector, of dimension *n*, containing all relevant variables, among which is the searched solution, from which the measurements can depend.
- **Y**: *Measurement Vector*: Vector of dimension *m*, containing all relevant measurements.
- ε_Y: *Measurement Uncertainty Vector/array*: Vector/array of dimension *m/mxm*, containing the uncertainties of all relevant measurements (when array includes also the covariance information).
- **A**: *Ancillary data*: set of *known/assumed* informations relevant to solve the problem: geographycal position, time, observation/illumination geometry, relevant geophysical variables from external data sources (e.g. climatology, forecast model).
- ***F***: Forward model. A model that given a geophysical scenario and acquisition conditions (geometry) gives the expected measurement vector: ***F(X)=Y***

Forward problem

From geophysical variables to measurements



Inverse problem

From measurement to geophysical variables

A non trivial problem

- Forward model ***F*** very often not linear and not explicitly invertible: .
- Measurements do not depend **uniquely** from the variable of interest
- *Hill posed* problems: different number of observations (known) and unknown. **Possibility of different combination of solutions that give the same result in terms of mesurements.**
- Uncertainites in the measurements and in the forward model

Inversion- Possible approaches

- **Analitycal:** not always possible: signal equation(s) should be analitically inverted for all relevant variable. Generally, need assumptions/ancillary data to handle second order effects. *An estimation of the uncertainty may be obtained from uncertainty propagation laws*.
- **Variational** – does not requires assumptions on the set of possible solutions (may limit their range). Numerically inefficient. *Very likely the method gives an estimation of the uncertainty*.
- **Regressions (including Artificial Intelligence and similar):** Computationally efficient. Need a training set. Assumptions on the functional form/structure. May have difficulties in finding a solutions for cases not included in the training data set. *Uncertainty estimation may not be straightforward*.
- **Lookup Table (LUT)** – computational efficiency dependent from the amount of LUTs, Search the solution within a set of tabulated (LUT) solutions. Set of possible solutions defined (difficulties in extrapolating). *Difficult to estimate the uncertainty of the solution*
- **Index (e.g. NDVI, AI)** – Relatively simple because defined from the measurements, but it does not represent a geophysical variable. It needs, for some application, a relationship with geophysical variables.

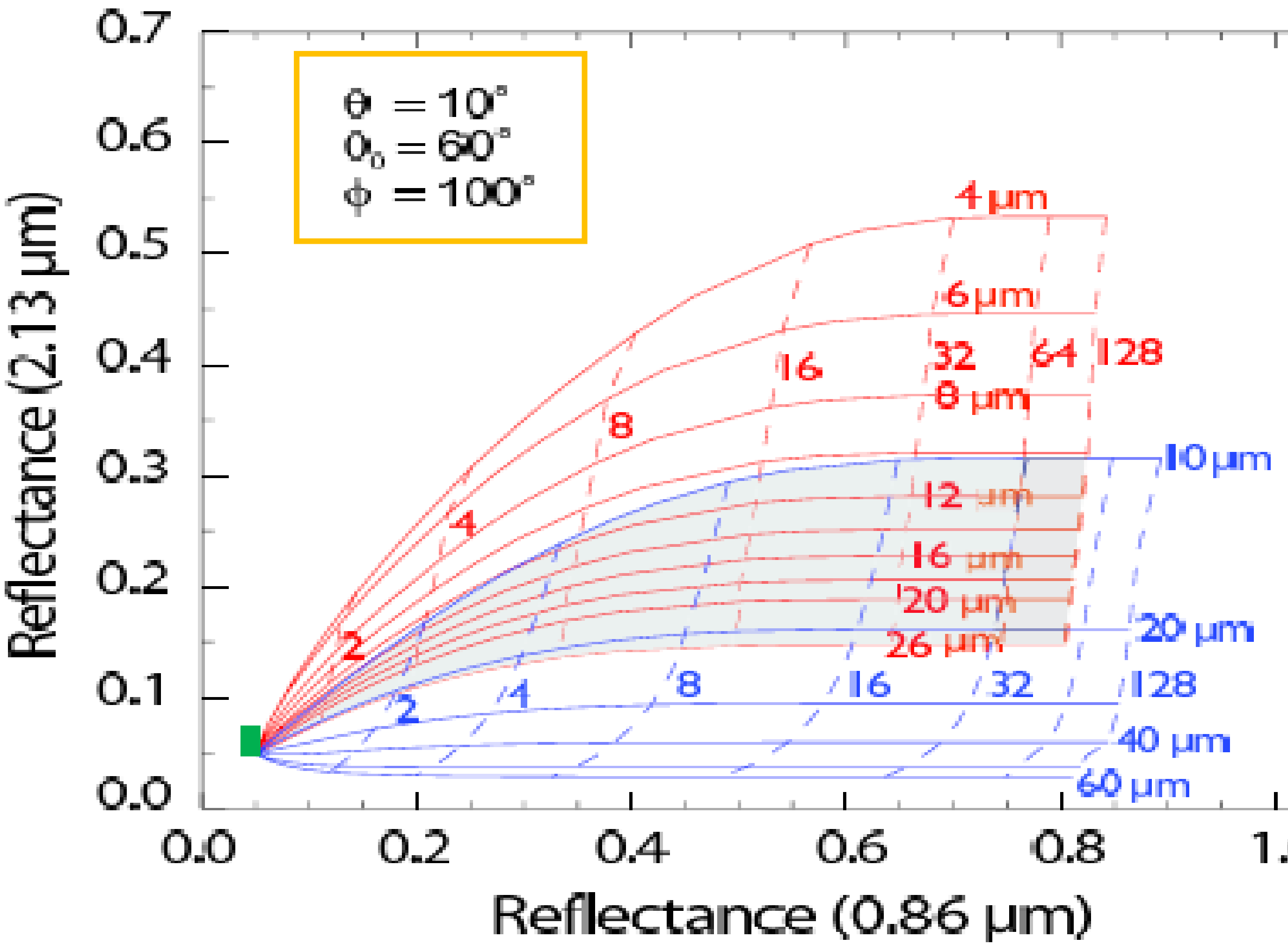
Example of LUT-based retrieval: cloud optical thickness & particle effective radius.

Inputs to select the LUT:

observation/illumination geometry, cloud top phase (liquid/ice), surface reflectance

Inputs to the LUT:

TOA reflectance @0.86 and @2.13



Variational

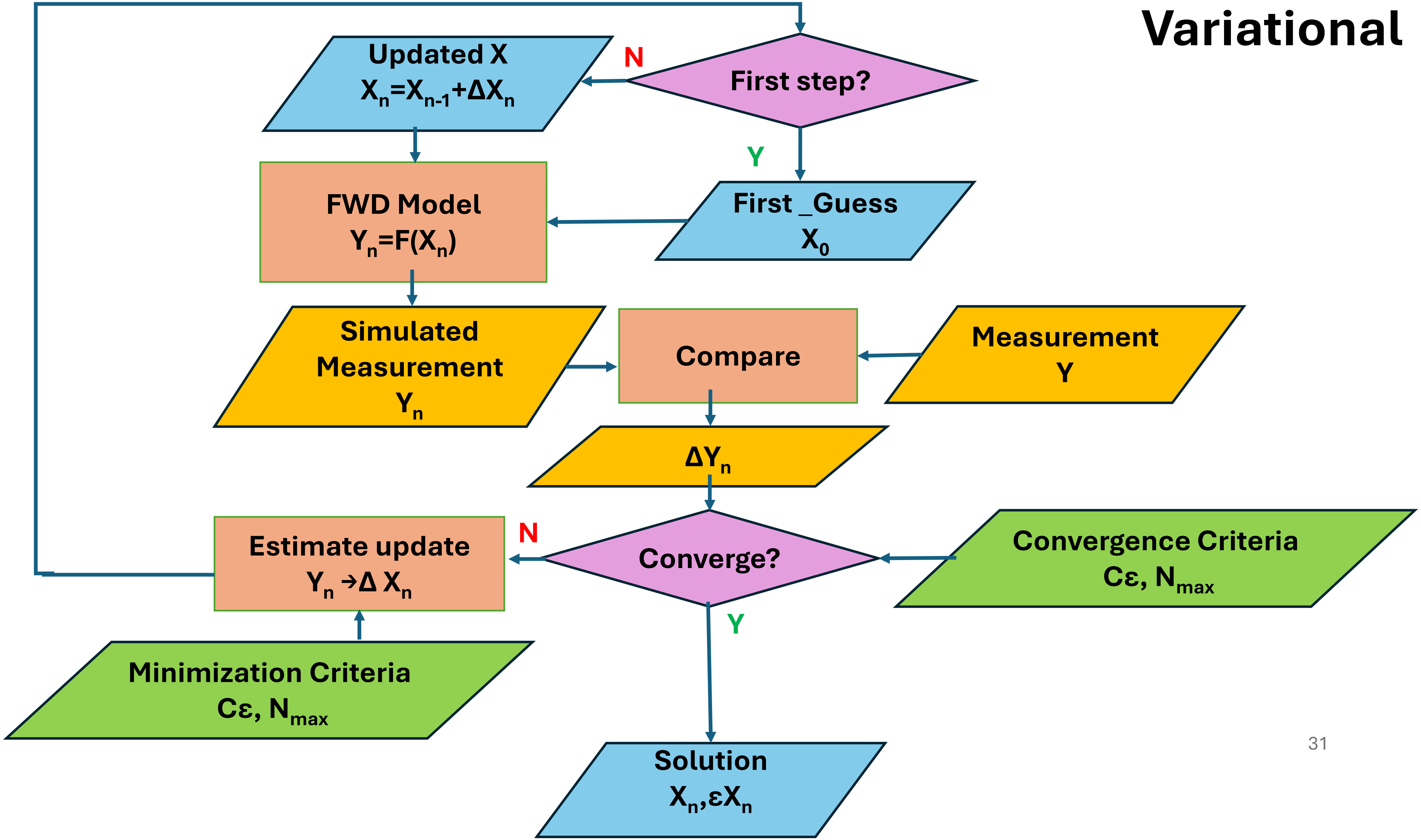
First _Guess
X_0

Measurement
Y

Convergence Criteria
$C\varepsilon$, N_{max}

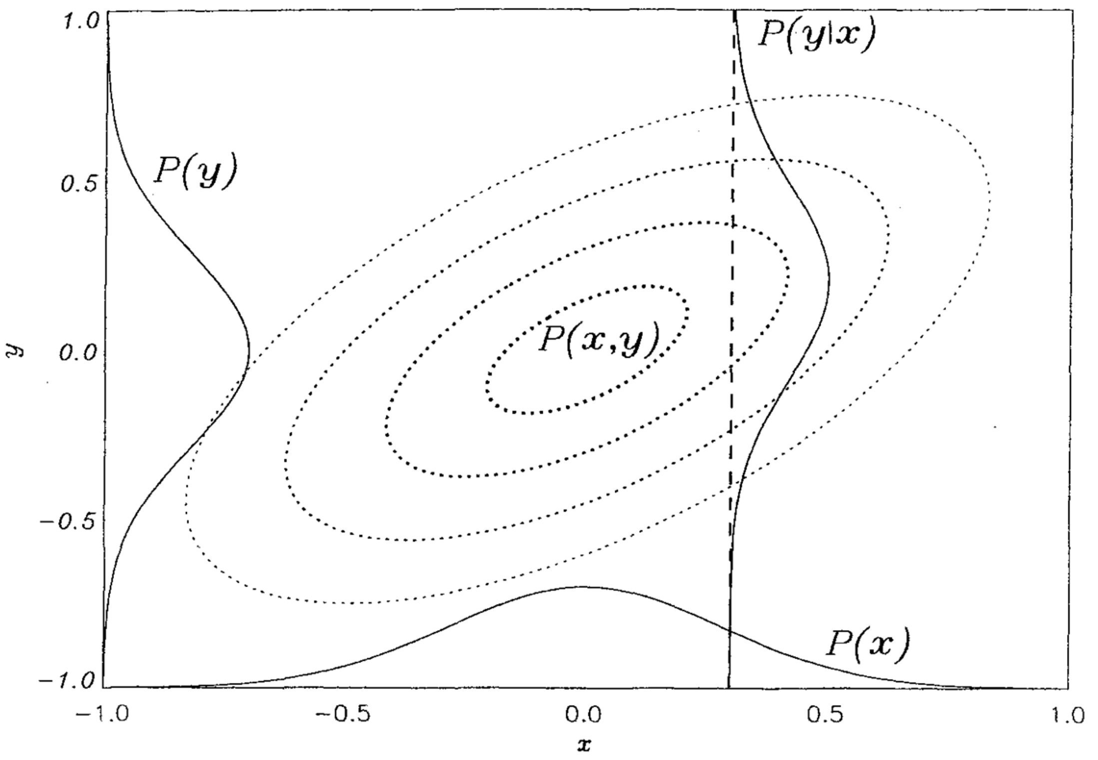
Minimization Criteria
$C\varepsilon$, N_{max}

Variational



Bayesian Interpretation

The problem is set as maximizing the probability that, given a geophysical scenario characterized by a *state vector* **x** (for ex: surface wind, temperature and water vapour amount profiles, cloud liquid water, sea surface temperature) the instrument measures the *measurement vector* **y**



Joint Probability

Conditional probability

$$P(x, y) = P(x \mid y)P(y)$$
$$P(y, x) = P(y \mid x)P(x)$$

$$P(x, y) = P(\mathrm{y}, x)$$

Bayesian Interpretation

PDF of the measurement given a certain Status (x) includes the uncertainties due to the instrument precision

Informazione a priori sullo stato. Probabilità che ci sia un dato stato indipendentemente dalla misura (es. climatologia)

BAYES THEOREM: $$P(x \mid y) = \frac{P(y \mid x)P(x)}{P(y)}$$

Normalization factor
(a priori PDF of the measurement)
P(y)=1

- Possiamo assumere una incertezza sperimentale con distribuzione gaussiana

$$P(y \mid x) = A\exp\left(-\frac{\left(y - F(x)\right)^2}{2\sigma^2}\right)$$

- Per il caso multidimensionale abbiamo invece

$$P(y \mid x) = A\exp\left(-\frac{1}{2}\left(y - F(x)\right)^T C_\epsilon^{-1}\left(y - F(x)\right)\right)$$

- Ragionevole assumere una distribuzione gaussiana anche per l'informazione a priori su x

$$P(x) = A\exp\left(-\frac{1}{2}(x - x_a)^T C_a^{-1}(x - x_a)\right)$$

- Otteniamo la seguente probabilità a posteriori

$$P(x \mid y) = A \exp\left(-\frac{1}{2}\left(\big(y - F(x)\big)^T C_\epsilon^{-1}\big(y - F(x)\big) + (x - x_a)^T C_a^{-1}(x - x_a)\right)\right)$$

- Noi vogliamo una soluzione, non l'intera PDF. Dobbiamo scegliere cosa ottimizzare, es: il valore più probabile, minimizzare l'incertezza, massimizzare la risoluzione

- MAP (Maximum A posteriori Probability)

$$x = maxP(x \mid y)$$

- Il massimo può essere calcolato in veri modi:
- - **Analiticamente** (se possibile)
- - **Ottimizzazione numerica** for ex.: Gauss-Newton, Gradient coniugato
- - **Monte Carlo**

- Nel caso **non sia presente una conoscenza a priori** di x, la soluzione MAP è la stessa della ML (Maximum likelihood)

$$P(y \mid x) = A\exp\left(-\frac{1}{2}\big(y - F(x)\big)^T C_\epsilon^{-1}\big(y - F(x)\big)\right)$$

- LSM (Least square method)

Cost function ——— $\Psi(x) = \frac{1}{2}\big(y - F(x)\big)^T C_\epsilon^{-1}\big(y - F(x)\big) = min$

$$\nabla\Psi(x) = \frac{\partial\Psi(x)}{\partial x_i} = 0$$

• Maximum likelihood and LSM

For a **linear*** system for which **f(x)=Kx** we can write the Cost Function $\Psi(x)$ as:

$$\Psi(x) = \frac{1}{2}(y - Kx)^T C^{-1}(y - Kx)$$

Minimising $\Psi(x)$ gives:

$$\nabla\Psi(x) = K^T C^{-1} K x - K^T C^{-1} y = 0$$

$$\downarrow$$

$$K^T C^{-1} K x = K^T C^{-1} y$$

Solving in x:

$$x = (K^T C^{-1} K)^{-1} K^T C^{-1} y$$

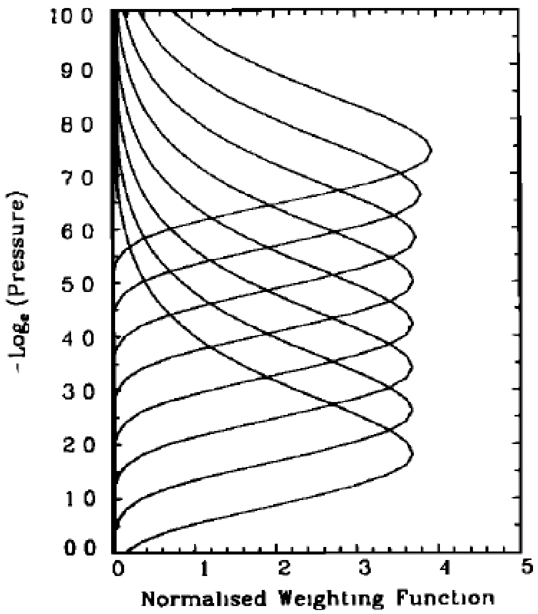
Valid if $det(K^T C^{-1} K) \neq 0$ and uncertainties have a gaussian distribution

- * It is possible to linearize a non linear operator f(x) in a given interval

Regolarizzazione

- Nel caso di problemi mal posti non posso invertire K

$$y = Kx \qquad \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} = \begin{pmatrix} k_{11} & k_{12} & \cdots & k_{1n} \\ k_{21} & k_{22} & \cdots & k_{2n} \\ k_{31} & k_{32} & \cdots & k_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ k_{m1} & k_{m2} & \cdots & k_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}$$



A set of idealized weighting functions normalized to unit area.

$$I(\nu) = \int_0^\infty B(\nu, z) \frac{dT}{dz}(\nu, z)\, dz$$

$$I_i = I(\nu_i) = \int_0^\infty B(\bar{\nu}, z) K_i(z)\, dz \qquad i = 1 \cdots M$$

$$B(\bar{\nu}, z) = \sum_{j=1}^{M} b_j W_j(z)$$

$$I_i = \sum_{j=1}^{M} b_j \int_0^\infty W_j(z) K_i(z)\, dz = \sum_1^M A_{ij} b_j$$

agupubs.onlinelibrary.wiley.com/doi/10.1029/RG014i004p00609

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$$p = rank(K)$$
$$m = dim(y)$$
$$n = dim(x)$$

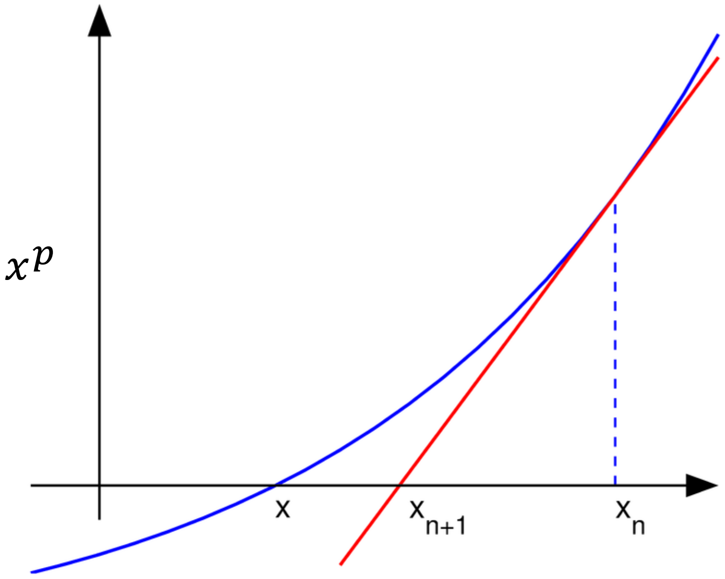
- **p=m=n** Well posed
- **p<m=n** Under and overconstrained
- **p=m<n** Underconstrained
- **p<m<n** Under and overconstrained
- **p=n<m** Overconstrained
- **p<n<m** Under and overconstrained

- In caso di funzioni non lineari possiamo risolvere l'equazione **y=f(x)** attraverso iterazioni basate su approssimazioni lineari e partendo da un valore iniziale
- Metodo di Newton

$$x^{p+1} = x^p - \Delta x^p$$

$$K_p \Delta x^p \approx f(x^p) - y \qquad K_p = \nabla f(x)\,|_{x^p}$$

$$x^{p+1} = x^p - K_p^{-1}(f(x^p) - y)$$



- Vogliamo risolvere $$\nabla\Psi(x) = 0$$
- Sostituiamo $f(x^p) = \nabla\Psi(x^p)$ e $y = 0$
- $$x^{p+1} = x^p - \Delta x^p$$

Normal system

$$A_p \Delta x^p \approx \nabla\Psi(x^p) \qquad A_p = \nabla\big(\nabla\Psi(x)\big)\,|_{x^p} \approx K^T C^{-1} K$$

$$x^{p+1} = x^p - \left(K_p^T C^{-1} K_p\right)^{-1} \nabla\Psi(x^p) =$$

$$= x^p - \left(K_p^T C^{-1} K_p\right)^{-1} K^T C^{-1} (f(x^p) - y)$$

Numerical method

Numerical inversion method: Newton-Gauss iteration algorithm (Rodgers, 2000)

$$x^{(n+1)} = x^n - \left(S_a^{-1} + J_n^T S_\epsilon^{-1} J_n\right)^{-1} \left(J_n^T S_\epsilon^{-1} \left(F(x^n) - y\right) + S_a^{-1}(x_n - x_a)\right)$$

$\mathbf{x}_a$ First guess vector

$\mathbf{y}$ Measurement vector

$\mathbf{F}(\mathbf{x}_n)$ Radiances vector at TOA generated by $\mathbf{x}_n$

$\mathbf{J}$ Jacobi matrix, $\mathbf{J}^T$ Transposed Jacobi matrix

$\mathbf{S}_\epsilon$ Instrumental error Covariance matrix

$\mathbf{S}_a$ First guess Covariance matrix

Example of numerical experiments

Spectra of % difference **first guess,** **final solution**

Simulated Spectrum measurement vector

First guess 1 2 3 4

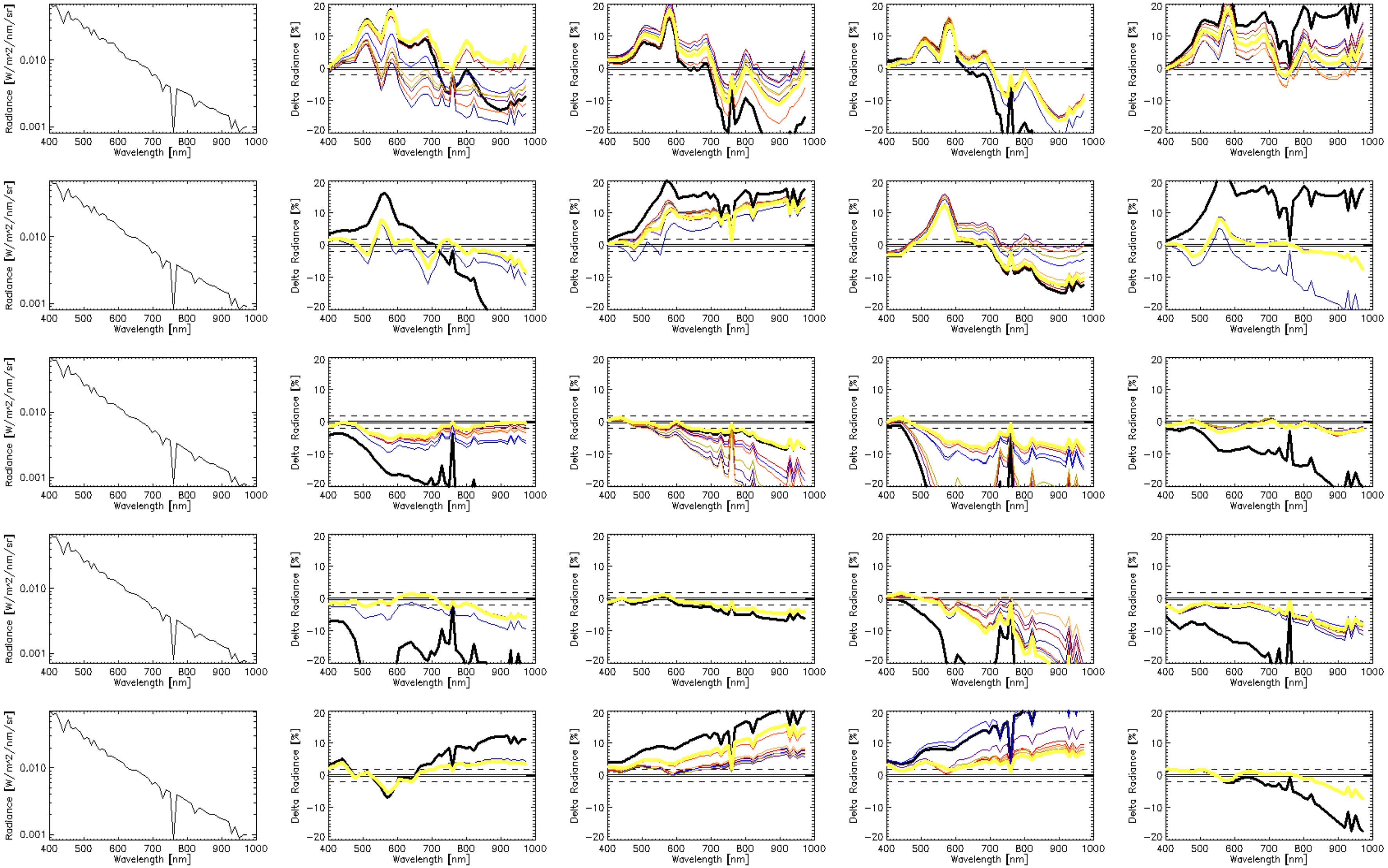
Exp.1

Exp.2

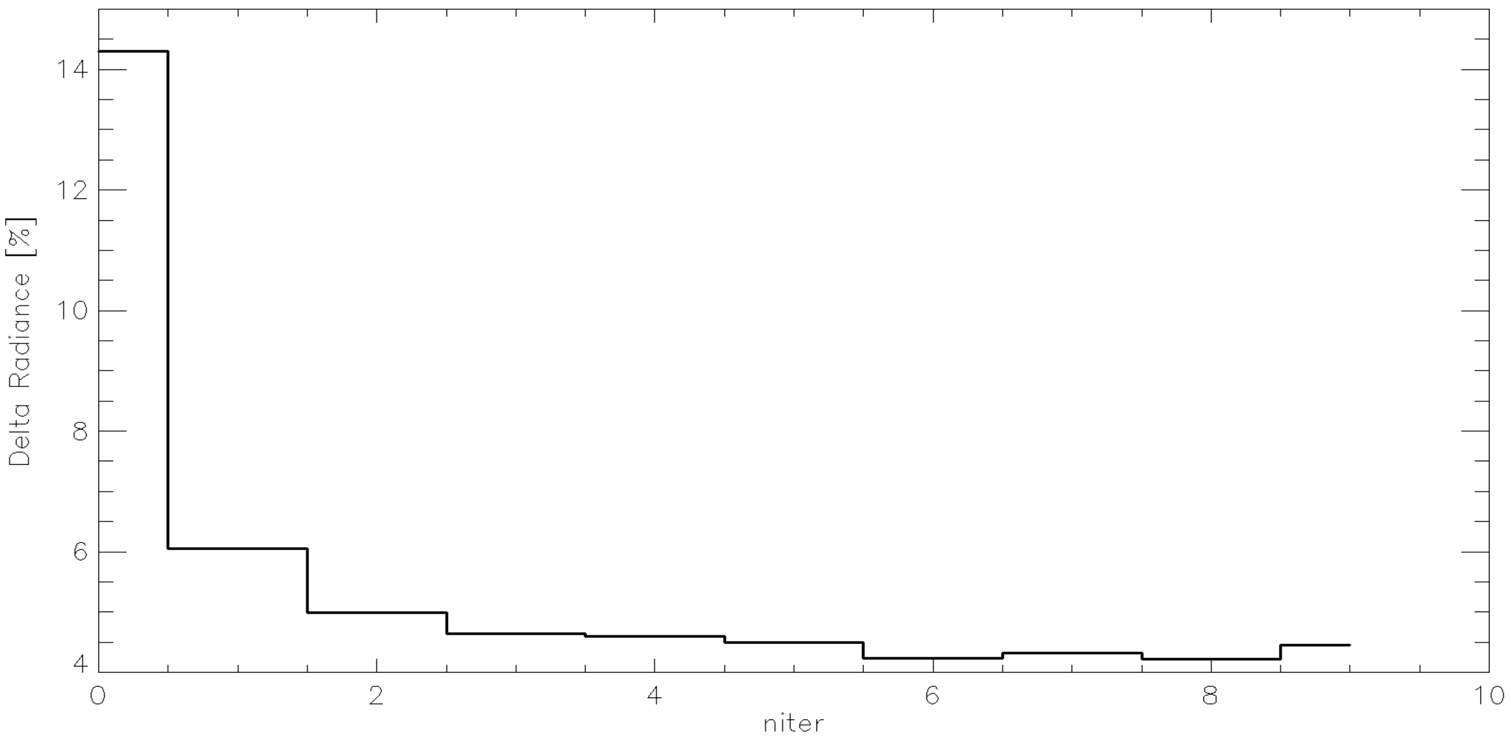
Exp.3

Exp.4

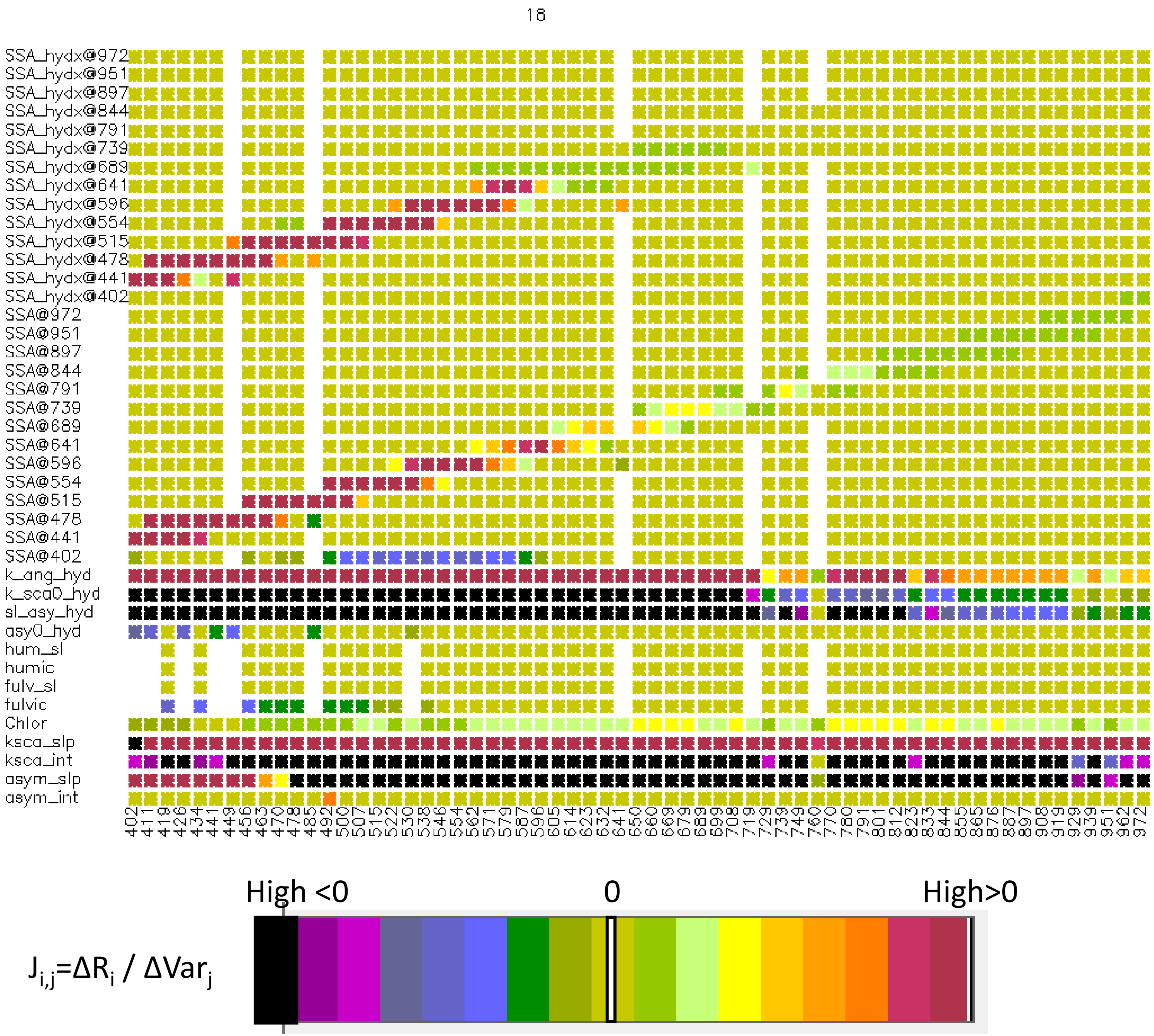
Exp.5



Average Δ Radiance [%] as a function of the iteration step

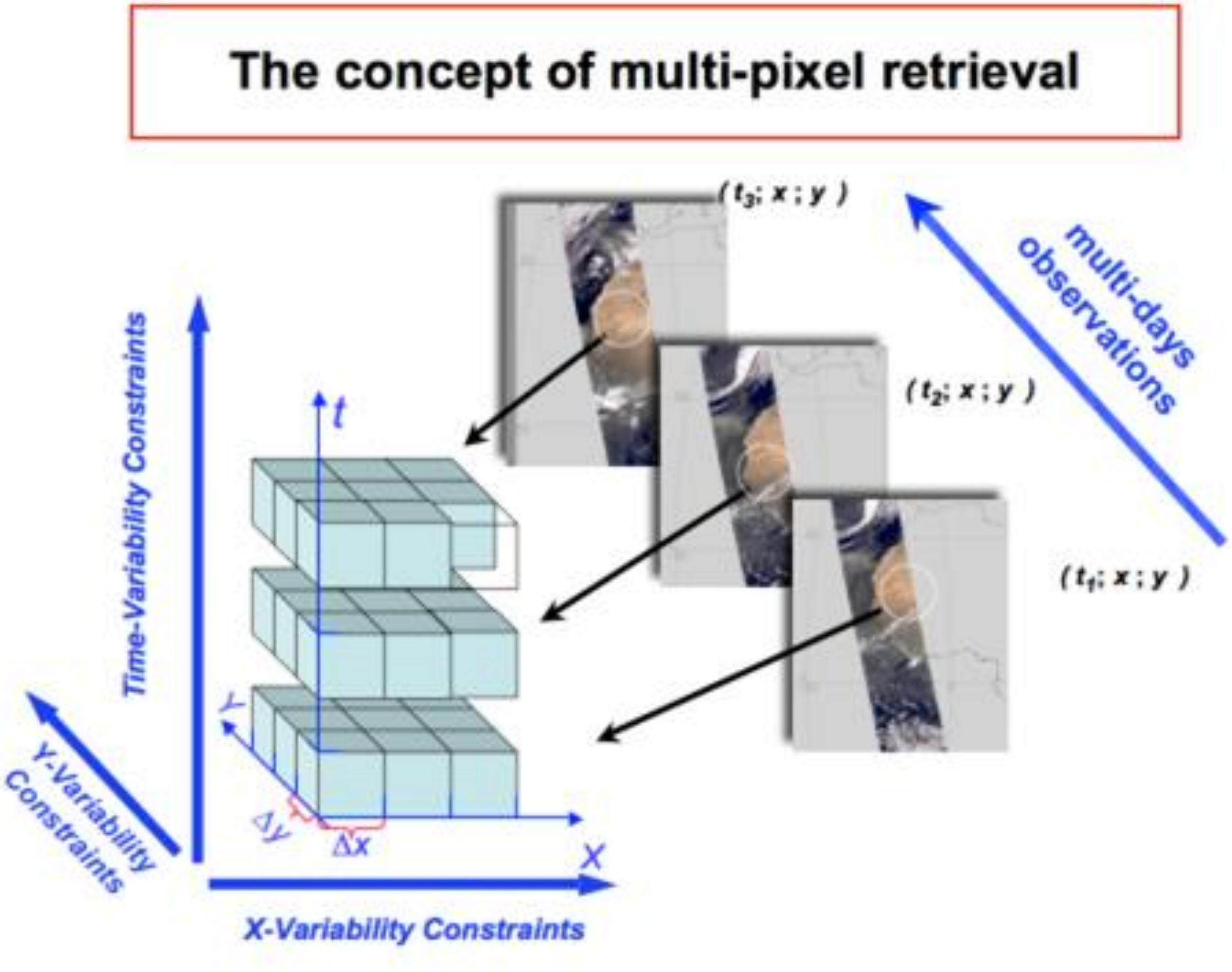


Example of Jacobian (average of 40 Jacobians)



$J_{i,j}=\Delta R_i / \Delta Var_j$

GRASP multi-pixel



REF: The GRASP Package. An overview. - General Retrieval of Aerosol and Surface Properties

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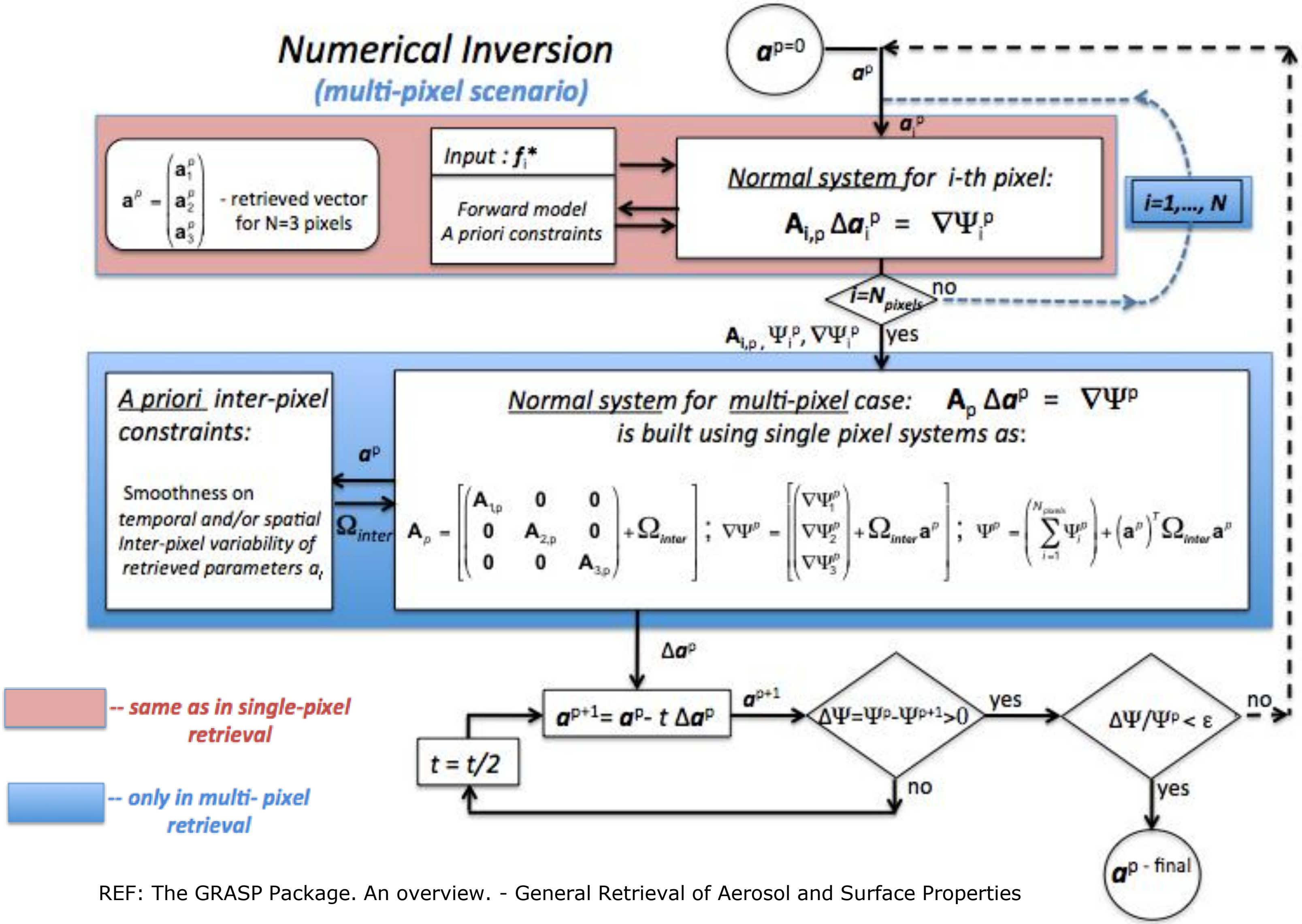

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