



XXII MEETING OF THE INTERNATIONAL
MINERALOGICAL ASSOCIATION
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A NEW HYPERSPECTRAL LIBRARY CONNECTED TO SOLSA OPEN DATABASES

for on-line-real-time analyses of Ni laterites & Bauxite

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ThermoFisher
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 Géosciences pour une Terre durable
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ERAMET

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 **EMC**
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 **ENSICAEN**
UMR6508

 VILNIUS UNIVERSITETAS
UNIVERSITAS VILNIENSIS
 Institute of Biotechnology



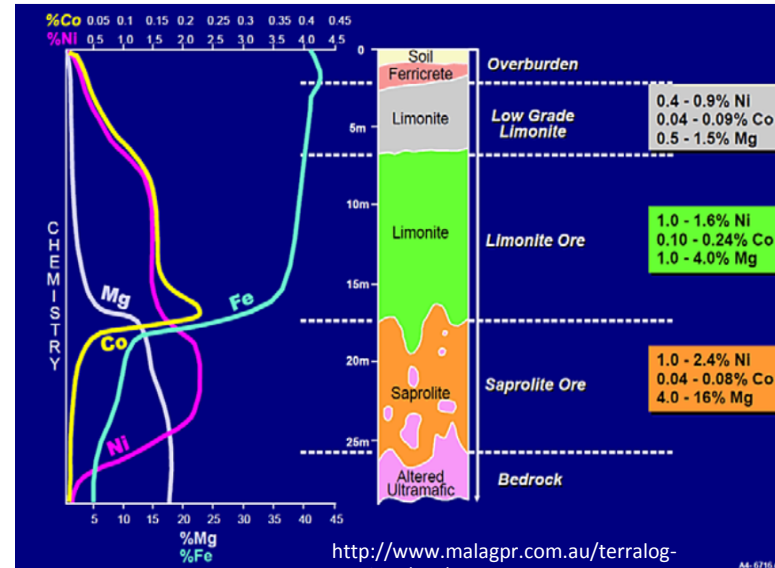
- Introduction
- Databases
 - Sample database
 - Raman open database
 - Hyperspectral library
- Hyperspectral imaging
 - Hyperspectral library
 - Sparse unmixing techniques
 - Results
- Conclusions and perspectives



1st SOLSA prototype validated for Nickel-laterites (ERAMET end user)

Ni-laterites (tropical countries): 70 % world's Nickel resources (40% of Ni production), but also Co, (Sc target) EU for steel-alloy-chemical industries => EU technologies

(Sub-) SURFACE ores



- Grade decrease (0.5 – 1 % Ni)
- Multiple metal (Ni, Co, Sc) carrier-minerals of different physico-chemical properties (part in swelling clays)
- Heterogeneities: hard – loose material

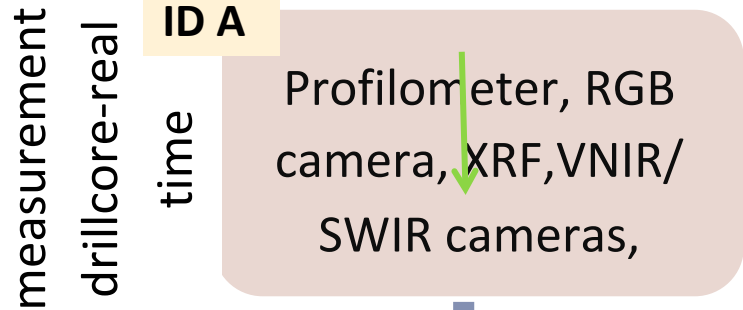
- Inaccurate resources & reserves estimates,
- Insufficient Metal Recovery
- Dysfunction in processing

Complex materials need a multi-instrumental approach

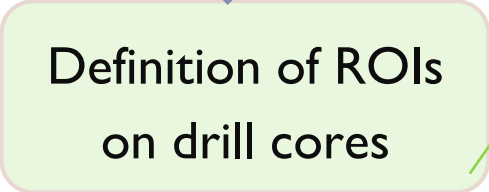
SOLSA ID

Analyse & Identification in field & industrial applications

on line-on-mine



processing

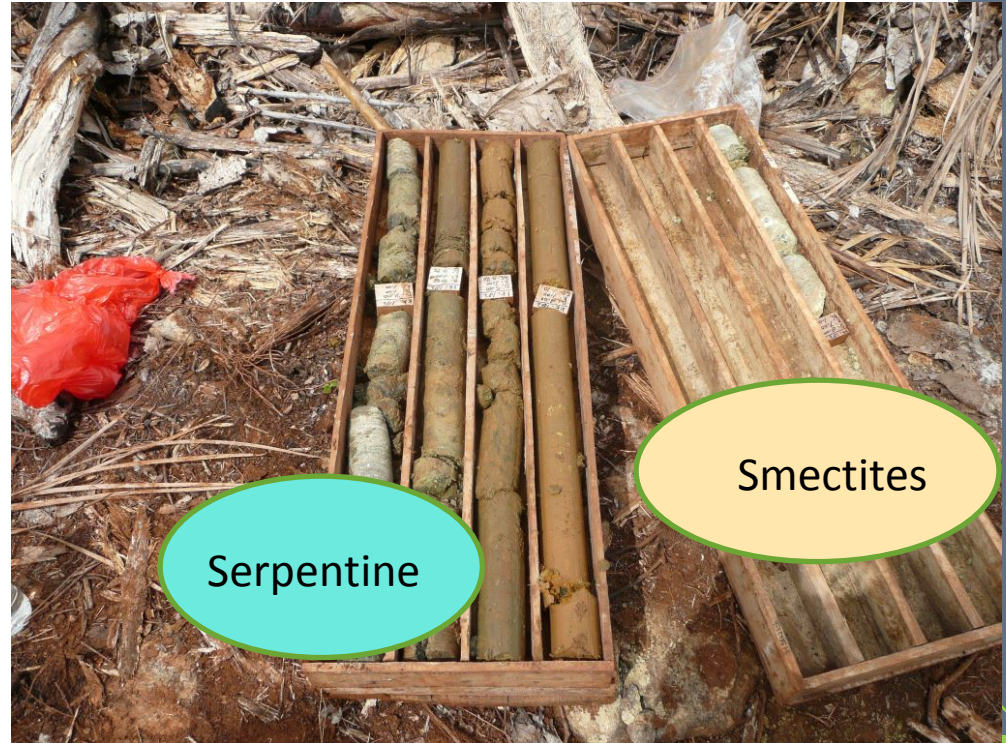
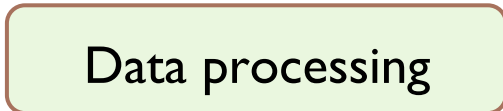


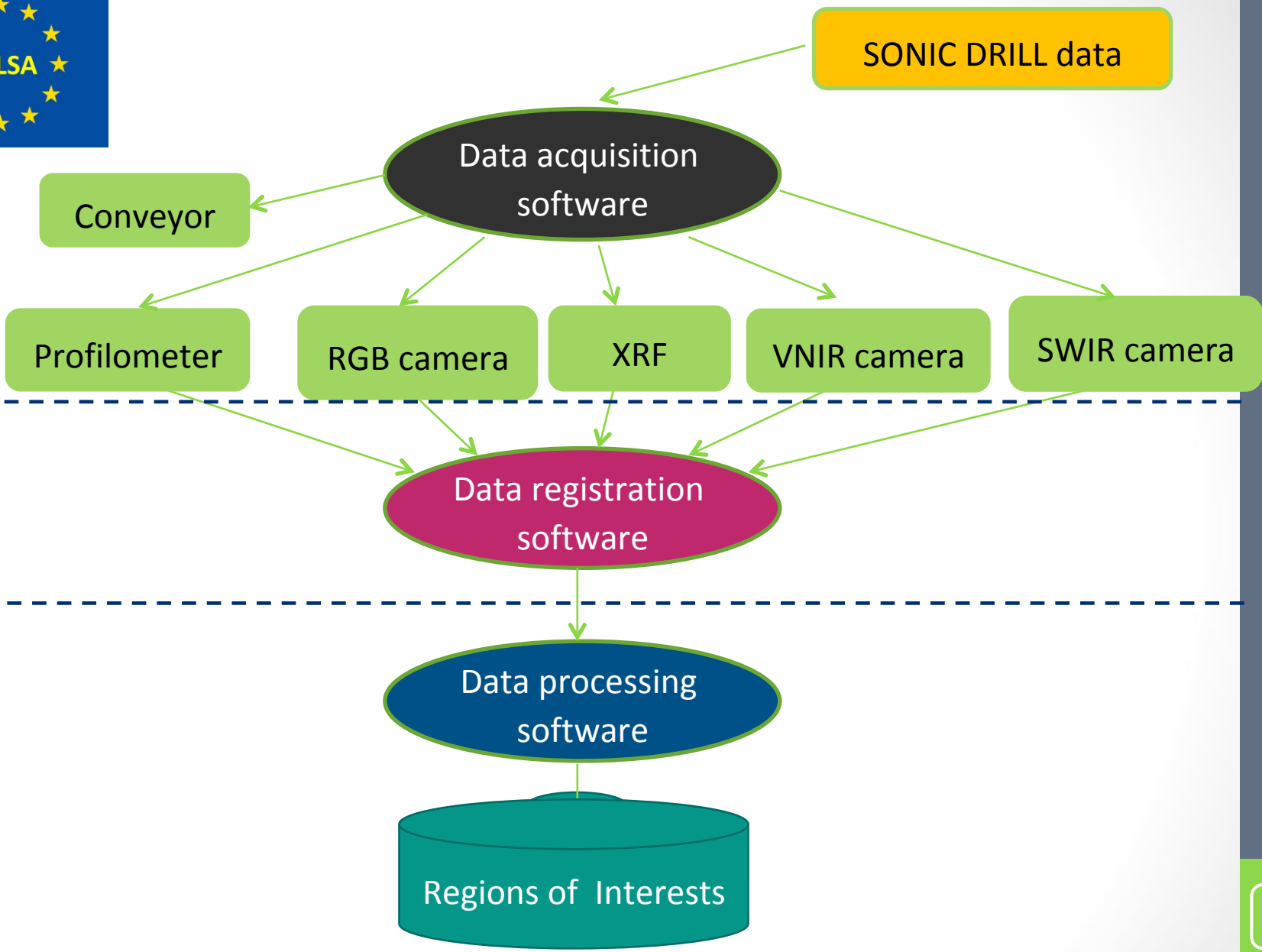
measurements
off-line

ID B



processing





Software development scheme



- Introduction
- Databases
 - Sample database
 - Raman open database (ROD) (*El Mendili et al, this session*)
 - Hyperspectral library
- Hyperspectral imaging
 - Hyperspectral library
 - Sparse unmixing techniques
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Sample database: Key issues



- ID cards of reference samples-sample library: geological-mine context, macroscopic and microscopic description (ISO 14688, 14689), laboratory analyses (XRF, EPMA, XRD), (mine specific here for Ni-laterites)
- Relational SQL database: comparing lab, handheld (pXRF, pPIR) and SOLSA on-line analyses.
- Definition of key parameters of the reference samples important for the mining company (based on macroscopic description).
- Definition of homogeneous units when implementing data



ROD and Hyperspectral library

- **Raman open database:**

- Collection of Raman spectra of standard samples.
- Available at
<http://solsa.crystallography.net/rod/>

talk: Yassine El Mendili et al. this session

- **Hyperspectral library (under construction):**

- Collection of spectra of pure minerals
- Will be available at
<http://solsa.crystallography.net/hod/>

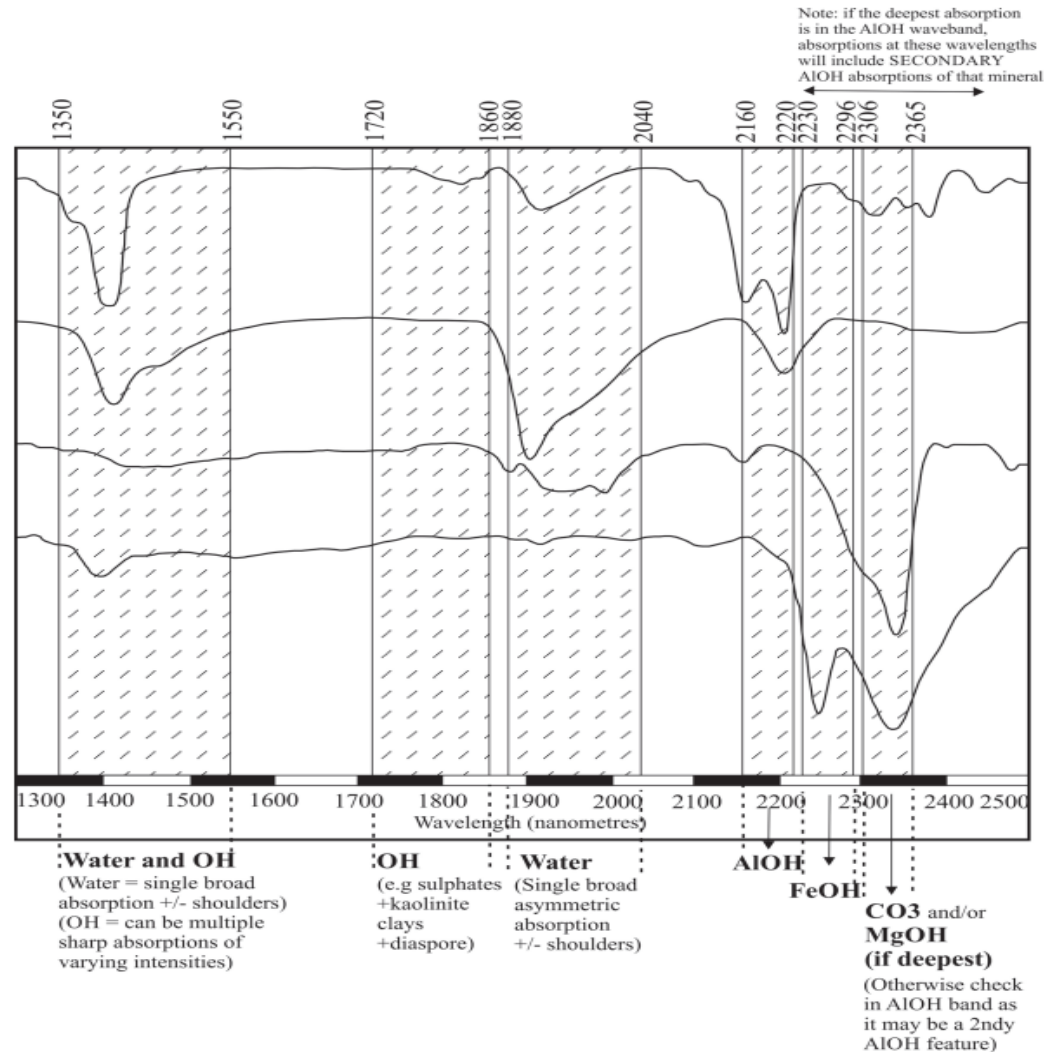


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Hyperspectral imaging for mineral identification

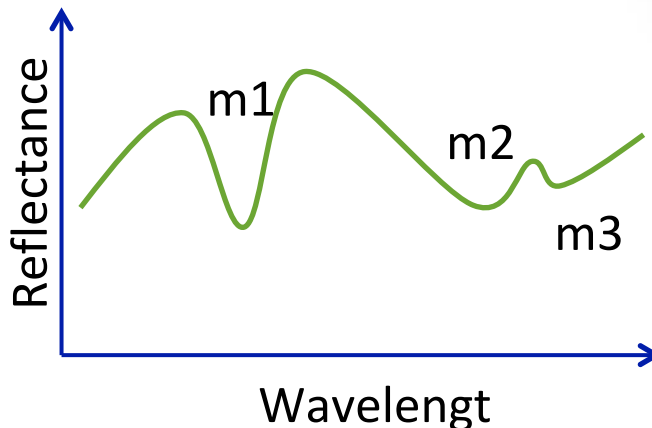
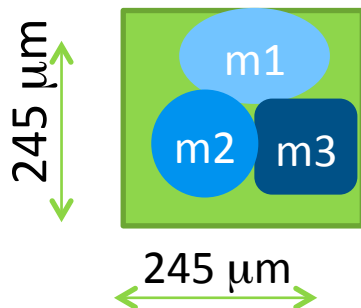
Molecules	Dominant absorption features
OH	1400nm (1550nm and 1750-1850nm in some minerals)
Water	1400nm and 1900nm
AlOH	2160-2228nm
FeOH	2230-2295nm
MgOH	2300-2370nm
CO ₃	2300-2370nm (and also at 1870nm, 1990nm and 2155nm)



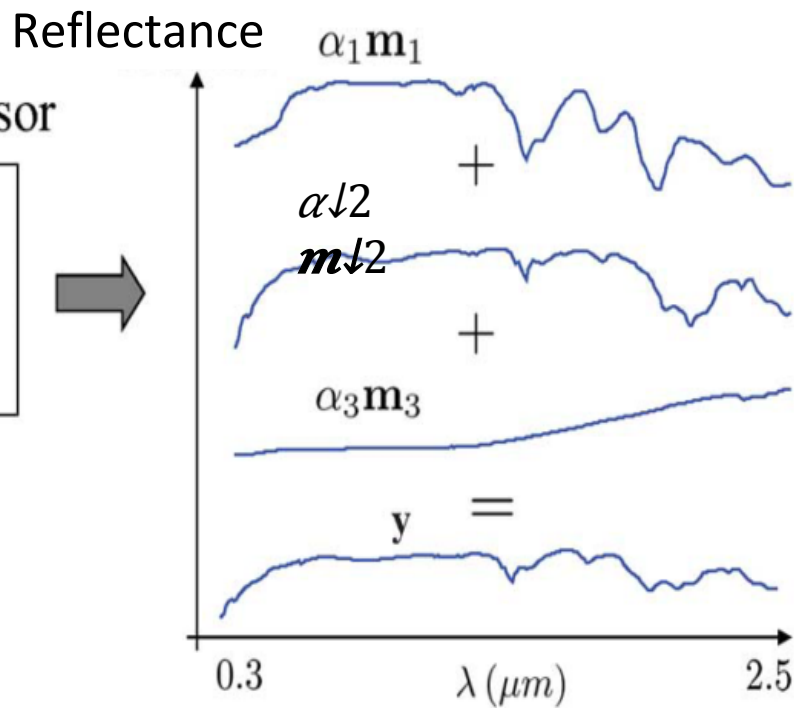
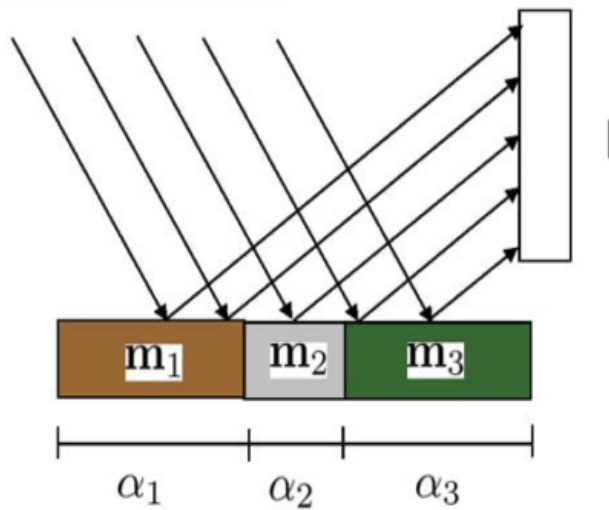
Crystallinity variations -> shape variations
 Compositional variations -> wavelength shifts

GMEX, 2008,
 Pontual et al. 1997

Hyperspectral unmixing



Halogen light



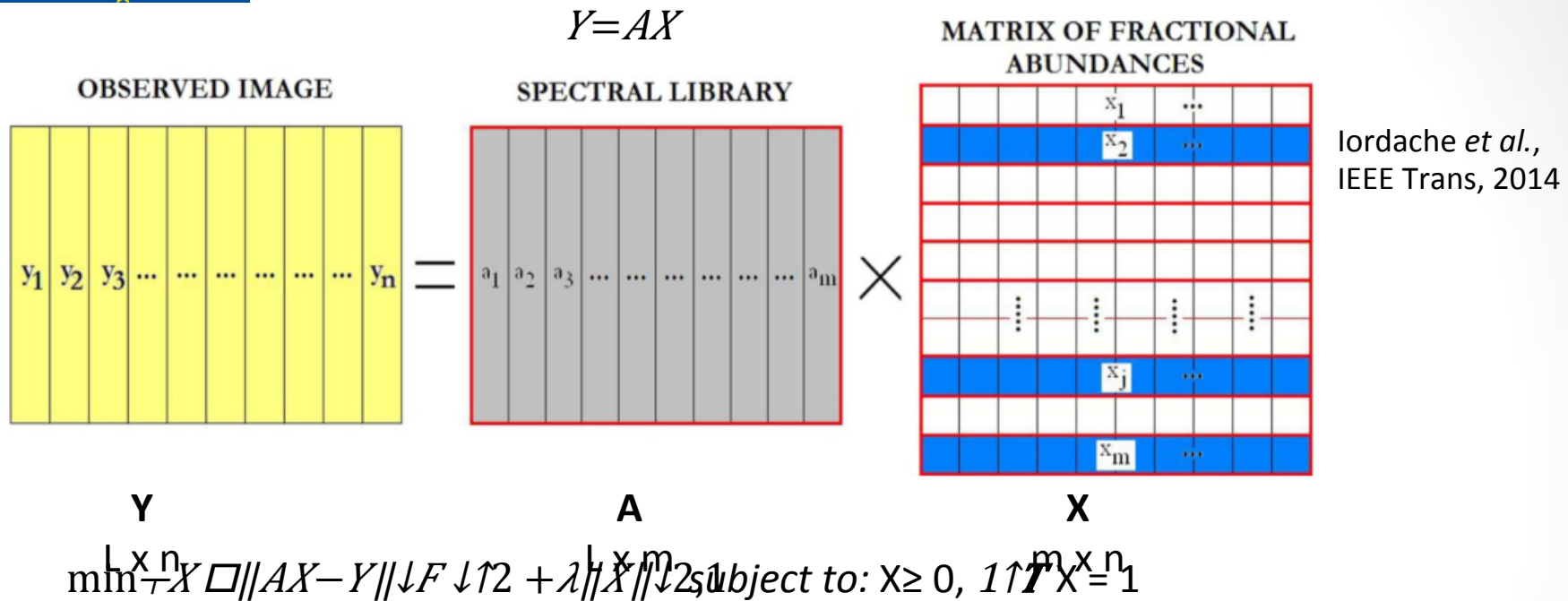


Hyperspectral unmixing

- Statistical approaches (*Debigion et al. 2008 ; Altmann et al., 2015*)
 - The likelihood: data generation models
 - Priors: constraints on the endmembers
- Geometrical approaches (*Nascimento et al., 2005; Bioucas-Dias et al. 2009*)
 - The observed hyperspectral vectors: simplex set whose vertices correspond to the endmembers.
- Sparse regression



Sparse unmixing



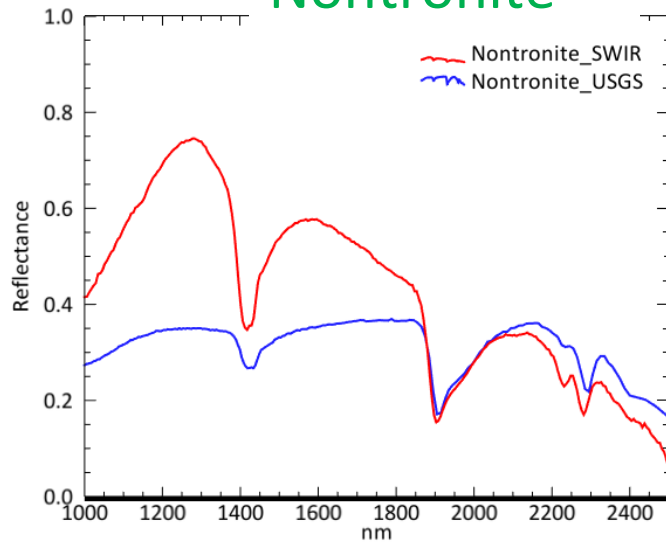
- The observed image signatures can be expressed in the form of linear combinations of a number of pure spectral signatures known in advance ([spectral library](#)).
- Unmixing amounts to finding the optimal subset of signatures in a [spectral library](#) that can best model each mixed pixel in the scene.
- The sparse unmixing exploits the usual very **low number of endmembers** (maximum of 4, Berman *et al.*, CSIRO, 2017) present in real images, out of a [spectral library](#).

Hyperspectral library

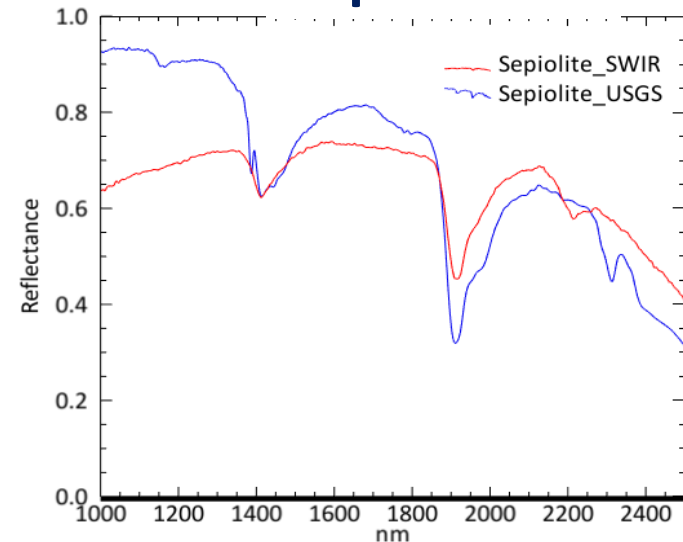


- Other libraries (e.g., USGS, CSIRO, John Hopkins Univ.) may not contain spectra of pure minerals.
- SOLSA includes spectra that are collected with our instruments used in our operational exploration.
- Minerals and mineral associations typical for Ni laterites (and different mine types) may not be present in other libraries.

Nontronite

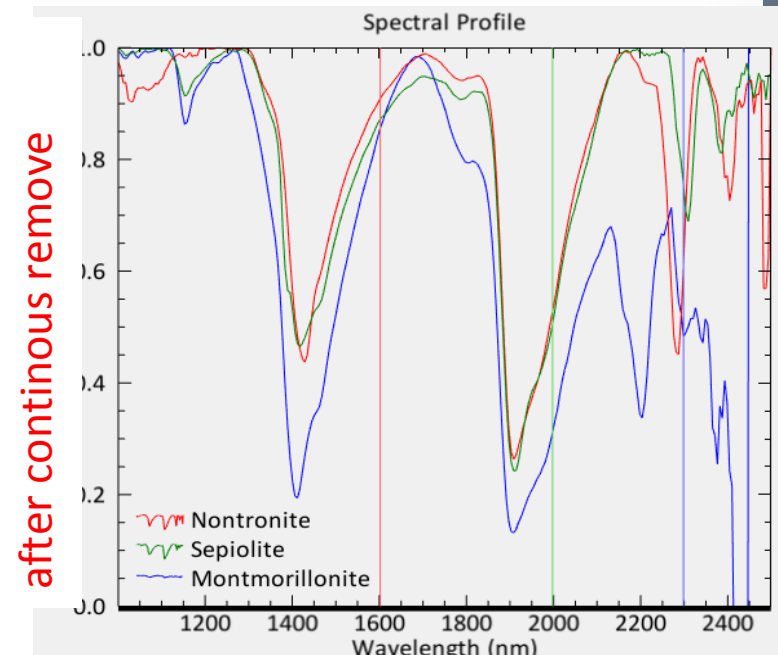
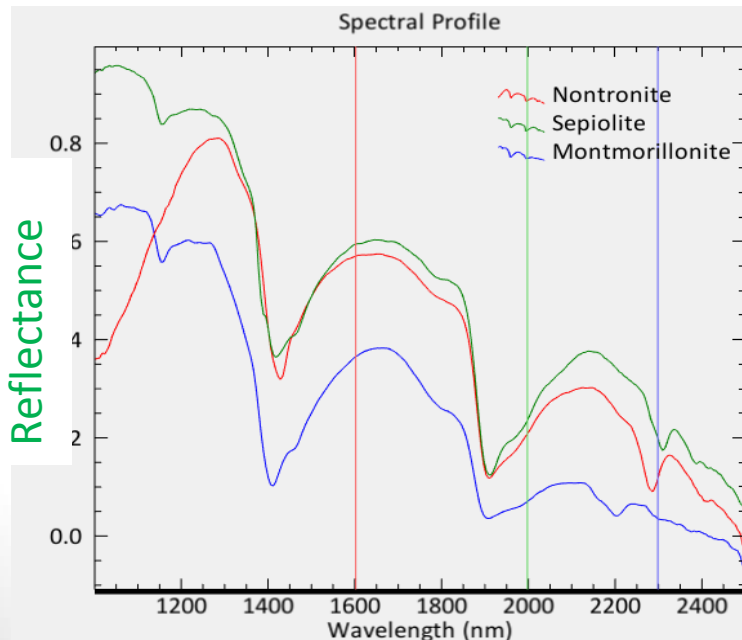
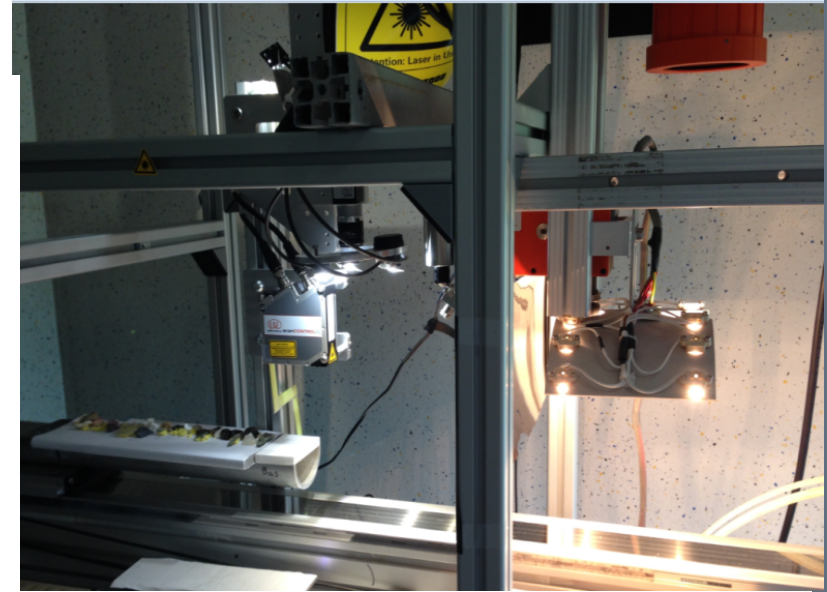


Sepiolite



SOLSA Hyperspectral library at present

- Rocks, pure mineral samples: BRGM, ERAMET, National Museum of Natural History, France
- Spectra extraction: ENVI 5.4 & G-MEX (taking into account: wavelength positions, the relative intensities of the absorption features).





Sparse unmixing techniques

CLSunSAL

(Collaborative sparse unmixing by variable splitting and augmented Lagrangian):

$$\min_{\tau, X} \square \|AX - Y\|_{F, \tau} + \lambda \|X\|_{2,1}$$

$$\text{subject to: } X \geq 0, \mathbf{1}^T X = 1$$

SUnSAL

(Sparse unmixing by variable splitting and augmented Lagrangian):

$$\min_{\tau, X} \square \|AX - Y\|_{F, \tau} + \lambda \|X\|_{1,1}$$

$$\text{subject to: } X \geq 0, \mathbf{1}^T X = 1$$

FCLS

(Fully constrained least squares):

$$\min_{\tau, X} \square \|AX - Y\|_{F, \tau}$$

$$\text{subject to: } X \geq 0, \mathbf{1}^T X = 1$$

The optimization is based on the alternating direction method of multipliers (ADMM)

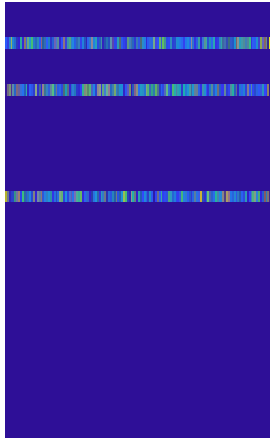
Bioucas-Dias et al., 2010
Iordache et al., IEEE Trans, 2014
Afonso et al., IEEE Trans, 2011



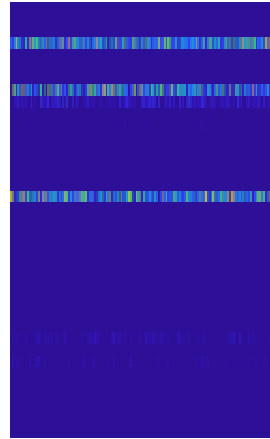
Hyperspectral unmixing

Simulated data

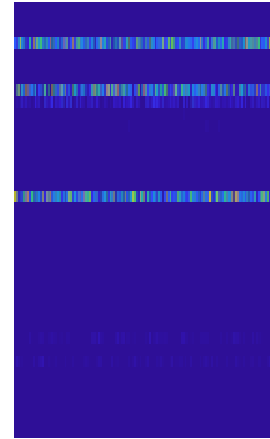
Original X



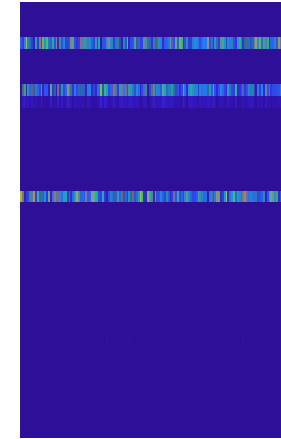
FCLS



SUnSAL



CLSUnSAL



Signal to reconstruction error (SRE) ratio:

$$SRE = 10 \log \frac{E\|x\|^2}{E\|x - \hat{x}\|^2}$$

SNR = 40 dB

K	FCLS		SUnSAL		CLSUnSAL	
	SRE	Time	SRE	time	SRE	time
2	14.24	0.022	14.94	0.254	16.74	0.228
3	6.41	0.019	7.45	0.259	11.95	0.230
4	5.25	0.022	7.07	0.499	7.16	0.453

FCLS: Fully constrained least squares

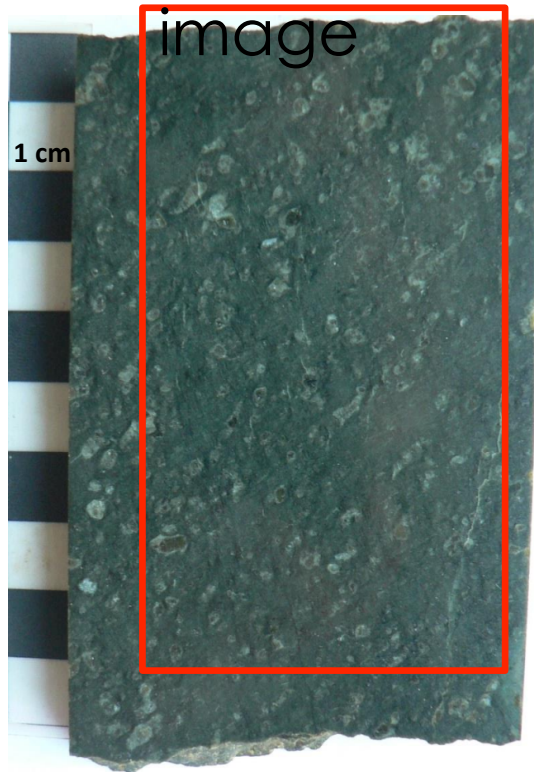
SUnSAL: Sparse unmixing by variable splitting & augmented Lagrangian

CLSUnSAL: Collaborative sparse unmixing by variable splitting & augmented Lagrangian

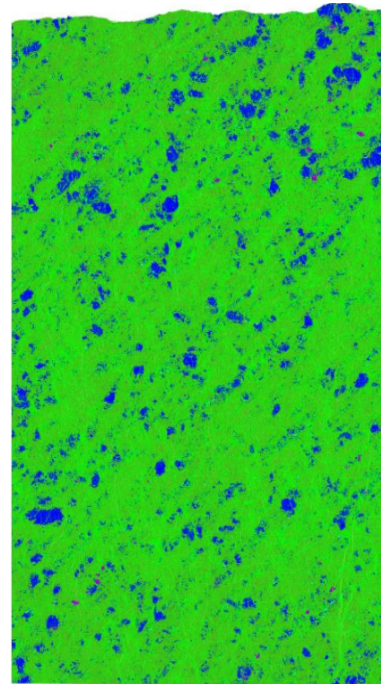
Hyperspectral unmixing

Data acquired: serpentized harzburgite sample

RGB
image



QEMSCAN results

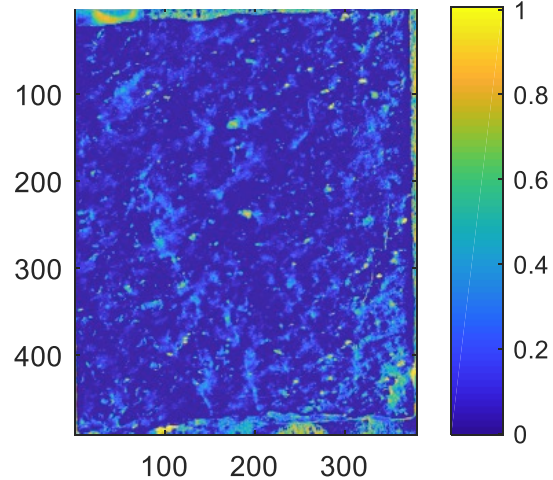




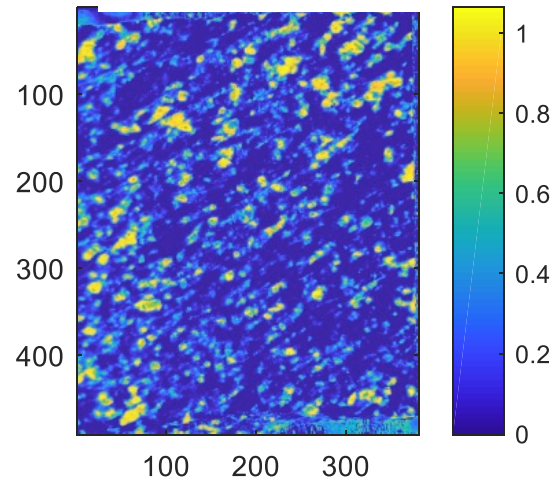
Hyperspectral unmixing

Proportion (abundance) of each mineral:

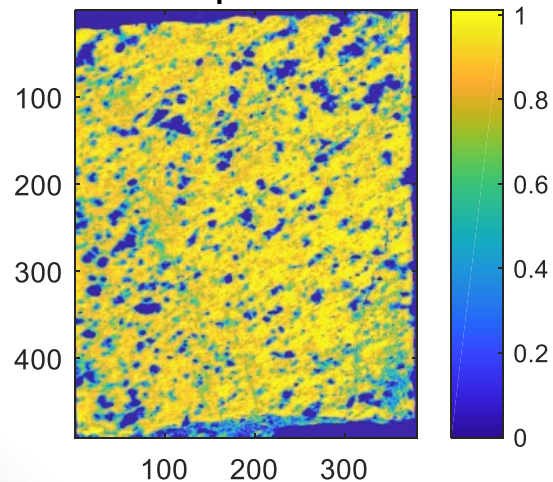
CHROMITE



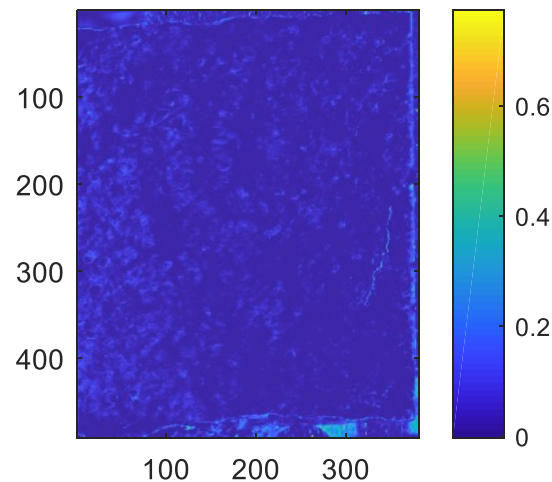
OPX



SERPENTINE



OLIVINE

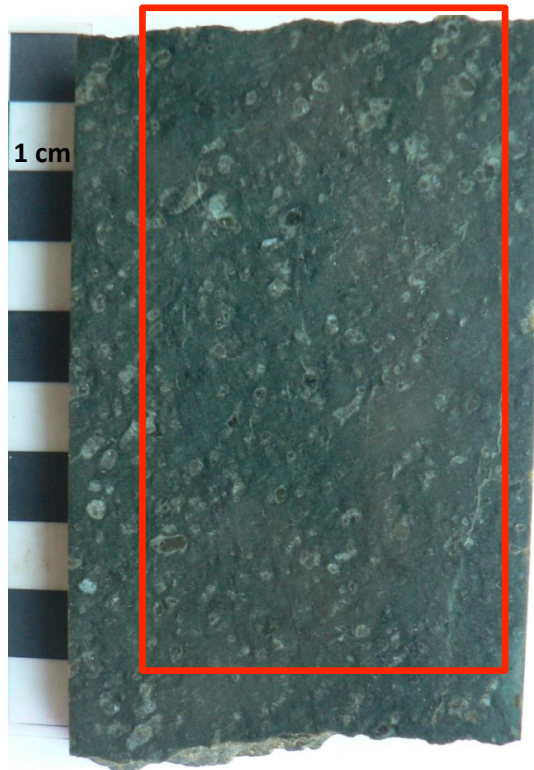


Computation
time: 4 mins

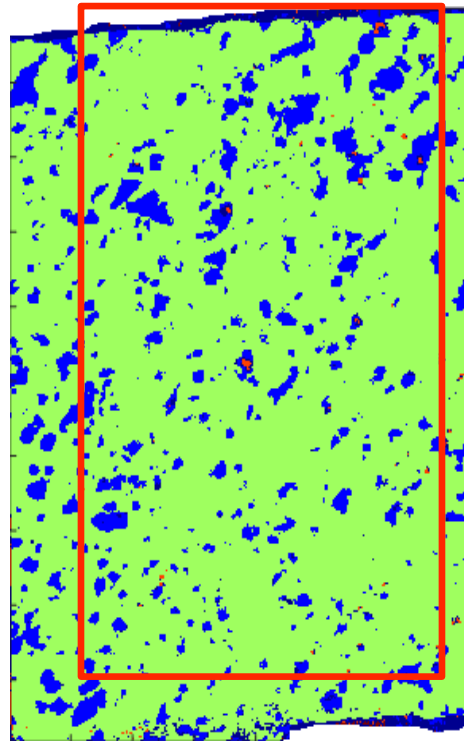
Hyperspectral unmixing

serpentinized harzburgite sample

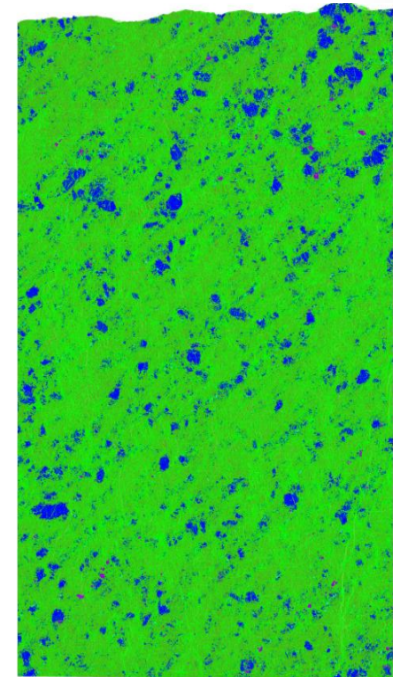
RGB image



Unmixing



QEMSCAN



Computation time: 4 mins



Conclusions and Perspectives

- Using our hyperspectral library, the CLSUnSAL provided the highest accuracy.
 - Need to improve the computation time.
 - Incorporate the spatial context to the unmixing problem
- The hyperspectral library is constantly extended
 - 257 spectra have been extracted for 49 minerals
- A graphic user interface is under development
- Machine learning classification approaches have been implemented.
- The connection between the databases will be done.



Thank you for your attention!