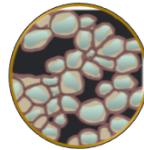


# Multibloc analysis of multimodal and multiresolution hyperspectral images Application to plant cell wall analysis



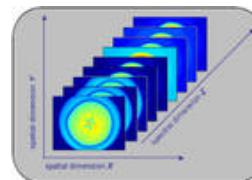
M-F Devaux  
F Guillon



*Parois Végétales  
&  
Polysaccharides  
Pariétaux*



M Hanafi



*Sensométrie  
&  
Chimiométrie*



F Jamme



*Dichroisme, Imagerie,  
Spectrométrie de masse  
pour la Chimie et la Biologie*

**PhD Fatma Allouche: 2009-2012**

# Plant cell wall

## Chemical composition

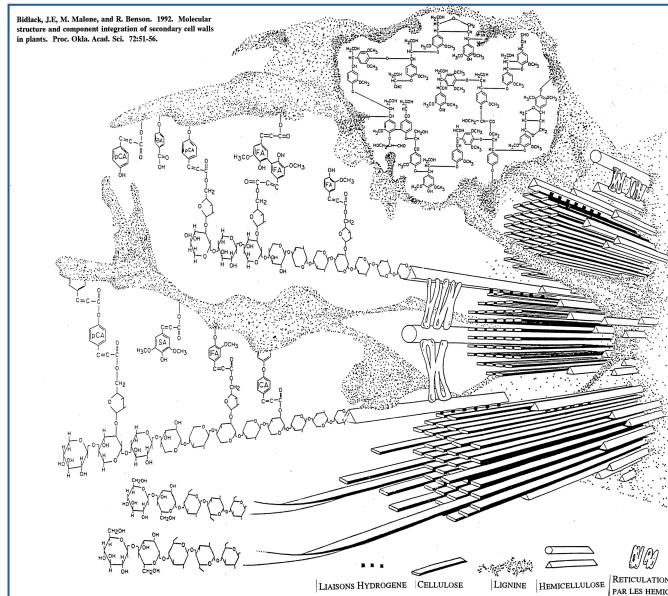
Major constituents  
are complex polymers

Carbohydrates  
Lignins  
Proteins  
Lipids

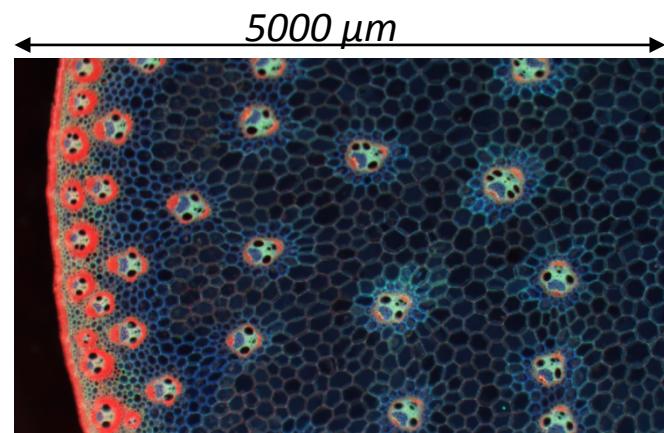
Constituents are organised....

In the plant

In the wall

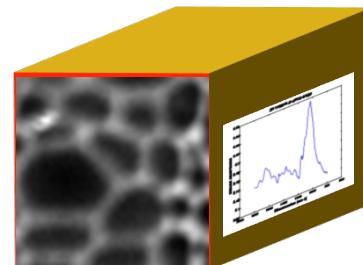
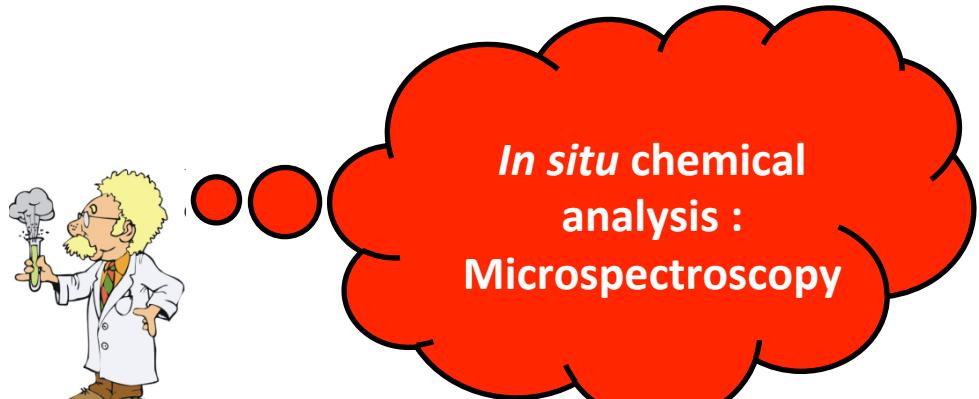


Bidlack et al., 1992



Maize  
stem

Autofluorescence:  
false color, Blue and UV fluorescence



hyperspectral  
images

# Multimodal image acquisition

hemicellulose

lignin

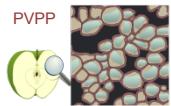
infrared



Vascular bundle in a Maize stem

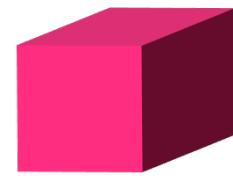
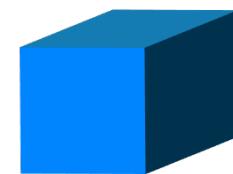
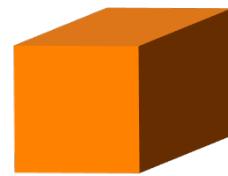
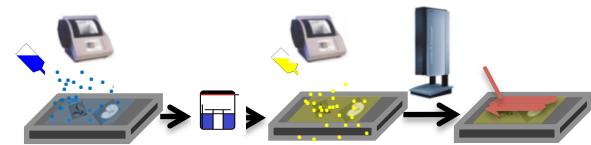


fluorescence



cellulose

Hydroxycinnamic acids

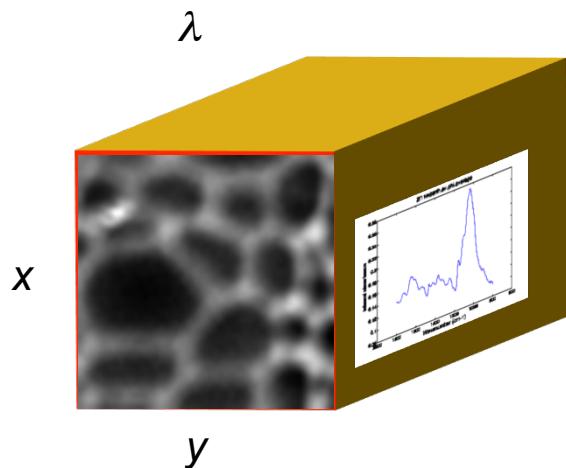


Blocks of multi and hyperspectral images

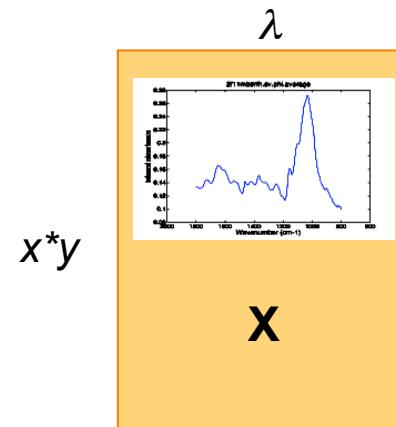
# Multi and Hyperspectral Image Analysis

## A chemometric Approach

Set of pixels acquired  
in different spatial locations



unfolded



Principal component  
Analysis



$$c = Xu$$

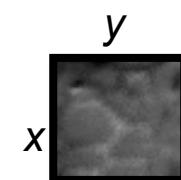
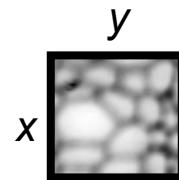
Scores

$$x^*y$$

C

refolding

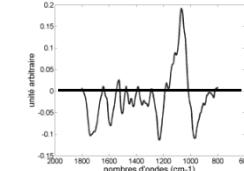
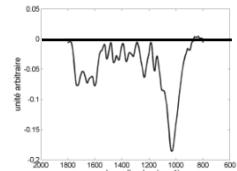
Score images : spatial interpretation



loadings

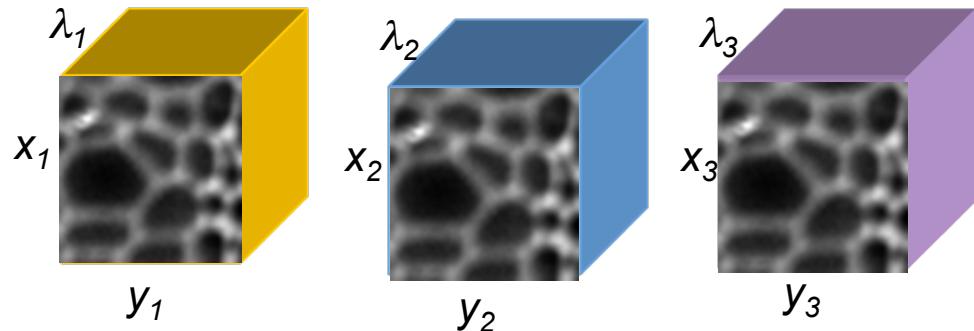
U

spectral interpretation

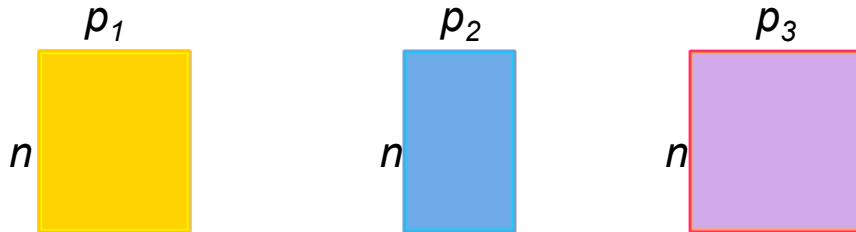


# Multimodal spectral images : Multiblock Data Analysis

Coupling different  
hyperspectral images

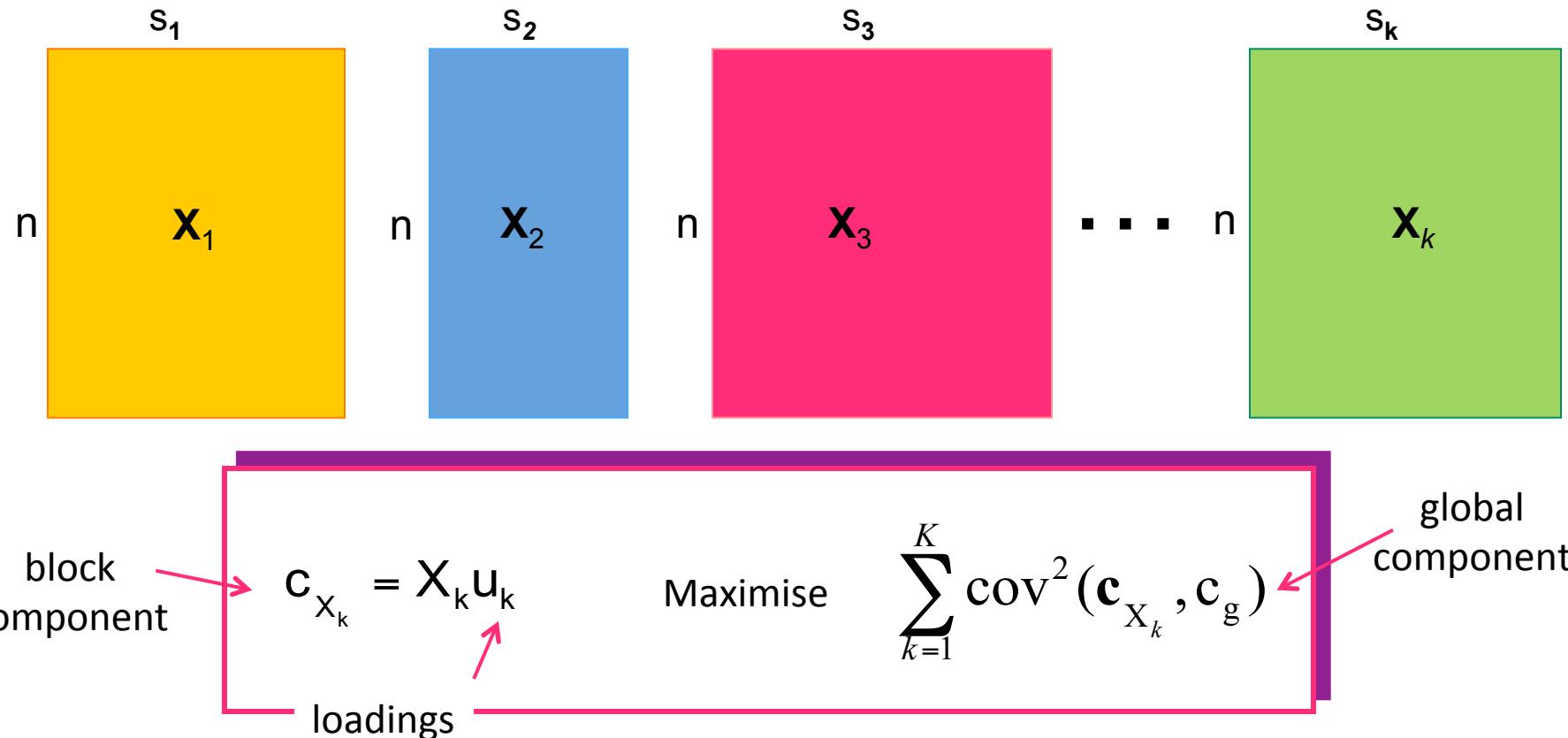


Joint analysis  
of different blocks of data

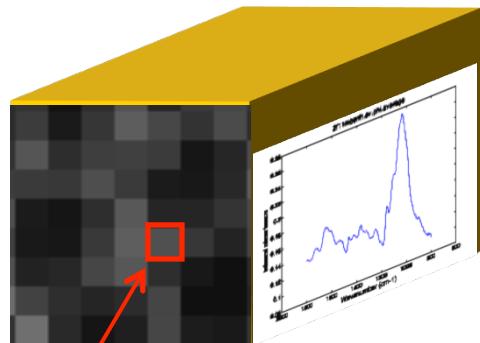


Parafac, Tucker, Multiple Co-inertia Analysis  
N-way Partial Least Square, Multiset Multivariate Curve resolution,

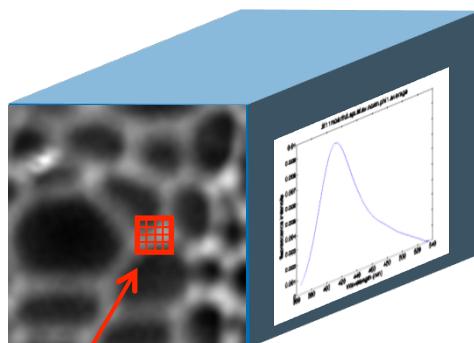
## Multiblock analysis: multiple co-inertia analysis



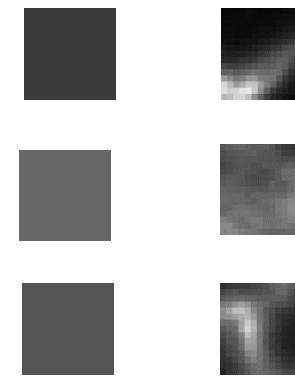
# Blocks of hyperspectral images with different spatial resolution



pixel

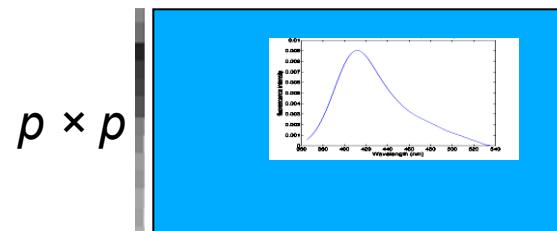
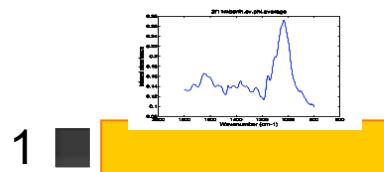


Small image



pixels      Small images

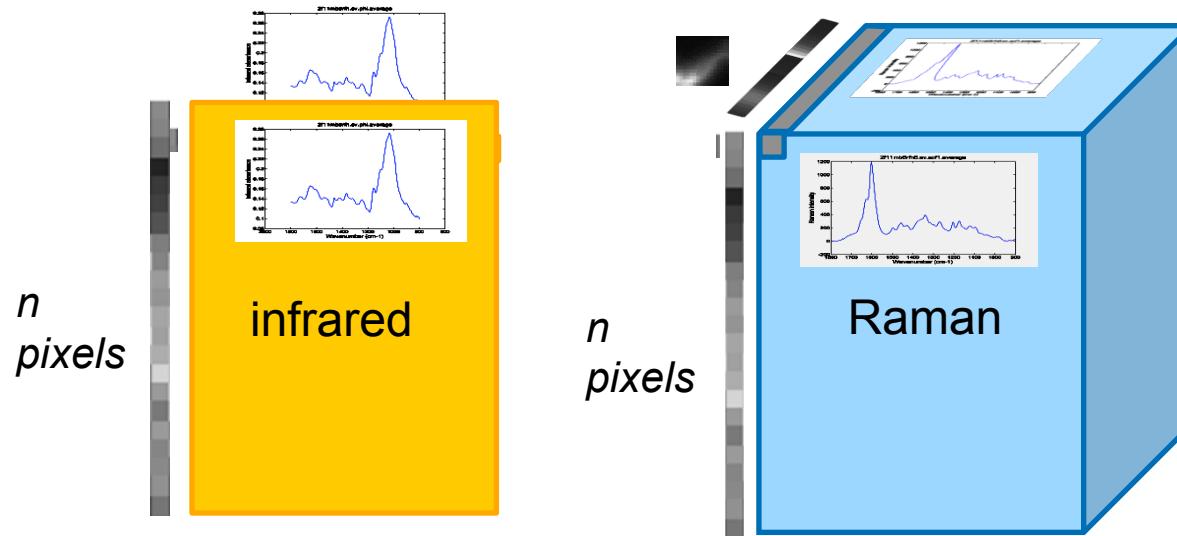
Low resolution pixels correspond to small images of size  $p \times p$  high resolution pixels.



Unfolding small images

Pairing multiresolution pixels

# Blocks of hyperspectral images with different spatial resolution paired data structure



How can we envision  
multiblock data analysis  
while preserving the full  
resolution of data tables

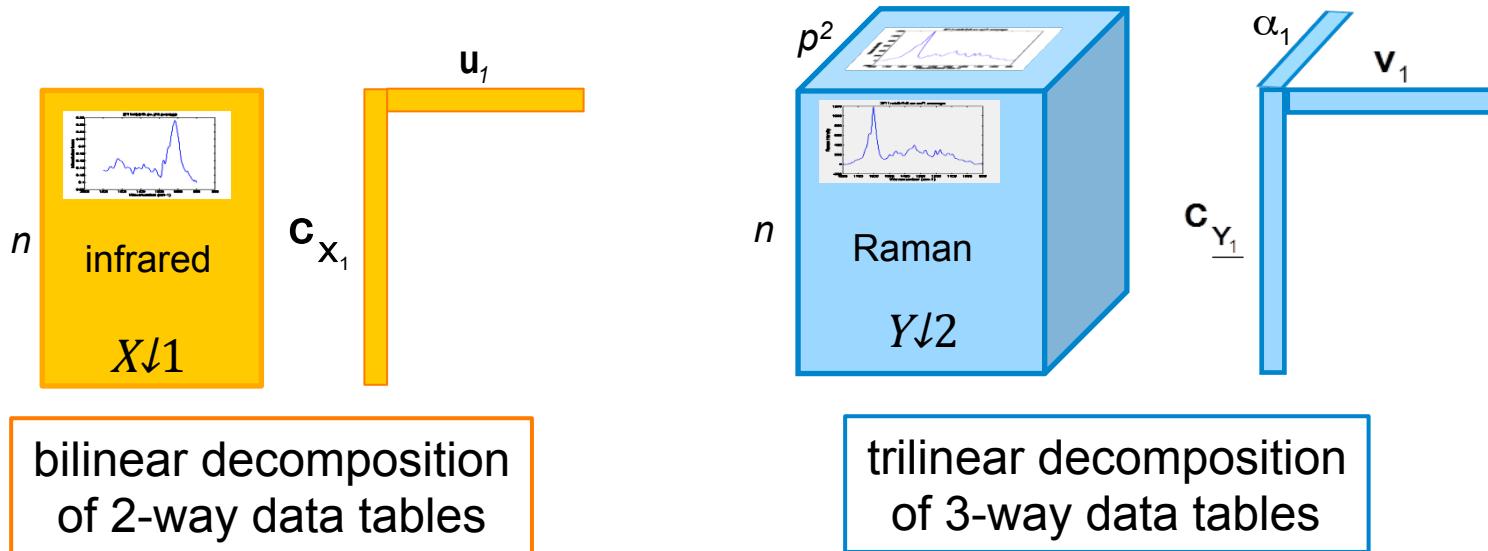


Extension of Multiple Co-inertia Analysis....



# Extension of Multiple Co-inertia Analysis

## Developing Trilinear Multiple Co-inertia Analysis



Assessing global and block components

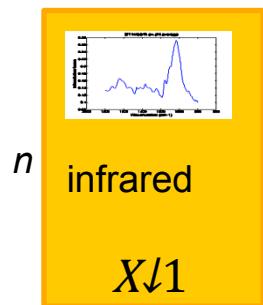
$$\text{Max } \text{cov}^2(c_{x_k}, c_g) + \text{cov}^2(c_{y_i}, c_g)$$

global component

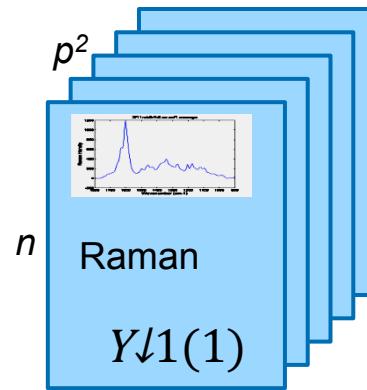
The equation shows the maximization of the covariance squared between the global component  $c_g$  and the block components  $c_{x_k}$  and  $c_{y_i}$ . The terms are highlighted with colored circles: orange for  $c_{x_k}$  and pink for  $c_{y_i}$ . Arrows point from these circles to a pink-bordered box labeled 'global component'.

# Trilinear Multiple Co-inertia Analysis

Assessing global and block components



consider 3-ways blocks  
as stacks of 2-ways blocks

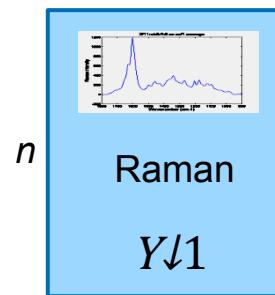
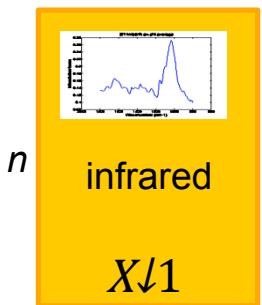
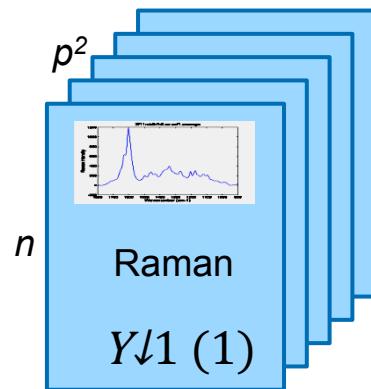
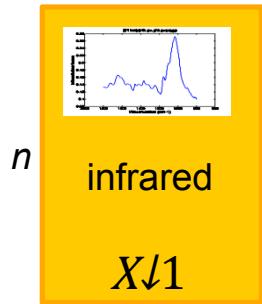


$$\mathbf{c}_{x_k} = \mathbf{X}_k \mathbf{u}_k$$

$$\mathbf{c}_{Y_{j(z)}} = \mathbf{Y}_{j(z)} \mathbf{v}_j$$

$$\text{cov}^2(\mathbf{c}_{x_k}, \mathbf{c}_g) + \sum \text{cov}^2(\mathbf{c}_{Y_{j(z)}}, \mathbf{c}_g)$$

# Trilinear Multiple Co-inertia Analysis



Assessing a weighted sum  
of block stacks

$$\bar{\mathbf{Y}}_j = \sum \alpha_{j(z)} \times \mathbf{Y}_{j(z)}$$

A diagram showing a vertical vector  $\mathbf{v}_1$  and a horizontal vector  $\mathbf{c}_{\bar{\mathbf{Y}}_j}$ . A pink circle highlights the scalar factor  $\alpha_{j(z)}$  in the equation. Another pink circle highlights the vector  $\mathbf{Y}_{j(z)}$ .

Multiple Co-inertia Analysis of the “weighted sum” data tables

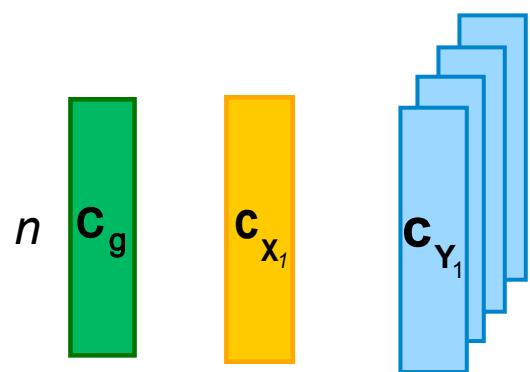


$\mathbf{u}_1$

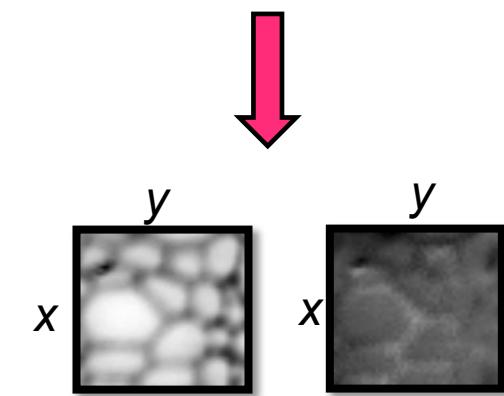
$\mathbf{v}_1$

Loadings

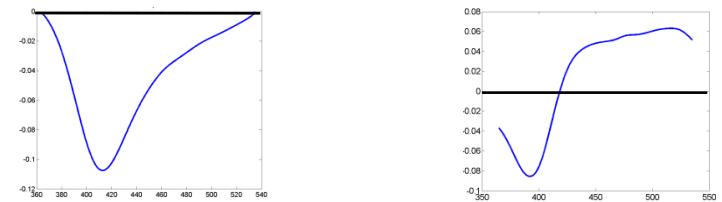
# Trilinear Multiple Co-inertia Analysis: results



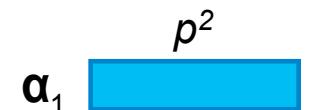
Global and block component



Spatial interpretation

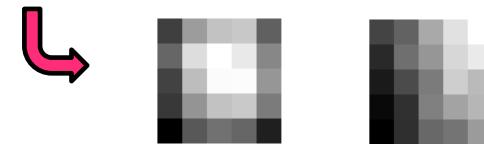


Spectral interpretation



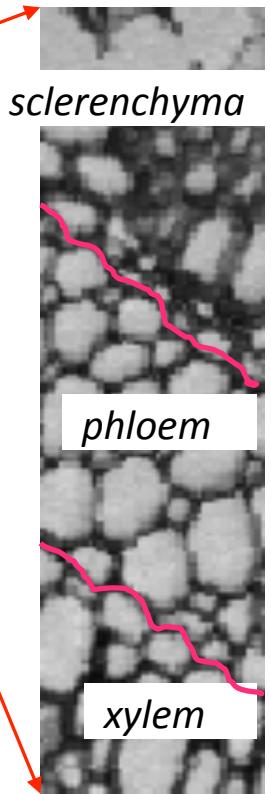
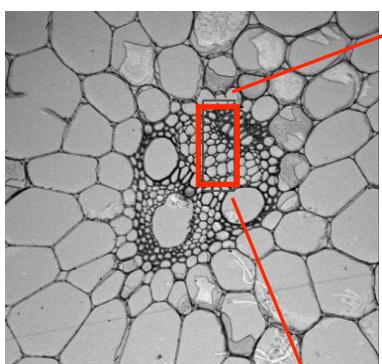
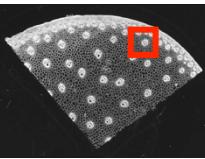
Weight vector

Refolding



Spatial interpretation

# Comparing cell types in maize stem



sclerenchyma

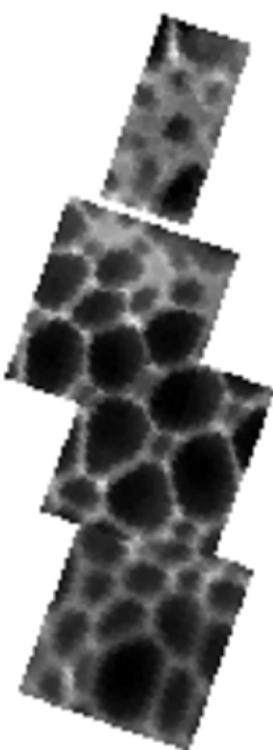
phloem

xylem

Infrared



Fluorescence



Raman



Registered images

Images of the spectral area between:

1200-950  $\text{cm}^{-1}$

360-540 nm

1800-800  $\text{cm}^{-1}$

Spatial resolution

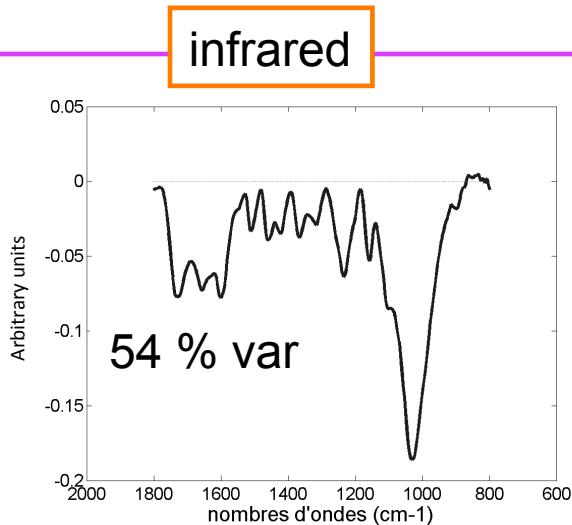
5  $\mu\text{m}$

1  $\mu\text{m}$

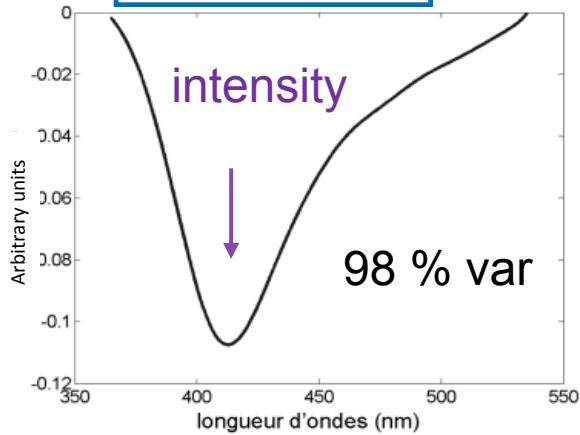
1  $\mu\text{m}$

# Trilinear Multiple Co-inertia Analysis: maize stem loadings

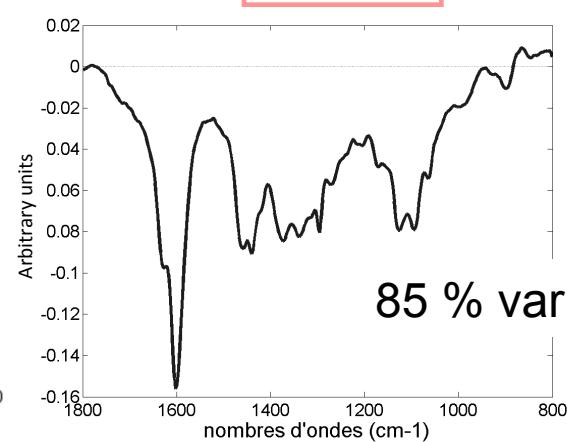
Component 1



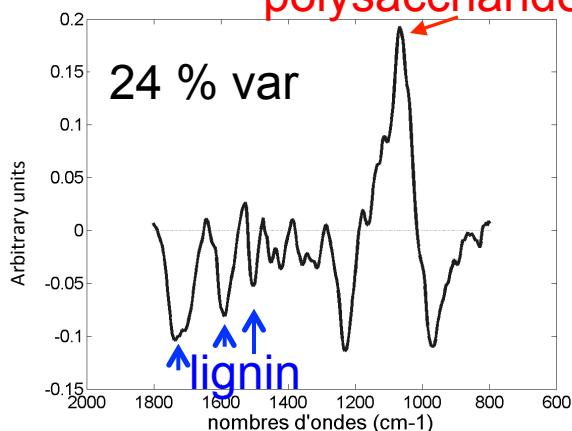
fluorescence



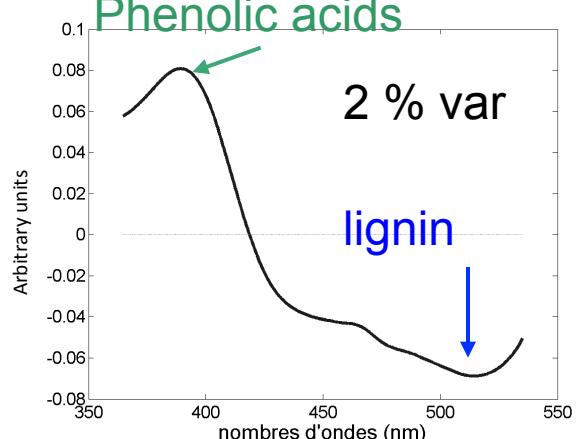
Raman



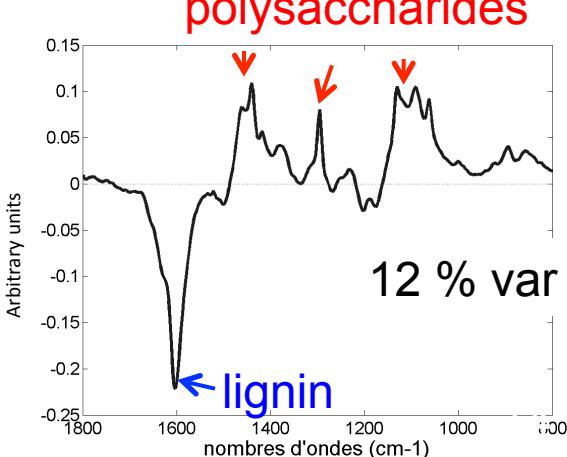
polysaccharides



Phenolic acids



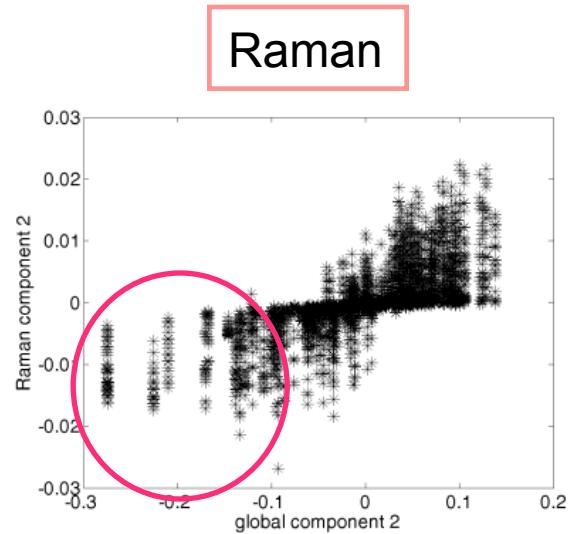
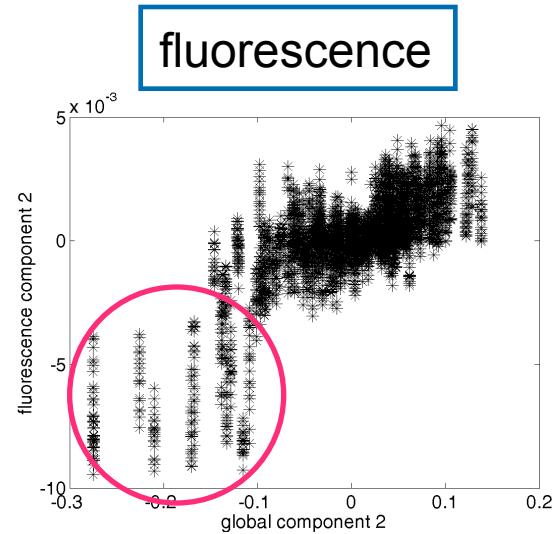
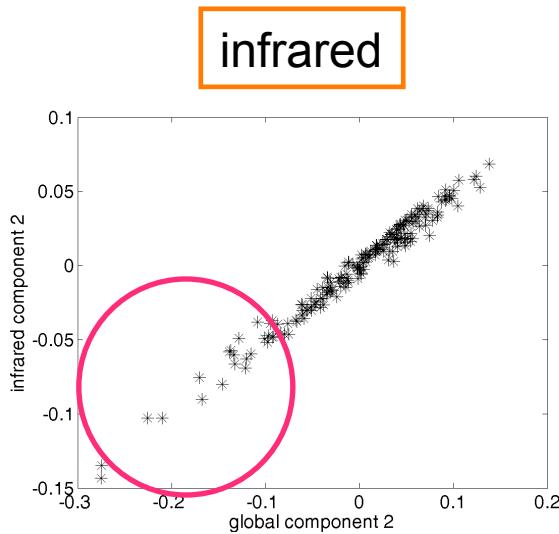
polysaccharides



Component 2

# Trilinear Multiple Co-inertia Analysis: maize stem Global and Block components

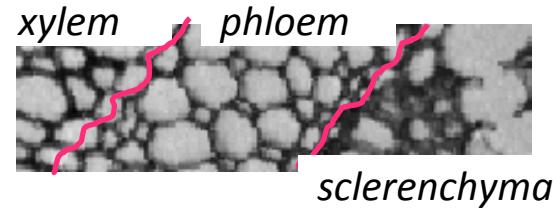
Component 2 : lignin / polysaccharides + phenolic acid



Segmented image:  $c_g < -0.1 \rightarrow$  lignin

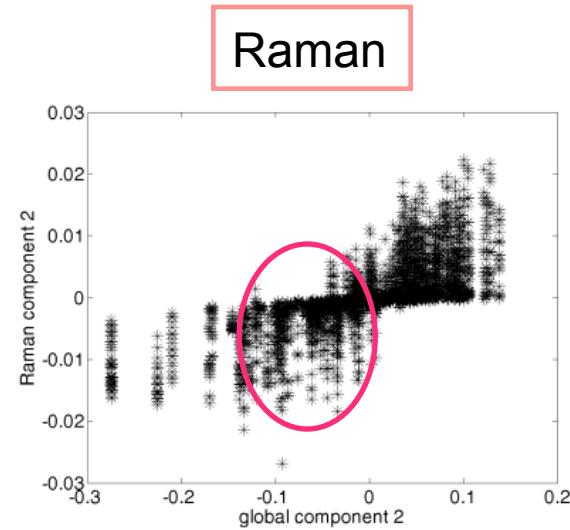
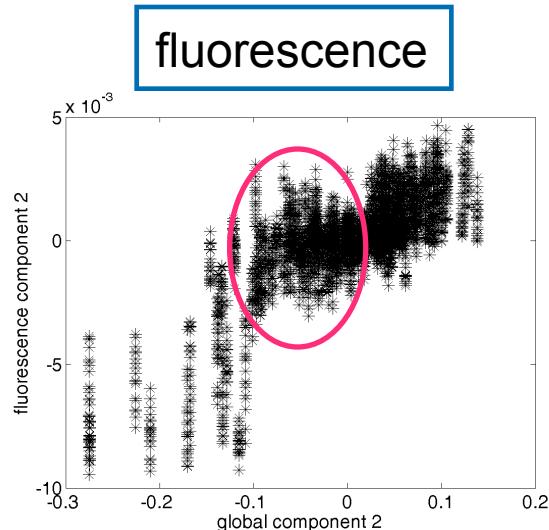
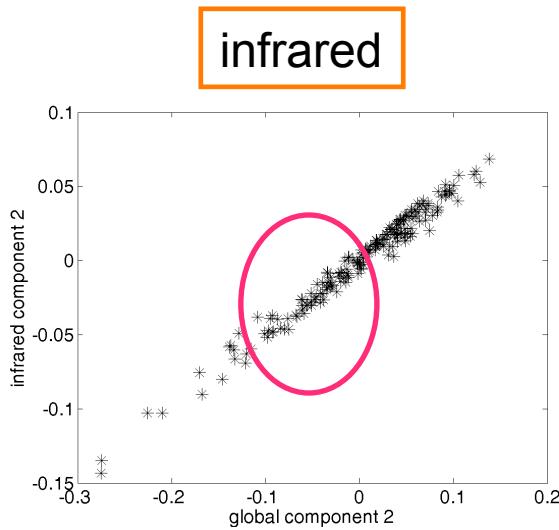


sclerenchyma



# Trilinear Multiple Co-inertia Analysis: maize stem Global and Block components

Component 2 : lignin / polysaccharides + phenolic acid



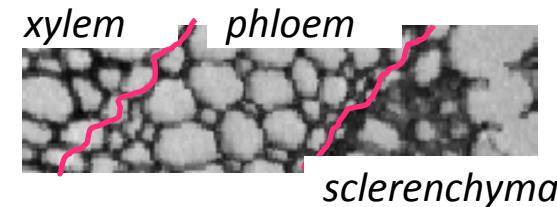
Segmented image:  $-0.1 < c_g < 0 \rightarrow$  lignin + phenolic acids



sclerenchyma



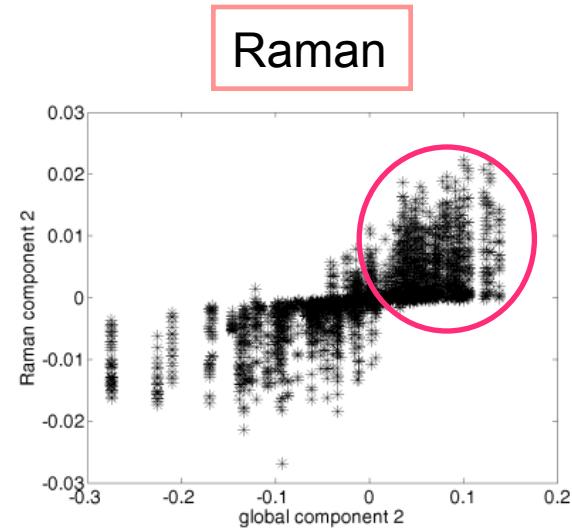
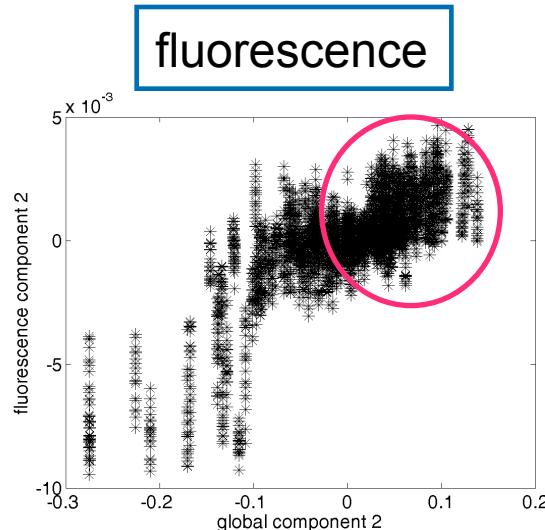
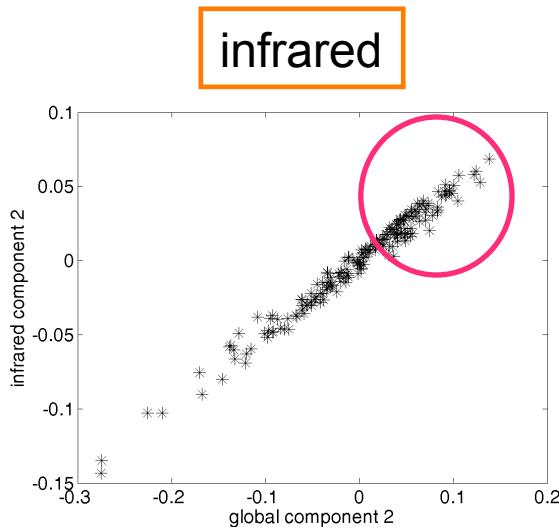
xylem



sclerenchyma

# Trilinear Multiple Co-inertia Analysis: maize stem Global and Block components

Component 2 : lignin / polysaccharides + phenolic acid



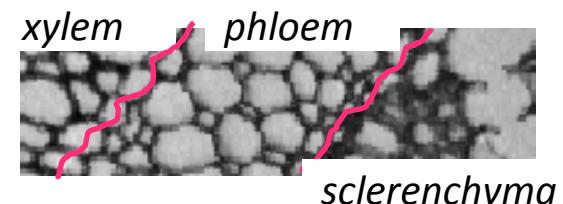
Segmented image:  $c_g > 0 \rightarrow$  phenolic acids +  
polysaccharides



sclerenchyma

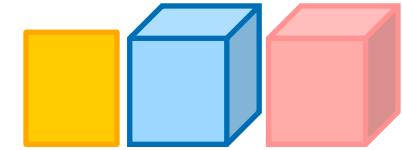


xylem



phloem

# Conclusion



**Designing data blocks that preserve spatial resolution**

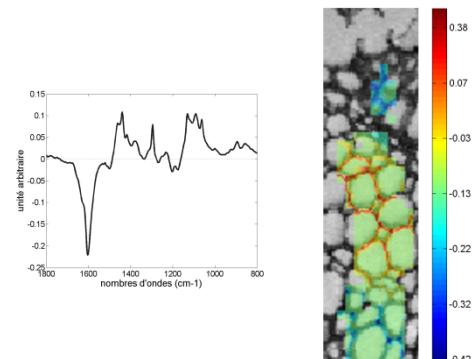
**Extension of Multiple Co-inertia Analysis to data tables with an heterogeneous number of way.**

**Application to hyperspectral images**

Loadings for spectral interpretation

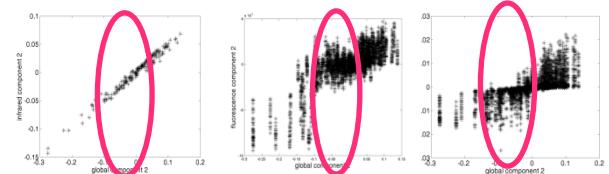
Component images for spatial analysis:

Maize stem: comparing cell types.



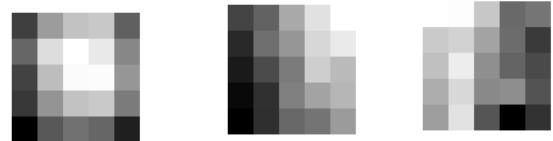
**Complementarity and common information**

Global and Block component

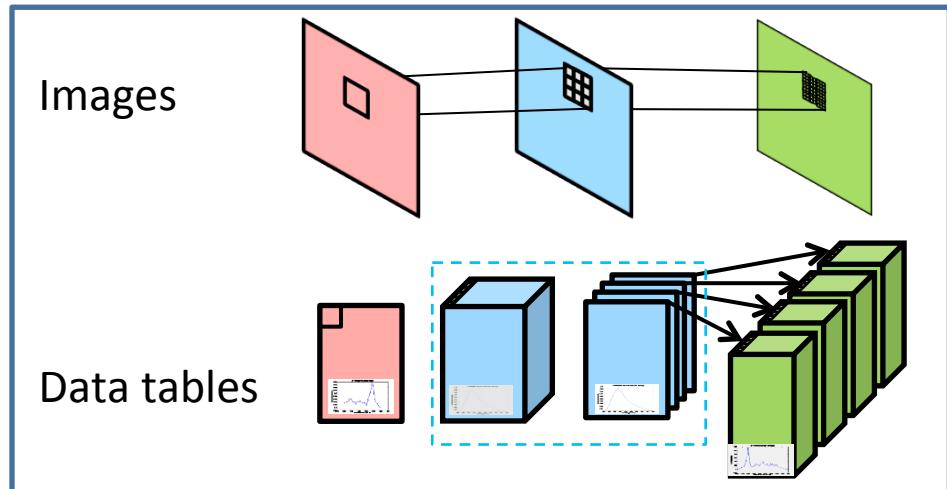


# Perspectives

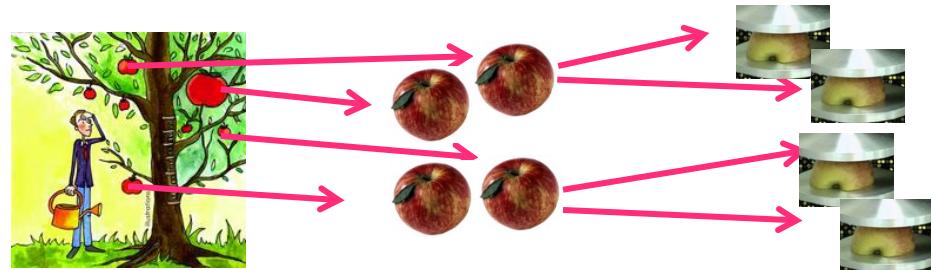
- Hyperspectral images: what about the third way?  
Spatial interpretation of the  $\alpha$  weight vectors

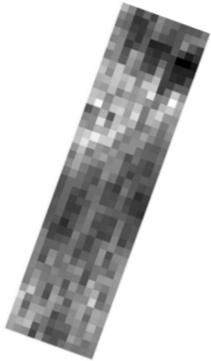
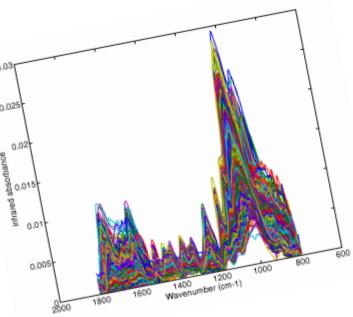


- With more than 2 spatial resolution

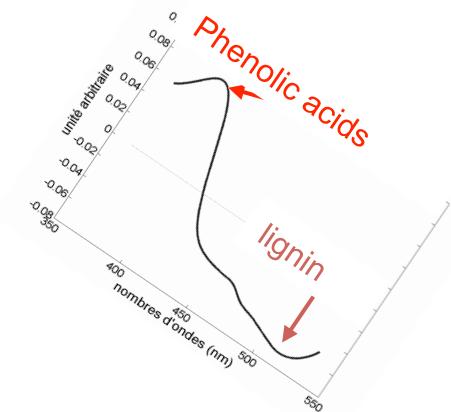


- Generic approach:  
multiscale context.  
anytime a vector can be  
paired to a set of vector

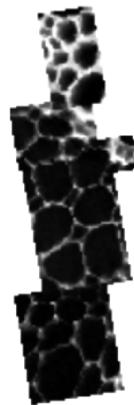
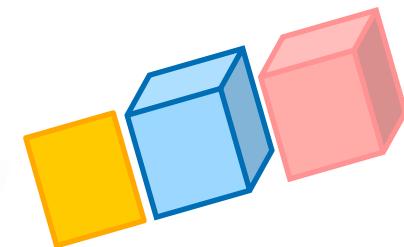
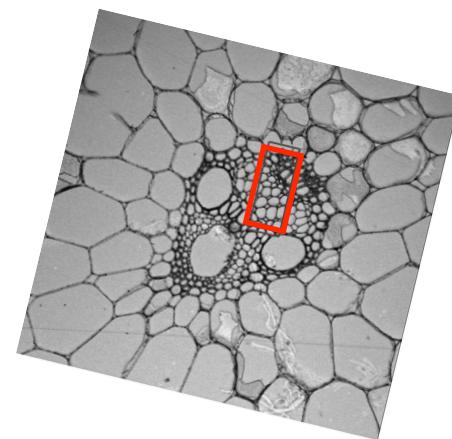
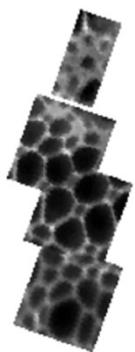
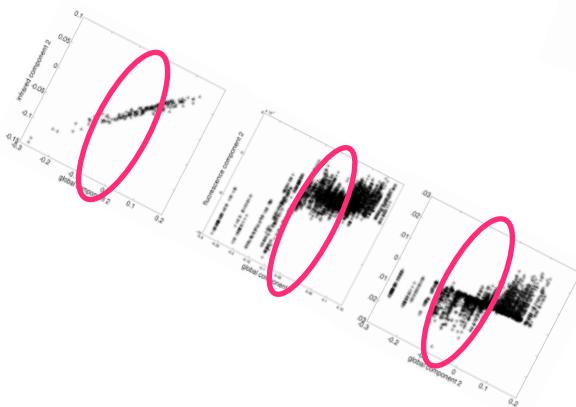
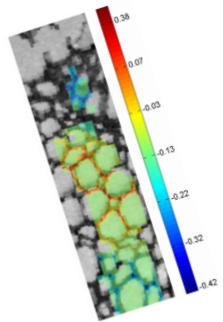




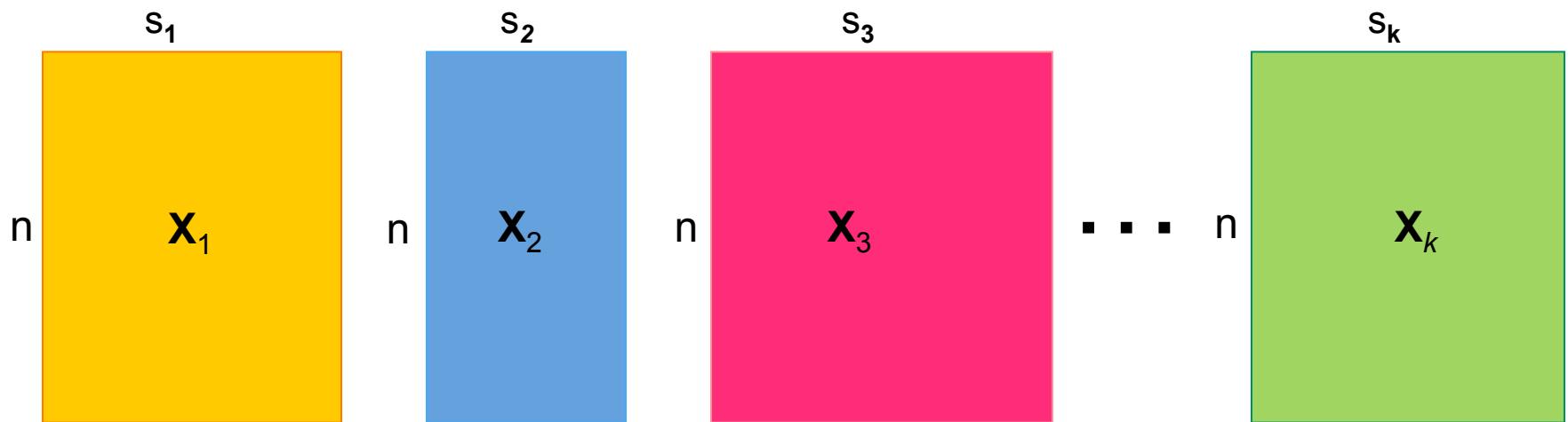
$c_{x_k} = X_k u_k$        $c_{Y_{j(z)}} = Y_{j(z)} v_j$   
 $\text{Max} \sum \text{cov}^2(c_{x_k}, c_g) + \sum \sum \text{cov}^2(c_{Y_{j(z)}}, c_g)$



Thank you for your attention !



# Multiblock analysis: multiple co-inertia analysis



block component →  $c_{X_k} = \mathbf{X}_k \mathbf{u}_k$  ← global component  
loadings ↑

Maximise  $\sum_{k=1}^K \text{cov}^2(c_{X_k}, c_g)$

Deflation :  $\mathbf{X}_k^{(h)} = \mathbf{X}_k^{(h-1)} - c_{X_k}^{(h-1)} \mathbf{u}_k^{(h-1)}$



subtract the information described in the block component

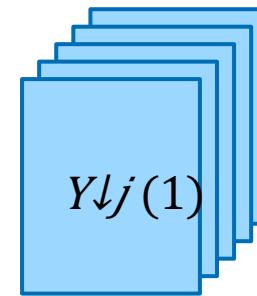
## Trilinear Multiple Co-inertia Analysis: deflation

Next components, loadings and weight vectors are assessed after deflation

Deflation is performed to provide orthogonal loadings per block

$$X_k^{(h+1)} = X_k^{(h)} - C_{X_k}^{(h)} U_k^{(h) \prime}$$

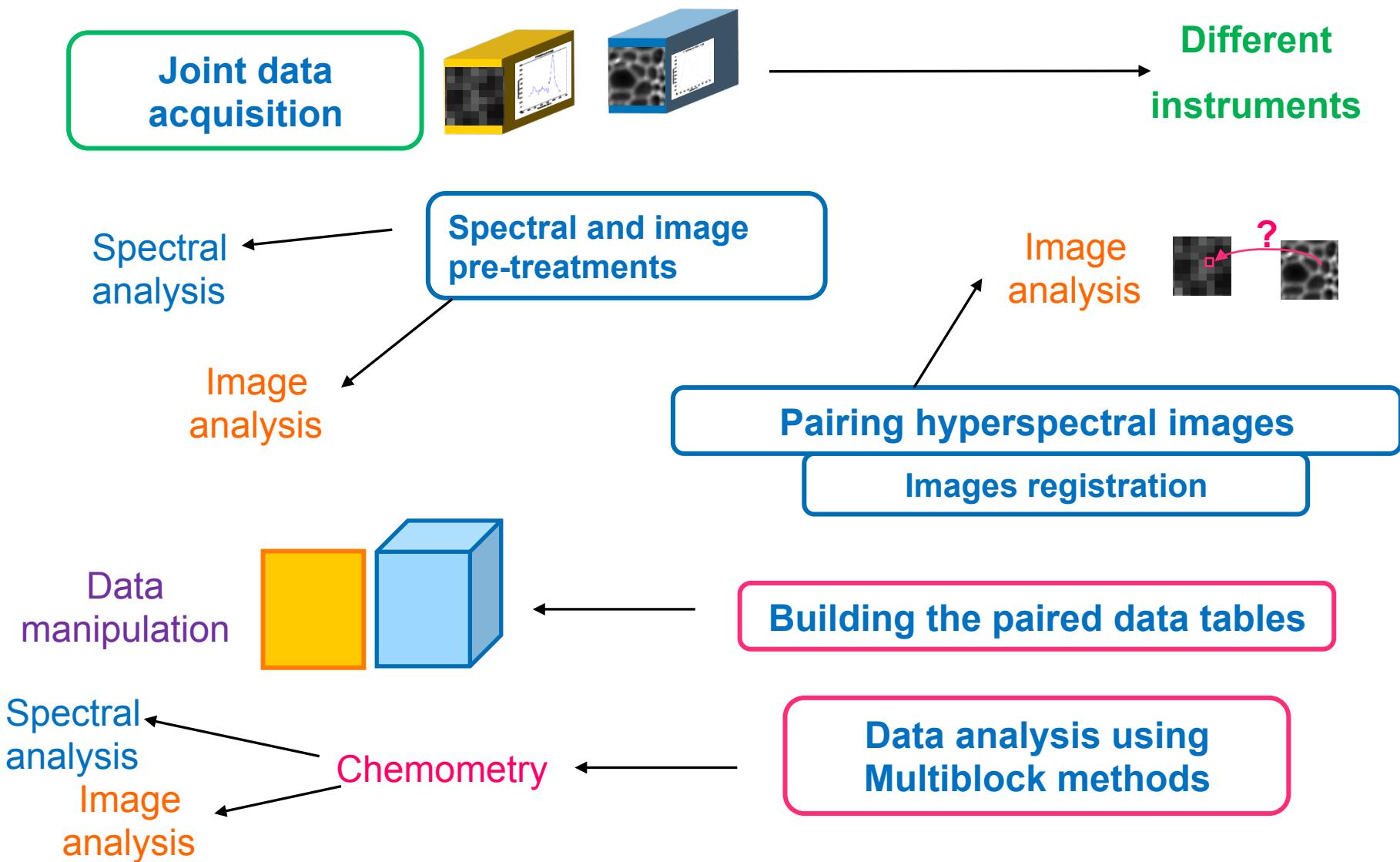
Deflation is performed on each stack of the three-way block



$$Y_{j(z)}^{(h+1)} = Y_{j(z)}^{(h)} - C_{Y_{j(z)}}^{(h)} V_j^{(h) \prime}$$

# Coupling multimodal hyperspectral images

## Multidisciplinary steps...

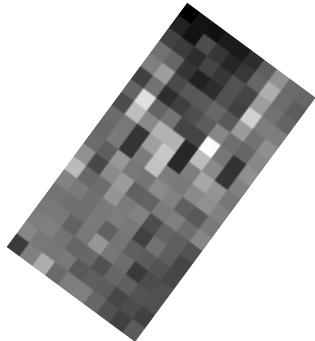


*Demonstration of the whole chain of analysis: PhD thesis F Allouche 2009-2012*

# Définir une image de référence Recaler, Fusionner ?

Définir une image de référence...

*Sum of intensities*



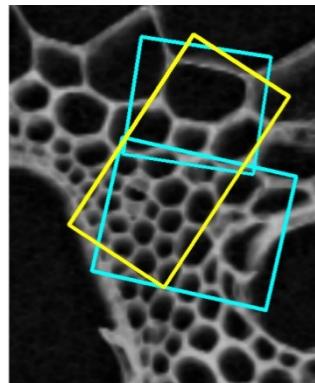
Infrared

Pixel size  
5  $\mu\text{m}$

Raman

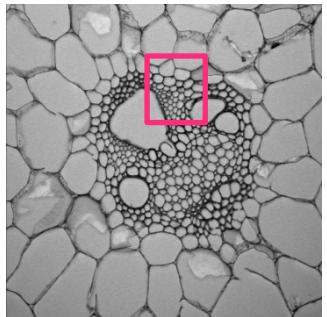
Pixel size  
1  $\mu\text{m}$

*Reference image inverted*



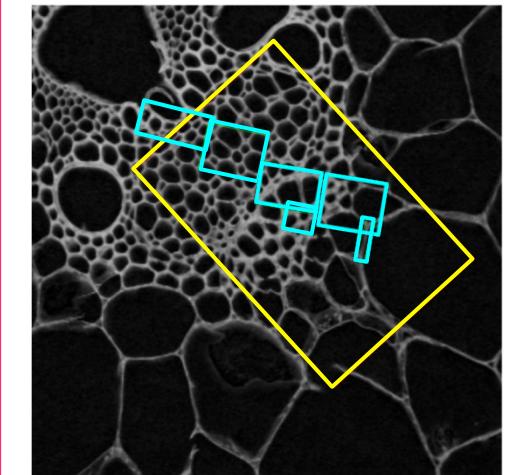
Registered image

Dataset 1



Reference image  
(confocal-brightfield)

Dataset 2



# Trilinear Multiple Co-inertia Analysis: algorithm

## Initialisation :

- Start with random  $\alpha$  weight vector with  $\|\alpha\|=1$

## Iteration :

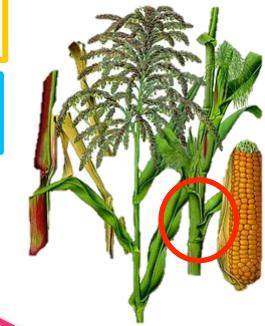
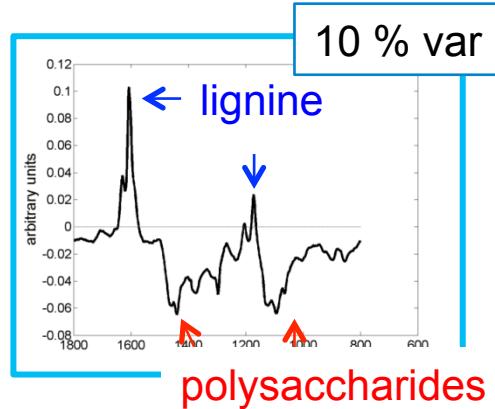
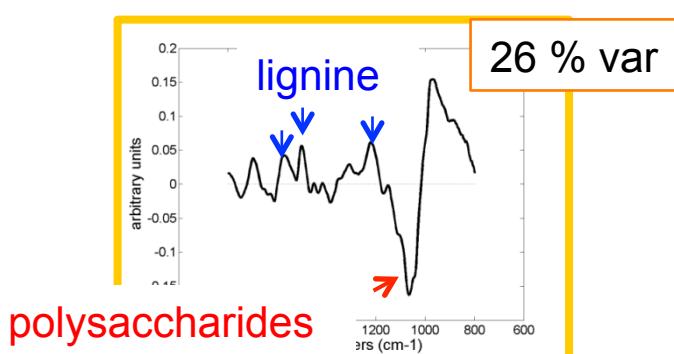
- Apply Multiple Co-inertia Analysis to weighted sum data tables
- Set  $\alpha$  weight vector:  
similarity between global and block component
- Normalise weight vector:  $\|\alpha\|=1$

$$\alpha_j^{p^2} = \begin{matrix} p^2 \\ \text{---} \\ \alpha_j \end{matrix} = \begin{matrix} n \\ \text{---} \\ c_g \end{matrix} \cdot * \begin{matrix} n \\ \text{---} \\ c_{Y_j} \end{matrix}$$

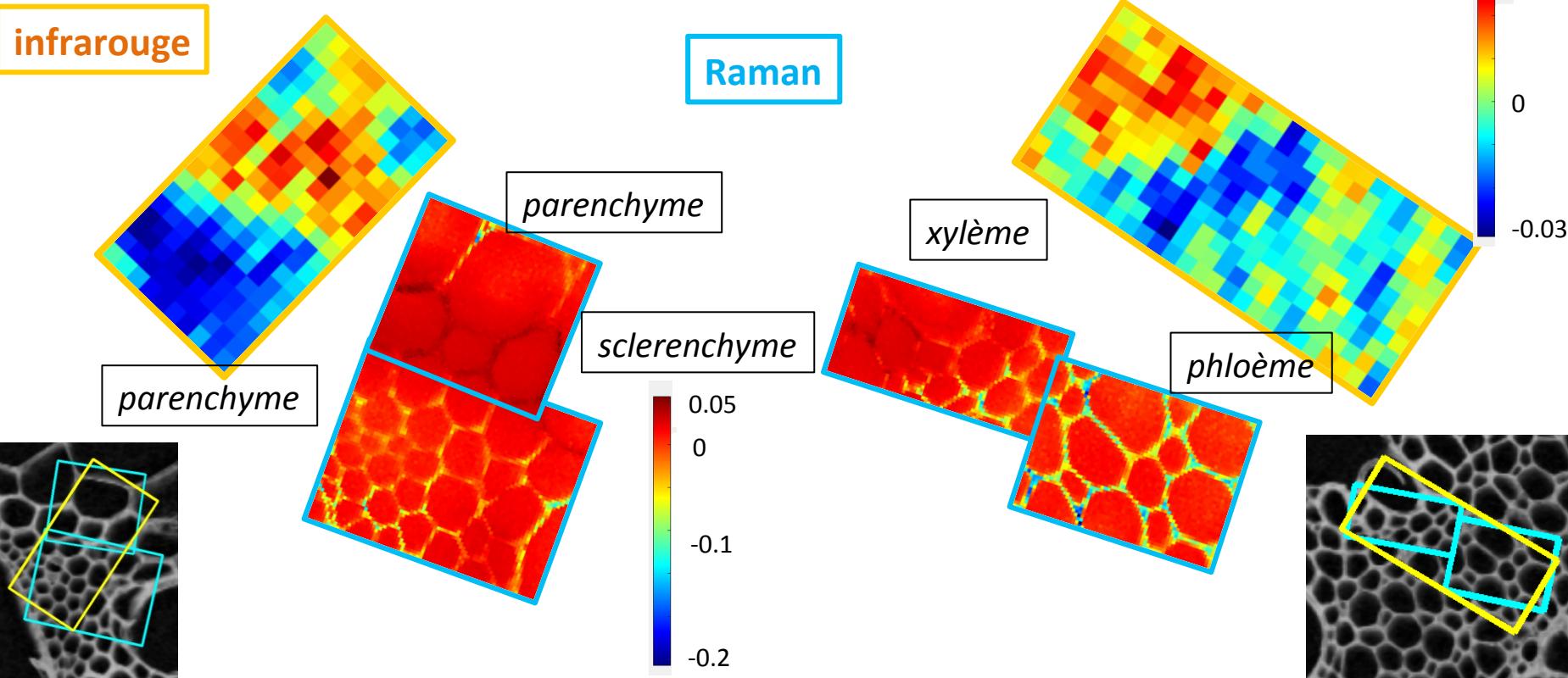
## Convergence :

- Stop when **loadings** and **scores** do not change between two iterations.

# Analyse Trilinéaire en Co-inertie Multiple *section de tige de maïs*



## Composante 2

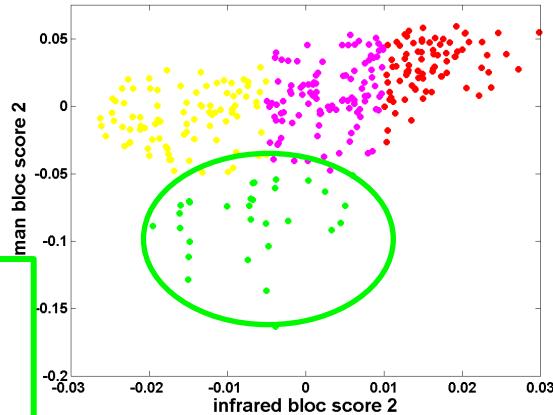


# Analyse Trilinéaire en Co-inertie Multiple

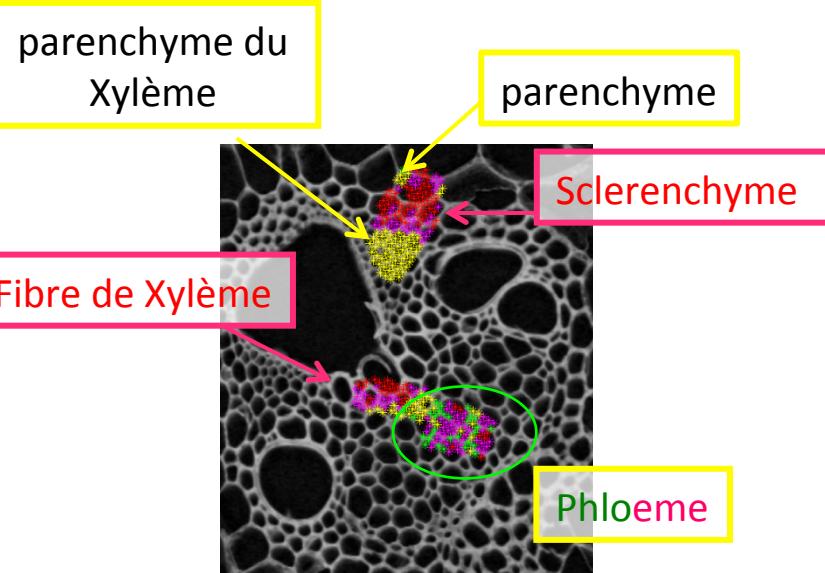
composante 2: lignin / polysaccharides

IR 5 μm / Raman 1μm

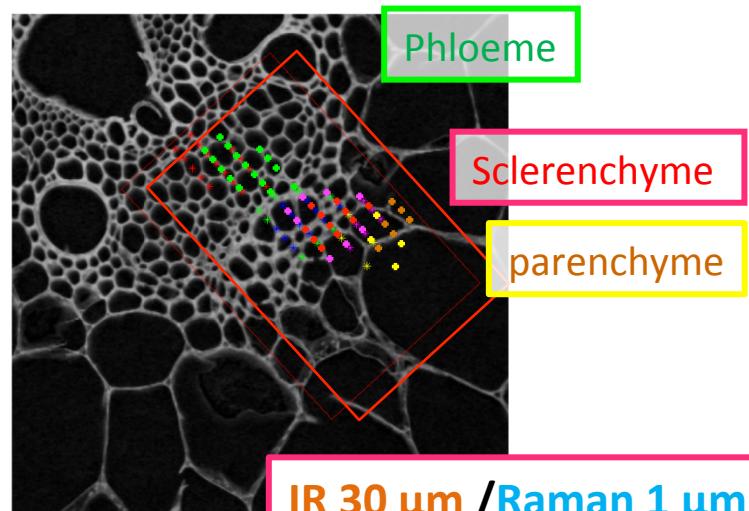
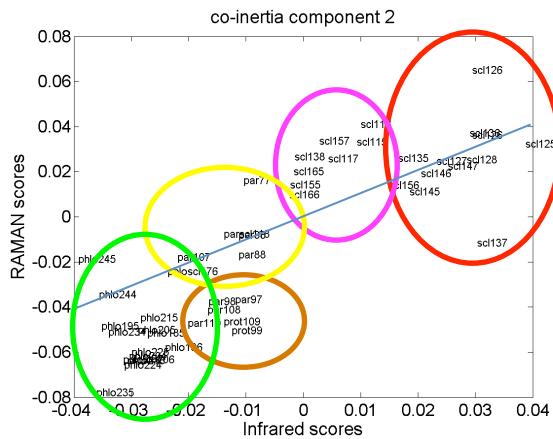
## Dataset 1



# Raman région non correlée



## Dataset 2



## Data structure

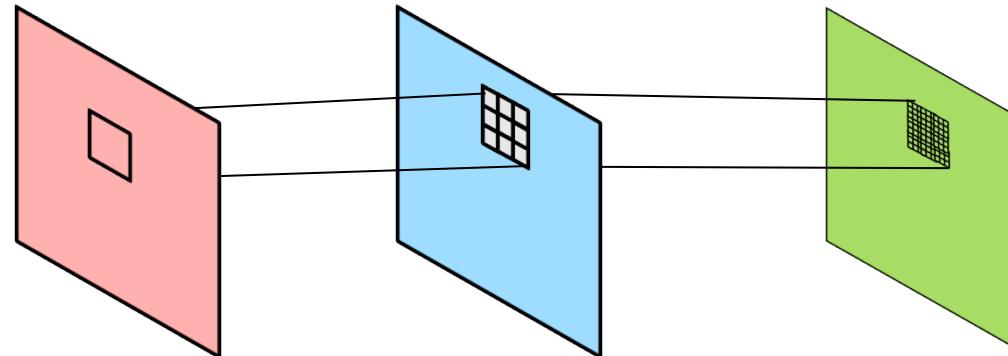
# Multiresolution hyperspectral images / Multiresolution data tables

Pixel size  $p_1 = s_2 * p_2$

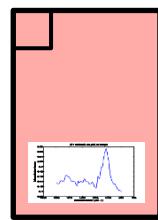
$p_2 = s_3 * p_3$

$p_3$

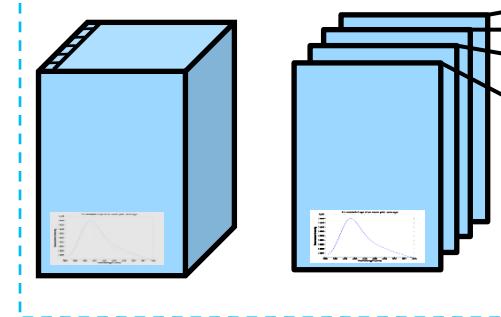
Images



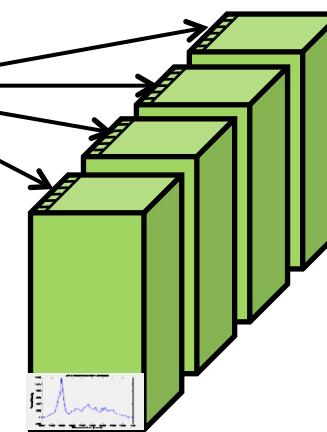
Data tables



$D^2(n, \lambda_1)$



$D^3(n, \lambda_2, s_2^2)$



$D^4(n, \lambda_3, s_2^2, s_3^2)$

Unfolding small images leads to multiresolution data tables  
=> multiway data tables with heterogeneous numbers of way

# Plant cell wall

## Chemical composition

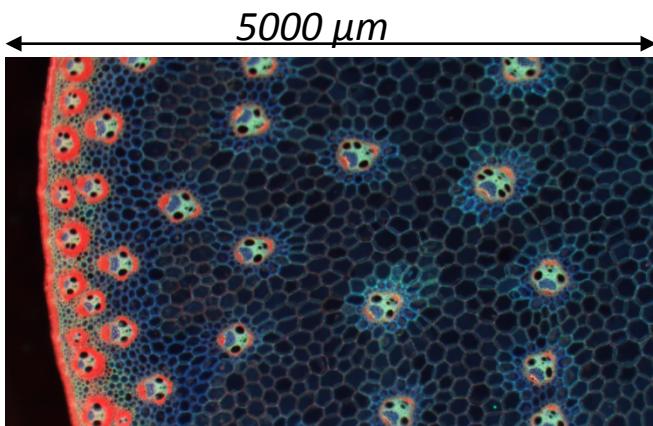
Major constituents  
are complex polymers

- Carbohydrates
- Lignins
- Proteins
- Lipids



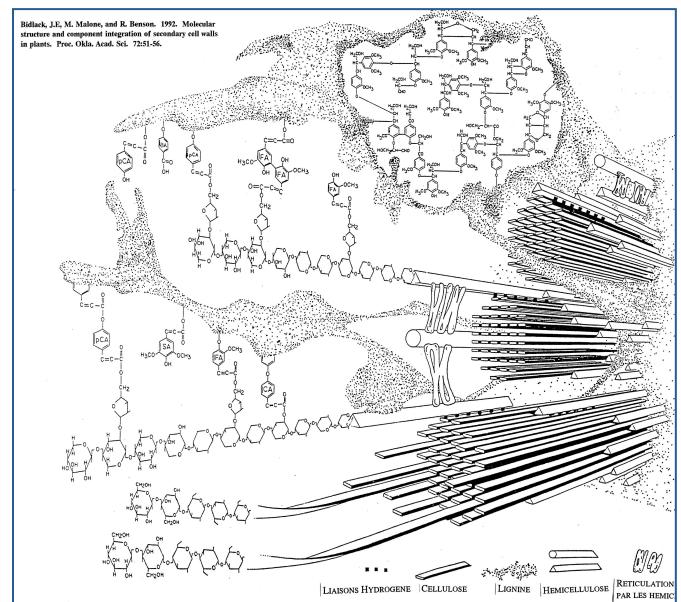
Constituents are organised....  
Ex: In cell walls

Maize stem



In the plant

Autofluorescence: false color, Blue and UV fluorescence



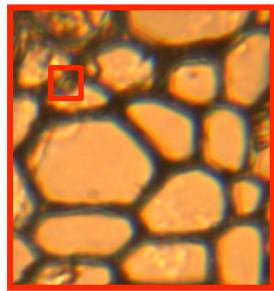
Bidlack et al., 1992

# **Microspectroscopy and hyperspectral imaging**

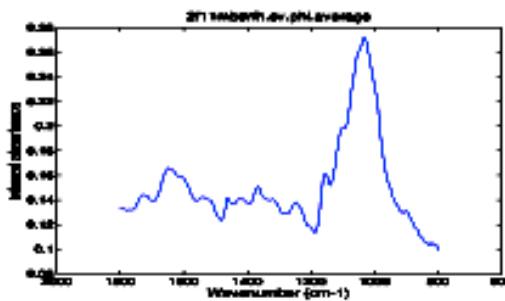
## *in situ* chemical analysis



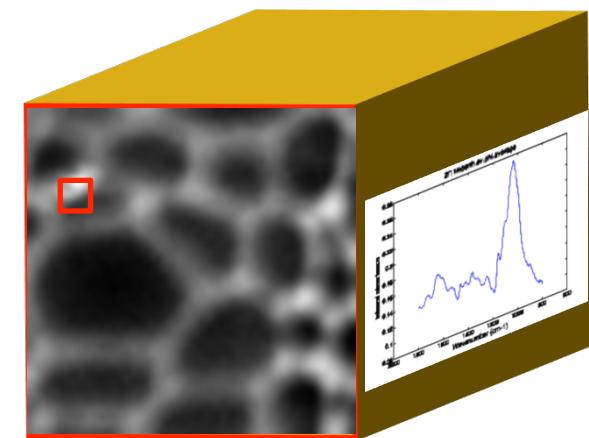
## Spectrophotometer + Microscope



## Sample region



One complete spectrum is acquired for each pixel



*pixels*

*pixels*

Scanning a region lead  
to one  
hyperspectral image