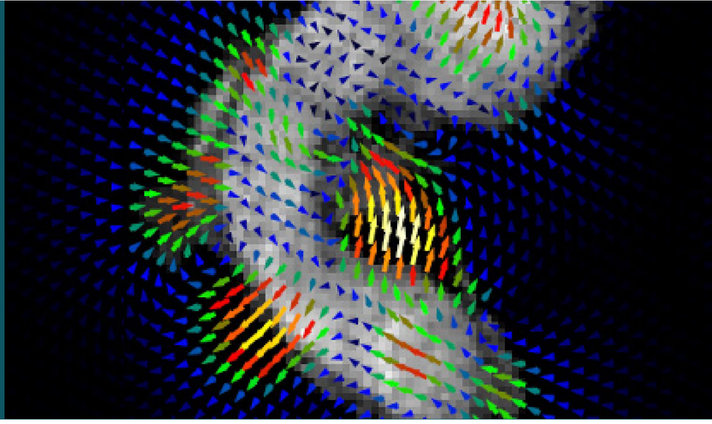

©Florent Grélard - Illustration of the deformations applied to a grain section observed in MALDI to superimpose it over its counterpart observed in MRI. The colour of the arrows reflects the intensity of the displacement (weak in blue, moderate in green, strong in yellow and red).

Coupling several imaging methods improves agronomic product characterisation

Read more

Grélard F. *et al.*
Esmraldi: efficient methods for the fusion of mass spectrometry and magnetic resonance images
BMC Bioinformatics . 2021
https://doi.org/10.1186/s12859-020-03954-z

Value creation

The set of methods developed is distributed in the form of a library in Python language and is available from the GitHub development platform. It has been integrated into a 'compute capsule' to facilitate analysis reproducibility.

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Context

Water and polysaccharides in cell walls are two components that have a strong impact on the technological or usage properties of agronomic products, especially cereals. Different imaging methods are able to characterise these two components: mass spectrometry imaging (MSI) can map the chemical composition of samples without any preconceived notions of the molecules to be analysed, and magnetic resonance imaging (MRI), a non-destructive method, reveals the anatomy of the organs and the state of hydration (content/mobility). To get a complete picture of the sample, researchers must be able to compare and merge the information obtained from these two methods. The difficulties concern the difference in image resolution, and the deformations caused by MSI during sample preparation.

Results

We developed a complete image processing workflow to merge the information obtained from both imaging methods. The workflow includes method-specific preprocessing steps, image registration to spatially match information, and dimension reduction to simplify the data. Spatialised information can be superimposed to match the chemical composition and mobility of the water and thus to understand, without any preconceived ideas, the molecules whose location correlates best with that of the water.

When applied to wheat grains at different stages of development, the method can be used to correlate the nature of hydration to the degree of substitution and acetylation of non-cellulosic polysaccharides present in the grain walls. In particular, the co-location of the most substituted and/or highly acetylated xylans in the most hydrated regions suggests a higher porosity of the walls related to the xylan modification. These two structural elements have been described as having an impact on wall organisation and polysaccharide interactions in the walls; however, to our knowledge this is the first clear evidence of this correlation at the plant level.

Future outlook

After having validated the approach on 2D sections, we are now studying the joint variations in composition and water content/mobility at the 3D grain scale, at different stages of development. We are also exploring multi-block methods for analysing data to take advantage of the abundant information.