PhD Position in Computer Science:
Multiscale Modeling of Plant Cell Wall Deconstruction

Applications are invited for a PhD position in spatio-temporal modeling of plant cell wall deconstruction.

Duration: 3 years
Start date: October 1st 2024
Key-words: Computational modeling, 4D (space + time) image processing, plant cell wall, enzymatic deconstruction

Context:
The environmental and economic challenges of climate change, and the growing global demand for energy, underscore the importance of a green transition from fossil carbon sources to alternative energy and material sources. The transformation of plant cell wall into bioproducts can be a sustainable, and carbon-neutral solution by recycling atmospheric CO2, and by cutting down our reliance on oil. A major challenge in converting the plant cell wall to bioproducts is the resistance of the plant cell wall, known as recalcitrance, which increases the cost of conversion. Over the past decades, extensive research has focused on recalcitrance, leading to the identification of key recalcitrance markers such as cell wall porosity and lignin content [1]. Notably, investigations have predominantly focused on markers at the nano-scale, while the enzymatic hydrolysis of plant cell wall at the cell and tissue scales remains under-investigated. Our team has recently overcome the experimental and computational challenges of studying the enzymatic deconstruction at micro-scale by developing a 4D (space + time) imaging pipeline including time-lapse fluorescence confocal imaging, and 4D image processing [2] together with first spatio-temporal computational models of enzymatic deconstruction. Mathematical modelling is a powerful tool to understand the underlying mechanisms of plant cell wall deconstruction [3].
This PhD position is part of the FillingGaps project (9 M€ budget) led by FARE laboratory and funded by the French National Research Agency under the B-BEST programme. FillingGaps aims to develop multiscale approaches for model biomass species to achieve a deeper understanding of the factors governing LB recalcitrance and the mechanisms underlying LB deconstruction.

PhD project:
The PhD project will involve:

- Interaction with engineers in charge of collecting time-lapse 3D acquisitions of maize stem samples during enzymatic hydrolysis using a fluorescence confocal microscopy. Collected datasets will include different maize samples (wild-type and mutant) under different conditions (e.g. enzymatic activity).
- Extraction of virtual representations of maize stem samples during hydrolysis from the collected time-lapse confocal datasets using the existing 4D image processing pipeline [2].
- Coupling these representations with computational models (e.g. partial differential equations that describe the underlying mechanisms of enzymatic deconstruction [3]) to reveal hidden variables that govern the hydrolysis.

The pivotal part of the project involves the seamless integration of these partial dynamics together with computational models into a comprehensive global model. This global model aims to provide a simplified and global representation of the enzymatic deconstruction of the entire maize stem which can guide further lab experiments.

We offer an outstanding scientific and technical infrastructure (such as computing facilities of the ROMEO HPC centre, state of the art confocal microscope facility to collect datasets, etc), a highly motivated research team, as well as an international and interdisciplinary working environment offering ideal conditions for successfully conducting the research project.

Requirements:
Candidates should have a master in computer science, engineering, applied mathematics, or related fields. Applicants should have good skills in the Python programming language. Experience in image processing and computational modeling would also be advantageous. Good communication skills are essential as the successful candidate will need to work in an interdisciplinary team gathering different researchers and write up their research work for presentation and publication.

Salary: Approximately 2100€ per month (gross), including health insurance and 35 days of annual leave.

Locations: The PhD student will be engaged in a collaborative project between two laboratories: FARE laboratory in Reims, France and MORPHEME team in Sophia-Antipolis, France. This arrangement provides the unique opportunity to benefit from the expertise and resources of both laboratories, offering a diverse and enriching research experience.

Application: Applicants should send a letter of motivation and a detailed CV to :
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References:
[1] Zoghlami, Aya, and Gabriel Paës. "Lignocellulosic biomass: understanding recalcitrance and predicting hydrolysis." *Frontiers in chemistry* 7 (2019): 874. https://doi.org/10.3389/fchem.2019.00874
[2] Refahi, Yassin, et al. "Plant Cell Wall Enzymatic Deconstruction: Bridging the Gap Between Micro and Nano Scales." *bioRxiv* (2024): 2024-01. https://doi.org/10.1101/2024.01.11.575220
[3] Jeoh, Tina, et al. "Mechanistic kinetic models of enzymatic cellulose hydrolysis—a review." *Biotechnology and bioengineering* 114.7 (2017): 1369-1385. https://doi.org/10.1002/bit.26277