

Developing WHEAMM, a new FSPM for the simulation of wheat cultivar mixtures. Feedbacks on model conception, sensitivity analysis and automatic calibration in Julia

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Developing WHEAMM, a new FSPM for the simulation of wheat cultivar mixtures. Feedbacks on model conception, sensitivity analysis and automatic calibration in Julia.

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The Green Revolution

Yield increase

- Breeding
- Chemical inputs
- Mecanization, irrigation



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Yield increase

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- Chemical inputs
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Negative externalities

- Landscape homogenization
- Loss of agro-biodiversity
- Pollution \rightarrow biodiversity, environment, human health



Climate change and yield stagnation



Figure from Schauberger et al. (2018)

 Agroecology : maximization of ecological processes to minimize the use of chemical inputs

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- Focus on cultivar mixtures
 - case study : winter wheat

Wheat cultivar mixtures

 17.5 % of wheat cultivated surface in France in 2022



in % of total cultivated wheat surface



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Wheat cultivar mixtures

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- Few assembling rules
 - except for resistance to fungal diseases
- Difficulties to study cultivar mixtures
 - combinatory explosion
 - difficult distinction between cultivars



in % of total cultivated wheat surface



RYT distribution

Meta-analysis on wheat cultivar mixtures (Borg et al. 2018) on the distribution of the Relative Yield Total (RYT = Yield mixture / Average yield in monoculture) \rightarrow large variance



RYT distribution

Large variance in the same environment: trial of 75 wheat cultivar mixtures at Le Moulon in France, 2014-2015 (Forst 2018)



Possible causes of RYT large variance

Expected yield from

Observed yield

 $\stackrel{\text{versus}}{\longleftrightarrow}$

of mixture

varietal proportions at sowing

and monoculture yields

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- inherent yield differences between monoculture and mixture for each cultivar (= phenotypic plasticity)

Hypothesis : these differences are caused by eco-physiological processes underlying plant-plant interactions

Differences in varietal proportions



Phenotypic plasticity



Source : Guntrip & Sibly (1998)

 $\label{eq:gmain} \mbox{Yield } (g/m^2) = \mbox{plant density x $\#$spikes/plant x $\#$grains/spike x grain weight}$



Number of plants per m²

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Grain filling

Tillering dynamics



 \rightarrow Focus on competition for light and its effect on tillering in conventional conditions

Research question

Understand the performance of cultivar mixtures from the evolution of varietal proportions between sowing and harvest by focusing on competition for light:

- Which traits are important for mixture performance?
- What is the importance of phenotypic plasticity for these traits and how is it shaped by plant-plant interactions?
- Are there differences in plastic responses among genotypes?

 \Rightarrow Interdisciplinary approach between field experiments and mechanistic modeling

- Experiments are essential but onerous
 - Diversification complicates combinatory designs
 - Difficulties raised by cultivar distinction in cultivar mixtures \rightarrow heavy and limited design (precision sowing)

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- FSPMs
 - Detailed 3D architecture + radiative model \rightarrow long simulation times (ADEL-wheat, CN-wheat, WALTer)
 - GreenLab models: simplified architecture + source-sink formalism \rightarrow short simulation times

Modeling strategy

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- Future applications: tool to support breeding for mixtures
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- Criteria
 - Short simulation time
 - Simulation of source-sink relations
 - Simulation of competition for light
 - Simulation of realistic and plastic tillering dynamics



- Organs: leaves, internodes, ears (no root system)
- \blacksquare Organogenesis \rightarrow thermal time calendar
- Biomass production by photosynthesis with the Monteith law

 $q(n) = PAR_n \cdot S_{el}(n) \cdot RUE$

 $\begin{array}{l} n: \mathsf{Day} \\ q: \mathsf{Produced biomass}\left(g\right) \\ \mathcal{PAR}: \mathsf{Photosynthetically Active Radiation}\left(MJ.m^{-2}\right) \\ \mathcal{S}_{el}: \mathsf{Exposed leaf surface}\left(m^2\right) \\ \mathcal{RUE}: \mathsf{Radiation Use Efficiency}\left(g.MJ^{-1}\right) \end{array}$

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• Approximation of S_{el} with a dedicated method for competition for light based on disks partition (Cournede et al. 2007)



 Biomass allocation with organ-specific beta functions (Baey 2014)



- Biomass allocation with organ-specific beta functions (Baey 2014)
- Height simulated as an independent process → final height of an internode of rank r (Lecarpentier et al. 2019) :

$$h(r) = (a \cdot r + b)^2$$



- Tillering dynamics
 - Emission
 - Cessation at R:FR ratio approximated by critical proximity Green Area Index GAI_c (Lecarpentier et al. 2019)
 - Regression when allocated biomass to an axis below threshold T_k (Larue et al. 2019) with protection delay Δ_{prot} (Lecarpentier et al. 2019)



Two model versions

- Individual plants (700 seconds)
- Average-plant (8 seconds) \rightarrow homogeneous canopy



Experimental data (Gawinowski et al. 2022)

- Field experiment (Perfomix project) at Le Moulon, France in 2019-2020 and 2020-2021
- 8 winter wheat elite cultivars with different heading dates or final heights → two contrasted quaternary mixtures
- Precision sowing for mixed stands by respecting spatial distributions
- Phenotyping
 - Growth: height, number of tillers, plant biomass, leaves surface and weight
 - Harvest: yield components



Global sensitivity of WHEAMM in pure stands

- GlobalSensitivityAnalysis Julia package (Rennels & Anthoff 2022)
- Computation of first and total order Sobol indices (Sobol 2001) for 24 parameters on different outputs
- Number of tillers at harvest



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- Experimental data \rightarrow Perfomix experiment for 8 elite cultivars grown in pure stands with variables throughout growth and at harvest
- Optim Julia package (Mogensen & Riseth 2018), simulated annealing algorithm with bounds (Goffe et al. 1994)
- 16 parameters jointly calibrated for each genotype and season separately
- Objective function (Seber & Wild 2003)

$$RMSE = \frac{1}{N_V} \sum_{\nu=1}^{V} \frac{1}{N_{T_\nu}} \sum_{t=1}^{T_\nu} \sqrt{\sum_{i=1}^{l_{\nu t}} \left(\frac{y_{\nu ti,obs} - y_{\nu t,sim}}{\sigma_{\nu t}}\right)^2}$$

Example of simulations with calibrated parameters for genotype Expert in 2019-2020



Better goodness-of-fit in 2019-2020 than 2020-2021

- Better goodness-of-fit in 2019-2020 than 2020-2021
- Calibrated parameters
 - Contrasted estimations between genotypes and/or seasons
 - 10% of parameters calibrated to their upper bounds
 - High values: extinction coefficient k_b , thermal time of emergence τ_{init} , biomass threshold activating regression T_k

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 - High values \rightarrow systematic activation, regression truly controled by $\Delta_{\textit{prot}}$
 - Solution: make regression irreversible and more progressive

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- Non conclusive validation
 - Another season \rightarrow joint calibration
 - Another density \rightarrow tillering misspecifications, calibration on several densities (Blanc et al. 2021)

Simulations in mixture

- "Individual plants" version
- Perspective to study differences in means and variances between pure and mixed stands on simulated data → implementation of stochasticity on the emergence date to simulate inter-individual variability between plants of the same genotype, even in pure stands

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- Sensitivity analysis in mixture
- Simulations in mixtures
 - Parameter values calibrated in pure stands in 2019-2020
 - Simulations of the two quaternary mixtures of the Perfomix experiment in 2019-2020
 - Mixture 1 (contrasted earliness)

Simulations Mixture 1 in 2019



 \rightarrow Satisfying tillering (although peak too early and regression too weak for Expert) but biomass often underestimated

 \rightarrow Simulated variability largely underestimated

Convergence of tillering dynamics in mixture

Simulated data for mixture 1 in 2019-2020



 \rightarrow In accordance with experimental data

Development of WHEAMM

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 - Realistic tillering dynamics in 3 phases with plastic responses to competition for light
 - Implementation of competition for light without detailed 3D architecture

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- All criteria
 - Source-sink formalism + minimalist 3D architecture \rightarrow fast simulations
 - Realistic tillering dynamics in 3 phases with plastic responses to competition for light
 - Implementation of competition for light without detailed 3D architecture
- Confrontation to reality
 - WHEAMM not fully validated on the PerfoMix experiment
 - Satisfying calibration for many cultivars in pure stands
 - Simulation of diverse plastic behaviors in mixtures
 - Emergence of tillering convergence in mixtures

Importance of sensitivity analysis and automatic calibration in a modeling cycle

 "The point of falsifying a model is not to learn that the model is false but rather to learn the ways in which a model is false" (Gelman & Shalizi 2013)

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- Essential to good modeling practices (Cournède et al. 2013) but too rare for FSPMs
- Manual calibration too subjective
- No consensus on calibration practices for crop models (Wallach 2011) but consideration of entire process

Modeling challenges \rightarrow computation time

 WHEAMM "average plant" 8 seconds vs WHEAMM "individual plants" 10 minutes

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Modeling challenges \rightarrow computation time

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- Parallel simulations → possible for sensitivity analyses but not always for automatic calibration (iterative process)
- Calibration → parallel computing within the one simulation (parallel computation of different plants at one timestep)
- Metamodeling: Gaussian processes (kriging) metamodels to approximate complex models coupled with a sequential EGO (expectation global optimization) method
 - Successful automatic calibration for tillering parameters in WALTer (Blanc et al. 2021)
 - Further developments required for WHEAMM \rightarrow plant scale, several variables

Conclusion

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- Use of Julia for model development
 - Efficiency
 - Accessible
 - Important number of packages
 - Community
 - But lack of solutions for some very specific issues...
- Perspectives
 - Solve identified tillering misspecifications, add sources of stochasticity and a root sink
 - Many possible applications, notably coupling WHEAMM with population genetics models to study heterogeneous populations over sowing/resowing cycles

Thank your for your attention!

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