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Reducing a model of sugar metabolism in peach fruit to explore genetic diversity

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1 Introduction

Nowadays, increasing efforts are made to select varieties that respond to a large panel of criteria, including abiotic and biotic stress tolerance, increased yield and quality of food products. Gene-to-phenotype models have been considered as the tools of the future since they can help to test the performance of new genotypes under different environment and management conditions. A kinetic model of sugar metabolism has been developed by Desnoues et al. (2018) to simulate the accumulation of different sugars during peach fruit development as a set of parametric ordinary differential equations. The model correctly accounts for annual variability and for the genotypic variations observed in ten peach genotypes issued from an inter-specific population. Two major drawbacks of this model are the number of parameters to estimate and its integration time that can be costly due to non-linearities and time-dependent input functions. Together, these issues hamper the use of the model for the whole genetic progeny of 106 genotypes, for which few data

are available (six data points or less per sugar). Several reduction and approximation approaches exist in literature, each one addressing a specific aspect of model complexity (Cariboni et al., 2007; Heinrich and Schuster, 1996). In this work, we present a model reduction scheme that combines different methods in several parallel steps. The purpose is i) to obtain a simplified model showing comparable predictions as the original model while reducing its calibration time and number of parameters. ii) to calibrate it for the genotypic progeny and develop an integrated genetic-kinetic model.

2 Methods

First, multivariate sensitivity analysis (Lamboni et al., 2009) was applied to identify those parameters having a significant influence on the outputs of the model, over the whole dynamics. Second, we operated three structural simplifications in terms of network and reactions rates to reduce the complexity of the model. Third, timescale-based approaches and quasi-steady-state approximation (López Zazueta et al., 2018) were applied to reduce the number of ODEs of the model. The quality of individual and combined reduction steps was systematically evaluated with respect to the original model according to three criteria of major importance for our application: the Akaike Information Criterium (AIC), the calibration time and the expected error over a population of virtual genotypes.

3 Results and conclusions

Results from the reduction steps were combined into a final reduced model (Fig. 1). This model has only 9 parameters to be estimated, linear flows, 9 ODEs and only one temporal enzymatic capacity, common to all genotypes. Comparison between the reduced and the original model showed an equivalent fit quality and confirmed a strong benefice for most genotypes. Results showed a satisfactory agreement between predictions and experimental data. Thanks to the reduced calibration time, the whole progeny of 106 genotypes 'could be' calibrated. The parameter values obtained were considered as quantitative genetic traits and used for a Quantitative Trait Loci analysis. Results from this analysis were then used to define a genetic model to be incorporated in the reduced kinetic model. This opens the possibility of predicting sugar metabolism of genotypes carrying diverse combinations of alleles at the markers controlling the parameters.

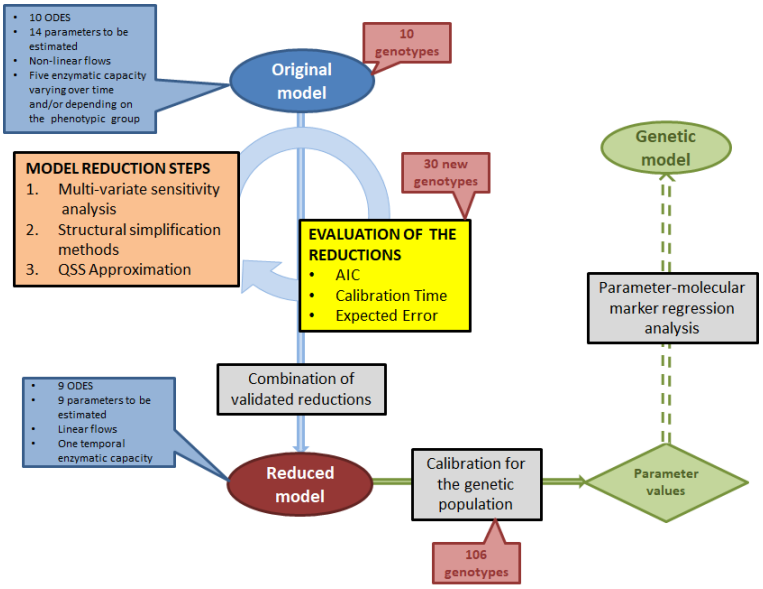

Figure 1: Graphical representation of the proposed strategy to calibrate 106 genotypes. Orange rectangle represent reduction methods. Yellow rectangle represent model evaluation steps by means of our 3 criteria: AIC, calibration time and expected error. The specificity of the original and reduced models are indicated in blue. Green dashed line represent the perspective part.

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