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MATHEMATICAL MODELLING IN THE SCIENCE AND TECHNOLOGY OF PLANT BREEDING

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Abstract. The livelihood of humanity depends crucially on the growing and harvesting of crops, the processing of crops to produce the various foods that are eaten and the distribution of the resulting products and produce to the various consumers. The underlying biological foundation on which the success of this complex industrial hierarchy of activity rests is the success of the ongoing process of plant breeding. Not only must plants be bred to ensure that the planned end-products, such as bread, cakes, pasta and noodles, are of acceptable quality, they must, in order to minimize crop failure and thereby ensure food security and supply, also be insect and/or disease resistant. The success of such endeavours rests on the quality of the underlying science, which has become highly sophisticated in recent years. Its utilization, in terms of the modern understanding of the genetics of plant growth and the increasing sophistication of experimentation and instrumentation, has greatly improved the speed and quality of plant breeding. The associated implementation of these new plant breeding protocols is generating a need for improved quantification through the utilization of mathematical modelling. In order to illustrate the diverse range of mathematics required to support such quantification, this paper discusses some illustrative aspects connected with the recent modelling of the flow and deformation of wheat-flour dough, information recovery from spectroscopic data (e.g. such as the determination of the protein content in wheat), antiviral resistance in plants and pattern formation in plants. Various aspects of the mathematics involved are highlighted from a mathematical modelling perspective, with a key secondary goal, using the discussion about these examples, of illustrating how applications impact on mathematics with the resulting mathematical developments in turn contributing to the solution of other applications with the process starting all over again.

Key words. plants, plant breeding, near infrared spectroscopy, hexagonal cell modelling, linear viscoelasticity, pattern formation, reaction diffusion modelling, derivative spectroscopy, causal modelling, rheology

1. Introduction

In traditional mathematical modelling, such as in the application of the equations of fluid dynamics [23] to the solution of practical problems such as flow of wind through and over plant canopies and the infiltration of water into soils [21], the underlying fundamentals are clearly understood to the point where well-defined and comprehensive mathematical models are available. In such traditional modelling, the first step often reduces to an assessment of the dominant robust behaviour of the phenomenon being modelled which should be utilized to capture the essence of the situation under examination (e.g. geophysical fluid dynamics [65]; industrial mathematical modelling [26]). The available experimental evidence and scientific background play a key role in this process. The second step reduces to solving and interpreting the resulting set of equations (e.g. numerical methods for the solution of differential equations [56, 22]).

There are also areas of biology where such modelling plays the key role. They include the modelling of human physiology [64], the design of artificial arteries [42] and reaction-diffusion modelling of pattern formation in plants and animals [74, 58].

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In other areas of biology, the modelling is still very much a hypothesis-and-test exploratory activity, in that there is insufficient information about the problem context to give a clear guide as to how to "uniquely" identify the likely solution from within the various possibilities [25, 38, 24]. This is the situation not only in biology, but also in sociology, economics and physiology and even in many areas of industrial mathematical modelling [33]. A number of proven strategies act as guides on how to progress the exploratory process. They include the formulation and utilization of allometric scaling laws [36], calibration-and-prediction [16], compartmental modelling and ordinary differential equation modelling [34].

In many situations, especially in areas of molecular biology, because only a partial picture of the assumed mechanism under examination has been tentatively formulated, success depends on coupling the modelling with complementary experimentation. In fact, the limiting factor is very much what can be performed and measured experimentally, not the plethora of possible models of the mechanism that can be formulated and solved computationally. The coupling, if properly managed, is the strength that mathematical modelling brings to the exploratory process. However, as explained in Anderssen and Waterhouse [17] and Groenenboom and Hogeweg [41], it is a chicken-and-egg situation: on the basis of experimental observations, a variety of models are formulated to simulate possible mechanism; as a proof-by-elimination activity, new experiments are performed to reduce uncertainty about the likely mechanism; the process continues inductively. For example, in areas like plant genetics, some of the questions to be resolved are quite speculative and their resolution depends on identifying and performing the more, rather than the less, appropriate experiments.

The overall goal of this paper is to illustrate, within the context of modelling biological aspects of plant breeding, the wide variety of mathematical modelling issues that arise when aiming to answer the real-world questions that orchestrated and orchestrates the associated modelling activity. In particular, discussion will focus on:

(i) The causal nature of mathematical models in biology with a specific emphasis on the modelling of the flow and deformation of wheat flour dough.

(ii) The role of the calibration-and-prediction methods as a surrogate for direct laboratory experimentation with a specific emphasis on the identification, from a large pool of pest resistant wheats, of the ones that contain the proteins that make good breads.

(iii) How insight, arising from the modelling of biological invasion, yields a possible foundation for modelling the antiviral response of plants. Such information is required for the design of biological protection for the plants selected through a plant breeding program.

(iv) Insight about how genetics controls the development of the various geometric features of plants is required to improve on current plant breeding protocols by identifying the presence or absence of key signalling proteins and hormones. Currently, such insight is being obtained by formulating simple rules for the control of the positioning of the hairs on the leaves of plants. The rules must not only reproduce the observed patterns in normal plants but also, for small changes in the parameters in the model, reproduce the known mutants.

A central underlying theme guiding the writing of this paper has been to illustrate "the impact of applications on mathematics". Sometimes, but always involving a mixture of mathematical expertise and lateral thinking, it only involves