An integrative modeling framework to evaluate wheat production systems: Fusarium head blight

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An integrative modeling framework to evaluate wheat production systems: Fusarium head blight

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\textbf{Abstract:} This paper describes a practical, integrated, web-based and user friendly analysis tool for crop model users that provides quality control of input data, tracks user selections in model parameterization, and enables visual analysis of model outcomes using a single graphical user interface. This allows the user to undertake numerous steps in crop modelling and analysis in a seamless and integrated environment. The analysis and visualization components of the system were enabled utilizing R (pplr) and the robustness of the underlying data structures and coupling point between crop and disease models were achieved through use of PostgreSQL database management system. The approach was tested to investigate changes in: 1) wheat yield between current climate and plausible future climate in the southern part of Brazil; and 2) climate-related risks such as Fusarium Head Blight (FHB), an important fungal disease that impacts wheat grain yield and quality. The integrative modeling framework (IMF) greatly enabled the assessment of impacts of climate variability/change on wheat. Application results found that wheat yields might benefit from higher rainfall in the projected climate scenario. In contrast, increase of FHB severity should contribute to reduced grain quality.

\textbf{Keywords:} database, crop models, climate change, Gibberella zeae, model coupling

\section{Introduction}

Agricultural productivity will have to improve in both developing and developed countries to achieve substantial increases in food production by 2050. This challenge is heightened as land and water resources become less abundant and the effects of climate change introduce much uncertainty [Antle, 2008]. There is a growing concern that global food security and the quality of food production may be affected by future climate and weather, with ramifications at both local and large scales. Adaptation to
climate change through changes in farming practices, cropping patterns, and use of new technologies will help to reduce the negative impacts [Huang et al., 2011] and grab any emerging opportunities.

Considerable efforts have been directed toward understanding climate change impacts on crop production in the past several decades. The resulting advances in our understanding of climate impacts have come from the compilation of better data and the real-time observation of changes in climate and affected sectors [Antle, 2008; Kurukulasuriya and Rosenthal, 2013]. Such knowledge is critical as we contemplate the use of crop models to design innovative technologies and policies to mitigate climate change and facilitate adaptation to the changes that now appear inevitable in the future. Crop production is affected by meteorological variables, including rising temperatures, altered precipitation regimes, and rising atmospheric carbon dioxide concentrations. Field observations and crop model simulations indicate that climate change impacts on agricultural production will be positive in some agricultural systems and regions, and negative in others. These effects will also interact with climate variability and vary through time [Parry et al., 2004; Rosenzweig et al., 2013a].

Progress on the impact of climate change and climate variability in agriculture is made difficult by a lack of shared data, tools and common language for communication. Digital data sources (e.g., datasets on expected future climate, historical weather, soil characteristics and crop genetic traits) could have a transformative impact on research, but only if they can be made available to multiple users in an integrated systems information technology (IT) environment. Such a system must contain not only data but also the software and tools to generate, synthesize and analyze them. The system should enable users to reproduce crop model simulations, to modify and re-simulate scenarios, and could also serve as a dynamic archive.

Much of the work crop modelers face concerns analyzing, transforming, and otherwise manipulating data stored in isolated files. These data can be categorized as belonging to one of a modest number of data types with well-defined formats. Therefore, much of the IT complexity impeding research progress is concerned with relatively tedious activities like finding and fetching datasets, converting one format to another, installing and combining programs into simulation runs to achieve some goal, executing the simulation runs, and recording the steps required to generating outputs.

Additional issues hampering scientists are those related to the wealth of statistical methods developed over the years which have led to a variety of potentially important new algorithms and tools. Many scientists may not have the necessary expertise or time to learn how to construct, install or maintain multiple programs.

The objective of our work is to demonstrate an integrative modeling framework that consistently and coherently manages the requirements of data and their use in model integration for crop modeling researchers. Here, we define information architecture as the structural design of an integrative information space to facilitate task completion and intuitive access to content. We seek to enable the user to run crop and disease models and present outputs through a single user interface, utilizing the most appropriate data handling and analysis tools without the requirement to continually update and install multiple programs on their own computers. The system was designed specifically to support simulations of a crop model coupled to disease models.

2 Implementation

2.1 Overview

Owing to the diversity of agronomist training, we sought to develop a system that takes advantage of the most recent information technologies while retaining a relatively simple, user-friendly front end. This allowed us to take advantage of new ways to publish and access information through components that
extend the capabilities of web applications and provide interactive and collabo-
ratwe system approaches without confounding the user with too much detail about the systems running beneath the surface. We
designed the graphical user interface to be recognizable to users by creating a stepwise workflow that
mimics the procedure common undertaken for a standard crop model simulation.

Our implementation of the framework integrates a set of existing software components, namely
PostgreSQL, R, Fortran, Java, PHP, Javascript, Shell script, etc (Table 1). Integration of existing and
established components allowed us to construct a sophisticated system quickly and focus our attention on
assembling the datasets, data types, and programs to attend crop modelers’ needs.

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2.2 Framework

The integrative modeling framework (IMF) combines several open-source technologies already available
to form a fully integrated user-friendly system. This allows the user to perform data management and
analysis tasks through a single web interface. The IMF consists of four major components: a database to
store and manipulate the data, the compiled crop and disease models, routing communication through a
database and a high-level interface to communicate with it.

PostgreSQL was a clear choice for the database, as it is the leading open source industrial strength
database, and is competitive in quality and performance with the major proprietary databases. Our
architecture builds upon the rigor of this system with the design and implementa-
tion of additional functionality built on top of the PostgreSQL database management system. PostgreSQL extends the
relational data model with support for complex objects and allows users to add new programming
languages to be available for writing special functions and procedures. A PL/R was implemented allowing the use of R from within a PostgreSQL database for advanced analytics in a simple, efficient, and
controlled manner. R is the leading free software environment for advanced mathematical and statistical
computation and graphics [R Core Team, 2013].

2.3 Data Management and Analysis

Import. Imported data, mostly climate data, are obtained from a number of different sources, types and
formats. In this way, the database was designed with a module enabling data conver-
sion from one format to another. This module is named integration (Figure 1), and it also stores the metadata for input
and output data needed by the crop and disease models. Weather observations are categorized as historical, recent, current and projected, and are stored as daily or hourly intervals.

Figure 1. Class Diagram of integration module, presenting the classes responsible for integration of input and output data

When importing data, each line of the input file is converted to a row in a temporary table in the database. Based on the data description, each row of the temporary table is subsequently examined for consistency, converted, and then stored in the database. The code that performs this operation is written inside the database. The procedural language PL/pgSQL, native to PostgreSQL, was used to implement the code.

Setting an experiment. Designing a virtual experiment involves describing which treatments (i.e., farm management approaches) are associated with specific options or factors that the user may want to explore. The user interactively selects the treatments and factors to be compared. In so doing, the user dynamically builds up a table describing the experimental design and model inputs.

To make crop model simulation outputs more intuitive and meaningful to users, on-line interactive visualizing tools were developed. These included geographical maps of data availability by region as well as tools to quickly analyze simulated outputs. These enable nearly instantaneous visual inspections and facilitate comparisons between different model configurations. The PL/R library allows R functions to be called programmatically within SQL statements. One of the main reasons for using PL/R (Procedural Language/R) is that it allows data to be passed directly from the database to the R environment and back again in a robust manner. New functionalities can easily be added to the system by wrapping R scripts into a PL/R function.

The completion of a simulation run triggers the creation of a dynamically built webpage that provides access to plots and R code from the simulated experimental design. It can be viewed with any standards compliant browser with Javascript and CSS support enabled.
2.4 An application example

Wheat (*Triticum aestivum* L.) is an important crop in Brazil; especially in the South where 90% of the growing area is established in the states of Rio Grande do Sul, Santa Catarina, and Paraná. In this region, weather conditions during the growing season favor the occurrence of wheat diseases, of which Fusarium head blight (FHB) is a major concern. Apart from losses in grain yield and reductions in baking and seed quality, the major peril due to FHB is the contamination of grain with toxic fungal secondary metabolites known as mycotoxins. Owing to these dangerous consequences of reducing wheat yield and quality around the world, computer models based on weather variables, have been developed to predict the likelihood of occurrence of FHB and mycotoxin contamination in wheat (Prandini et al., 2009). Disease modeling and improved information technologies for agricultural impacts assessment are major emphases of model development in the Agricultural Model Intercomparison and Improvement Project (Rosenzweig et al., 2013b).

In our test case, we used a crop-disease model to assess the impacts of climate variability/change over the state of Paraná, Brazil, using historical and projected climate scenarios.

2.5 Crop and disease model description

An FHB infection-risk simulation model [Del Ponte et al., 2005] implemented in a generic disease model coded in JAVA [Pavan et al., 2009] was linked to a wheat simulation model code in FORTRAN [Jones et al., 2003]. The wheat crop model simulates biological processes of wheat growth and development that operate on a daily time step. The inputs required to run the models are daily weather variables (temperature, rainfall, and moisture level), crop management information (planting date, fertilizer use, irrigation, etc.), cultivar characteristics and soil profile data. Selected output from the models included grain yield and FHB severity. Model inputs used in our example included initial water and nitrogen content in the soil profile, and dates of planting according to agroecological zoning. Planting density, sowing depth, date and rate of fertilization were specified according to standard local commercial practices. Cultivar was set to the Louro variety adapted to the all locations in the state of Paraná. Climatic inputs were historical observations or climate model-based scenarios of daily maximum and minimum temperatures, precipitation and solar radiation.

We developed a communications-based approach where the wheat crop model and the FHB model run concurrently while exchanging data through an intermediate relational database management system (Figure 2). The routing communication was based on the work reported by Solano et al. [2013]. The wheat model passed to the FHB model the day of the year that the first spike emerged, which in turn, dispatched the disease model.

2.6 Model inputs

Wheat varieties’ genetic coefficients, site specific soil profile characteristics and observed weather data (1980-2009) from Simpar weather station network were used as input for running the coupled wheat and FHB model. An ensemble of projected climate change scenarios (2070-2099) (drawing from the relatively more extreme A2 scenario of the third Coupled Model Intercomparison Project [Meehl et al., 2007; Nakicenovic et al., 2000] was also used to drive the models in order to understand how projected climate changes (particularly related to moisture) affect crop growth and the incidence of FHB in a probabilistic approach.
3 Results

The integrative framework was a flexible, lightweight, and agile workflow for fully-reproducible crop model simulation runs. The interface proved to be very useful in assisting to design multiple-factor virtual experiments, run the experiments and analyze simulated results from individual treatments. The coupled wheat and FHB models interacted with the coupling infrastructure correctly and heading date of the wheat crop was passed to disease model appropriately.

The coupled system produced simulated values for wheat yield and FHB severity for 27 locations in the Paraná state, 5 sowing dates and 30 years using observed and projected climate scenarios as inputs. The results indicated that, in the state of Paraná, the wheat crop would benefit from the increase in rainfall projected in the future climate scenarios (Figure 3). However, FHB severity will increase in more humid and warm climate scenario to the detriment of wheat quality (Figure 4). A similar work also projected that, with climate change, wheat anthesis dates will be earlier and fusarium ear blight epidemics will be more severe, especially in southern England, by the 2050s [Madgwick et al., 2011]. Visualization tools present in the integrative framework were extremely helpful for understanding data and model outputs.

The visualization of results is an important piece in our technological architecture. As the database is the core of our architecture, various technologies and methods for the visualization of data can be employed. The hypsometric maps, presented on Figures 3 and 4, were built using the spatial and interpolation R packages.
**Figure 3.** Hypsometric maps and empirical cumulative distributions with average of the normalized values of wheat grain yield for the Paraná state in the decades 2000-2009 (observed weather data) and 2090-2099 (projected climate scenarios)

**Figure 4.** Hypsometric maps and empirical cumulative distributions with average of the normalized values of FHB severity, in the decades 2000-2009 (observed weather data) and 2090-2099 (projected climate scenarios)

## 4 Concluding Remarks

By leveraging the power of relational databases, the IMF offers integrated management and manipulation of data for crop model applications. It was demonstrated that the IMF is a practical and extensible solution for investigators who seek to deploy crop models to evaluate impact of climate change and climate variability on agricultural crops.

The IMF architecture is flexible and scalable to allow new crop models, analysis algorithms and tools to be added with relative ease and to cope with large increases in data volume. It integrates the power of the software R for model input and output data analysis.

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