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Towards Community Driven Food Safety Model Repositories

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Abstract

Transferring predictive microbial models from research into real world food manufacturing or risk assessment applications is still a challenge for members of the food safety modelling community. Such knowledge transfer could be facilitated if publicly available food safety model repositories would exist.

This research therefore aimed at identification of missing resources hampering the establishment of community driven food safety model repositories. Existing solutions in related scientific disciplines like Systems Biology and Data Mining were analyzed.

On the basis of this analysis, some factors which would promote the establishment of community driven model repositories were identified – among them: a standardized information exchange format for models and rules for model annotation. As a consequence a proposal for a Predictive Modelling in Food Markup Language (PMF-ML) together with a prototypic implementation on the basis of the Systems Biology Markup Language (SBML) has been developed. In addition the adoption of MIRIAM guidelines for model annotation is proposed. In order to demonstrate the practicability of the proposed strategy, existing predictive models previously published in the scientific literature were re-implemented using an open source software tool called PMM-Lab. The models are made publicly available in the first community Food Safety Model Repository called openFSMR (<https://sites.google.com/site/openfsmr/>).

This work illustrates that a standardized information exchange format for predictive microbial models can be established by adoption of resources from Systems Biology. Harmonized description and annotation of predictive models will also contribute to increased transparency and quality of food safety models.

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1. Introduction

Here we present the current status of an initiative aiming at the establishment of community driven and open Food Safety Model Repositories (FSMR). The motivation for this research arises from the understanding that there is a strong need for publicly available, collaboratively maintained and curated resources that allow software independent exchange of predictive models in the field of food safety modelling¹. Currently there exist quite a number of different and sophisticated modelling and prediction tools (an online tool inventory is available at: <http://sourceforge.net/p/microbialmodelingexchange/wiki/Tools/>). However, there is no standardized way of exchanging information or data between these tools. For business operators and governmental agencies this lack of interoperability is a significant obstacle hampering the broad application of models generated by the scientific community. It also limits the applicability of existing software tools itself, averting efficient knowledge exchange and hindering quality control and transparent documentation of modelling results.

2. Results

Related efforts in the Systems Biology domain showcase that the successful establishment and long-term provisioning of model repositories depend on certain prerequisites:

1. Existence of a standardized file format for software-independent encoding of models
2. Existence of rules / guidance for the annotation of experimental data and / or models
3. Software tools supporting the adoption of file formats and annotation rules
4. Technical infrastructure for hosting web-based model repositories
5. Community support (creation, sharing and quality control of models)

This research therefore addressed each of these issues and makes newly developed resources publicly available in order to promote joint future developments.

2.1. Predictive Modelling in Food Markup Language (PMF-ML)

PMF-ML is a standard allowing the encoding of arbitrary food safety models into XML-formatted text files. PMF-ML adopts SBML, version 3². It provides software developers with guidance on how to implement the SBML standard in the domain of food safety modelling. Such guidance is necessary in order to avoid e. g. misinterpretation of SBML concepts that have to be mapped to concepts used in the domain of food safety modelling. For example, a central SBML concept is “Species” which “... refers to a pool of entities that (a) are considered indistinguishable from each other for the purposes of the model, (b) may participate in reactions, and (c) are located in a specific compartment.”². PMF-ML clarifies that the SBML “Species” concept should be mapped to the “Organism” concept which is widely used in food safety models. In addition certain food safety domain-specific conventions are made inside the PMF-ML guidance document. For example, PMF-ML defines that certain model metadata, e.g. the reference to file(s) containing experimental data used for model generation, have to be provided inside the SBML annotation container using a newly introduced “pmf” namespace. The full specification is freely available at the website of the community project “OpenML for Predictive Modelling in Food”: (<http://sourceforge.net/projects/microbialmodelingexchange/>).

2.2. Rules / guidance for annotation of models

The assignment of meaningful, standardized and exhaustive metadata for food safety models is one of the biggest challenges for food safety data scientists. In this domain there is currently no standard or guidance available defining how a predictive model should be annotated and which terms or description scheme should be used. We therefore

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