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Abstract

Background — Scientific software incorporates models that capture fundamental domain knowledge. This software is becoming increasingly more relevant as an instrument for food research. However, scientific software is currently hardly shared among and (re-)used by stakeholders in the food domain, which hampers effective dissemination of knowledge, i.e. knowledge transfer.

Scope and approach — This paper reviews selected approaches, best practices, hurdles and limitations regarding knowledge transfer via software and the mathematical models embedded in it to provide points of reference for the food community.

Key findings and conclusions — The paper focusses on three aspects. Firstly, the publication of digital objects on the web, which offers valorisation software as a scientific asset. Secondly, building transferrable software as way to share knowledge through collaboration with experts and stakeholders. Thirdly, developing food engineers' modelling skills through the use of food models and software in education and training.

Keywords

scientific software, software re-use, modelling, model exchange, collaborative modelling, education

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1. Introduction

Knowledge transfer[1] based on models is a vital driver of scientific research and for putting research into practice. Particularly, the development of digital Information and Communication Technology (ICT) offers great opportunities to create interactive media that facilitates the communication for research partnerships (de Wit-de Vries et al., 2019). In food science, there is a growing interest in knowledge transfer among researchers and with stakeholders at large (e.g. industry, public institutions, consumers) (Thomopoulos et al., 2019; Erdogdu et al., 2017; Aceves Lara et al., 2018; Filter et al., 2015; Perrot et al., 2011; Plaza-Rodríguez et al., 2018). However, reviews show that the deployment of knowledge transfer by food scientists and food engineers is marginal (Djekic et al., 2019; Braun and Hadwiger, 2011). The inherent properties of food products and related processes (e.g. variability of raw materials, not fully formalized physics, heterogeneity of the structure) hamper knowledge transfer (e.g. Perrot et al., 2011). In food science, a major problem is the lack of *codifiability* (i.e. the ability to translate knowledge into symbols, such as equations and computer code), which expresses the degree of communicability and understandability of the domain knowledge. A computer code is an unambiguous codification of domain knowledge that can be readily shared, contrary to tacit (not encoded) knowledge. Moreover, food scientists that build mathematical models and software often lack the knowledge transfer expertise to make their work accessible to a larger audience. As a result, the (re-)use of scientific software in the food industry in Europe is limited and as such an outstanding challenge.

Software essentially captures expert knowledge formalised as equations (i.e. a mathematical model) and implemented as executable code (Davenport and Prusak, 2000). The hindrances to wider (re-)use of food research software are diverse, such as the lack of user-ready research software tools, the cost of getting acquainted with existing models, and the difficulty of designing adaptive reusable applications. Several papers address this knowledge transfer bottleneck. Datta and Halder (2008) and Saguy (2016) propose a road map for wider deployment of food models in industry. Datta (2016) discusses computer-aided food engineering to promote the use of virtualisation in the food industry. Perrot et al. (2011) describe opportunities offered by complex systems approaches to overcome limitations encountered by physics-based approaches. Della Valle et al. (2014) present prerequisites that favour the assimilation and the use of simple models in the baking industry. Plaza-Rodríguez et al. (2018) present a strategy for making a model publicly available and transfer predictive microbiology knowledge into operational applications. Haberbeck et al. (2018) present an open information exchange format for integrating and sharing knowledge captured in mathematical models in the food safety domain. Filter et al. (2015) present a strategy for developing expert-systems with broad end-user acceptance.

The food modelling community has a responsibility in strengthening the transfer of software conveying encoded domain knowledge, both, by making existing scientific software easier to find and (re)use, and by creating software that is easier to transfer to stakeholders. The former is a one-way[2] mechanism based on the dissemination of research results that requires post-treatment of the software (Plaza-Rodríguez et al., 2018). The latter is a bi-directional[3] mechanism that involves interaction between the modellers and the recipients of the software

[1] See Battistella et al. (2016) for a review on technology and knowledge transfer.
[2] A m*echanism of output* according to Battistella et al. (2016).
[3] A m*echanism of process* according to Battistella et al. (2016).

and entails that the software meets certain requirements; for example, the production of outputs that are of interest to end-users (Datta and Halder, 2008).

To encourage knowledge transfer in the food domain, a comprehensive overview of knowledge transfer enabling methods, frameworks and approaches is needed. Our paper aims at initiating this overview. It adheres to the broad definition of knowledge transfer as the communication of thoughts, ideas, hypotheses, theories, etc. that alters the recipient's knowledge state[4] (Braun and Hadwiger, 2011).

This paper focuses on academia and industry as sources and recipients of knowledge related to food. It considers software and models as objects transferrable between stakeholders. The paper reviews transfer initiatives in food software and modelling, and discusses what the food community may learn and adopt from other scientific communities in terms of knowledge transfer strategies and approaches, and how this may benefit the food community. The paper is organized in four sections, each illustrating a different set of knowledge transfer mechanisms. Section 2 discusses ongoing efforts in knowledge transfer through physics-based models and phenomenological models embedded in software. Sections 3 & 4 present collaborative initiatives and strategies for building software that captures knowledge shared by specialists from different domains pertaining to a particular subject. Section 3 focuses on collaboration through software reuse, while section 4 discusses collaboration through shared understanding. Section 5 presents initiatives in education and training that promote modelling in food engineering curricula.

2. Knowledge transfer in food science modelling

The application of modelling techniques in the food domain is challenging due to intricate physical structures (e.g. foams, emulsions, suspensions, networks, gels), which are typically dynamic, undergo significant changes during manufacturing and exhibit varied behaviour during consumption (Mohammed et al., 2020). Food researchers in industry and academia increasingly produce mathematical models embedded in software that capture relevant knowledge of such phenomena. These models, referred as physics-based and phenomenological models, are potential vectors for Knowledge Transfer (KT) among researchers and with stakeholders at large. This section focusses on KT using such models.

2.1. Physics-based food science models

Physics-based modelling deploys a theoretical framework involving mathematical expressions of phenomena. When computed, a physics-based model generates virtually animated objects (evolving in time and space) that describe the considered system, matching observations (Saguy, 2016). These simulations result from analytical (i.e. exact) or numerical (i.e. approximate) models. Due to the complexity of food, the former has limited applicability for food products (Bimbenet et al., 2007). The latter, on the other hand, has much more deployment within the academic and industrial food community. There is a vast range of numerical techniques available including Finite Element Analysis (FEA), Discrete Element Methods (DEM), and Smoothed-Particle Hydrodynamics (SPH), which can be used to simulate a wide variety of phenomena involving solid and fluid-like materials.

[4] Complies with the *frame of reference* in Battistella et al. (2016).

Numerical models have typically been deployed in three ways:

1. **Industrial manufacturing processes.** To determine and simulate important variables of process operation, e.g. the exit shape and the roll force of the torque for the rolling sheeting of dough (Chakrabarti-Bell et al., 2010; Chen et al., 2020). Another example is heat transfer modelling, which is probably the most common application of numerical techniques in food processing (Erdogdu et al., 2018), as the temperature of a product is critical for food safety and quality.
2. **Predicting complex phenomena**. To predict food breakdown during oral and gastric processes in humans (or pets) consider the interactions taking place in the oral cavity during the chewing for various food products (Harrison and Cleary 2014; Skamniotis et al., 2020). For example, the flow of a bolus resulting from the peristaltic waves inside a realistic stomach geometry (Ferrua et al., 2011) and food transport through the oesophagus during the swallowing of fluid food (Yang et al., 2007). The latter studied the effects of tissue properties, bolus properties (e.g. viscosity) as well as contraction and wave speed on the food transport process.
3. **Multiscale simulation design tool.** For linking the structure and behaviour of food in small scale processing to the bulk response of foods in larger scale processing. Multiscale numerical modelling is gaining importance in food science (Ho et al., 2013). For example, the texture of cereal solid foods can be predicted using FEA, by combining information about the product density (macro-scale), product cellular structure (meso-scale) and the mechanical properties of the constitutive materials (micro-scale) (Guessasma et al., 2011).

Numerical models are of interest to the food industry as well as the non-food industry, e.g. for the design of innovative bio-based materials. However, KT based on these models is limited. Models often need to be re-engineered and adapted to specific problems, which requires technical skills from the user, and measurements of material properties. Additionally, there is the fear of sharing sensitive data, as well as budget and time constraints, which hamper corporate investments in a dedicated modelling service or department. As a result, the numerical models available in the scientific literature are hardly transferred beyond the community of modellers that developed them.

2.2. Phenomenological models: empirical & simplified

The development of phenomenological models from experimental results (also known as semi-empirical models) can be seen as a lightweight approach compared to the physics-based models discusses above. Phenomenological modelling sacrifices the mechanistic foundation and predictive power to provide pragmatic solutions to practical problems within time and budget constraints. Phenomenological modelling is common in food engineering and many models of this kind can be found in the literature (Baudrit et al., 2011).

Basic Knowledge Models (BKMs) are a specific type of phenomenological models that rely on statistical or machine learning techniques to cope with unknown aspects. They have three main characteristics that facilitate KT (Della Valle et al., 2014):

- **Relevant knowledge.** BKMs capture relevant knowledge about the mechanisms that change a product during a process. This principle ensures that the model conveys only knowledge about the food product or process that is relevant to users.
- **Use-property information.** BKMs provide information on the use properties of a product. Firstly, to be of value to the food sector, a BKM must model a system that is recognisable and of interest to potential users, such as process operators in the domain of food manufacturing (e.g. mixing, rolling, frying). Secondly, the BKM outputs should serve practical use (e.g. predicting product quality criteria).
- **Understandable and modifiable.** Using and modifying BKMs requires limited knowledge of mathematics and physics as BKMs use relatively simple equations. Additionally, modelling languages from the field of Artificial Intelligence, such as causal graphs, can make BKMs understandable to users that are not skilled modellers (Kansou et al., 2017; Baudrit et al., 2010). The main challenge is to separate the BKM's structure from its mathematical and implementation details.

To further illustrate BKMs, consider the models describing a bacterial response to temperature, pH, and water activity. They associate a standard bacterial growth model, usually a sigmoïdal model either a Gompertz or logistic (Zwietering et al., 1992) with thermal inactivation (Leguerinel et al., 2005), while the parameters are fitted to the data. Along the same lines, Romano et al., (2007) proposed a BKM that simulates the wheat dough expansion leavening process from the dose of yeast using Gompertz function and a linear-regression model. Kansou et al. (2013) extended this model by introducing a BKM for dough stability, using an exponential decay function. One can think of building a third BKM of dough expansion by coupling both models. This shows how phenomenological models can be reused and adapted to meet specific needs.

More elaborate BKMs integrate stochastic modelling to manage complexity, uncertainty and tacit knowledge (Perrot et al., 2011). Baudrit et al. (2010) present a Dynamical Bayesian Network (DBN) of cheese ripening that simulates the evolution of practical product properties such as odour, percentage of coating, and humidity. The DBN integrates a knowledge model of the microbial activity with imprecise information in the form of probability distributions learned from data. More precisely, the DBN is a causal graph whose nodes (variables) and edges (causal dependencies) represent the coupled dynamics of dominant microorganism growth with their substrate consumptions. With the help of experts in cheese ripening, the graph was built in such a way that it is explicit and understandable even for a person with modest or no modelling skills. Determining the conditional probability distributions, i.e. the parameters of the DBN, required a significant experimental effort and a large dataset to account for the kinetics. In return, the prediction accuracy of the model was rather high.

2.3. Transfer channels for scientific software

Mathematical models are valuable means of KT, particularly when formalised as scientific software, which ranges from a simple script written by a single researcher to an elaborate software package (e.g. modelling software) developed by several groups in a joint effort. Currently, the main routes for transferring scientific software to stakeholders in the food domain are:

1. scientific publication, with some information about the implementation of the model;

2. simulation results as required by clients, but without sharing the code that produces these results;
3. software distribution via university or a university spin-off company; and
4. software hand-over to a company that handles the engineering and commercialisation.

These four routes basically reflect two approaches for sharing scientific software: (*i*) the academic approach, in which authors of the scientific software take care of the software use and dissemination (i.e. route 1 and 2), and (*ii*) the commercial and open-source approach, in which the software maintenance and the business aspects are entrusted to software specialists or a platform (i.e. 3 and 4). As food model developers are typically familiar with the academic approach, the next section focusses on the latter approach.

2.3.1. Hand-over scientific software to a development team

It can be beneficial to hand-over code to a software company, which then handles the software engineering tasks (e.g. user interface development, software development, maintenance, code testing, documentation) and the business aspects (e.g. licensing and distribution). Typical approaches for commercialisation are: (*i*) the development of fully integrated proprietary packages by a software company, (*ii*) proprietary packages set up for integration with external open-source packages, and (*iii*) the Independent Software Vendor (ISV) model, in which a software company offers a platform to ISVs (i.e. separate companies) that integrate their solutions in the platform (e.g. as packages) and offer it to their clients (e.g. ANSYS). ISVs are charged for the integration of their products in the platform, while they fully handle the development and the business aspects of their products (Goldbeck, 2017).

A primary market for scientific software commercialisation is research and development activities. In food, this concerns the development of innovative food products or packaging or the creation of new processes. Downstream in the R&D chain, scientific software can support product quality-assessment (e.g. safety risk, nutrition, conformity assessment), process optimisation and control, and supply chain or market trends analysis.

The Ludovic® case illustrates scientific software commercialisation. Ludovic® is a simulation software for the twin-screw extrusion of polymers and biopolymers developed and distributed by Sciences Computers Consultants (SCC)[5]. Twin screw extrusion has been developed in the 70's for various foods (e.g. snacks, breakfast cereals, infant flours, pet-foods). At that time, the approach to extrusion in industry was essentially empirical. In the eighties, the INRA and ARMINES institutes investigated theoretical and experimental aspects of the extrusion of starchy and other polymeric products. They developed a model based on continuum mechanics to rationalize the design of extruded starchy products (Della Valle et al., 1993; Vergnes et al., 1998). This model computed the temperature and the pressure profiles along the screw, as well as the Specific Mechanical Energy (SME). SME mainly determines the extent of the starch transformation and its viscosity, which in turn determines the product expansion at the outlet of the die. About six years after the model's main publication (1993), Ludovic® was released as the result of a business agreement between the two research institutes and SCC (Fig. 1). The initial model, written in FORTRAN, was given to SCC along with the Intellectual Property (IP) rights in return for a royalty on sales and free in house use of the software. SCC carried on the software engineering tasks (i.e. cleaning the code, developing a GUI, writing documentation,

[5] https://www.scconsultants.com/en/ludovic-twin-screw-simulation-software.html

with the help of the authors of the models to ensure scientific adequacy) and the distribution and maintenance. Several companies use Ludovic®, which is now in its 6th version, at the early stages of product design innovation and process optimisation to reduce the number of costly trials. The research groups that initially contributed to Ludovic® have since been using the commercial version in many research activities, for example to account for the texture properties of extruded products.

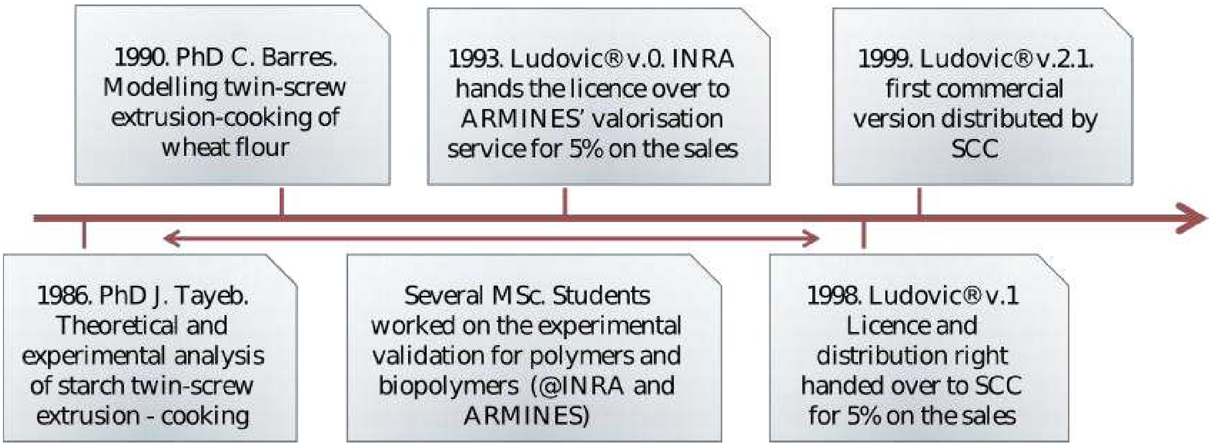

Figure 1. Timeline illustrating the origin and development of Ludovic®.

2.3.2. CAE solutions, when end-users are modellers

Physics-based modelling and more specifically numerical modelling is generally used to create a virtual space in which replications of products, processes or equipment are manipulated and tested (i.e. Datta, 2016). Modelling, simulation, optimisation and dynamic studies are a part of a wider scheme that is referred to as virtualisation (Marra, 2016). A number of manufacturing sectors have invested in this approach, e.g. automotive, aerospace, packaging, and adhesives. Virtualisation is used for product design and development; it offers an alternative to physical trial-and-error exploration. In the food industry, the design of innovative products is one of the applications that could benefit from this virtualisation approach (Saguy, 2016).

Numerical models can provide accurate predictions of the behaviour of a material under a variety of boundary conditions, whilst conveniently highlighting important parameters of the process analysed through parametric studies. Another advantage is that these models provide results in an accessible format, such as colourful contour plots and explicit graphs, which enable end-users to build a mental model of the phenomenon and subsequently use the knowledge gained for product and process optimisation. Additionally, there are strong arguments for the strategic importance of a wider use of virtualisation to support innovation in the food sector (Saguy, 2016).

The preferred KT channel for this type of model is commercial Computer-Aided Engineering (CAE), i.e. a software that assists end-users in the process of developing their own numerical models. The growing interest for such computational models has been driven by the increase in available processing power as well as the multiplication of commercially available software packages dedicated to materials and chemical processing (e.g. Comsol[6], ANSYS[7]). These commercial solutions are typically accompanied by technical manuals, training, free student

[6] http://www.comsol.com/products
[7] https://www.ansys.com/solutions/solutions-by-industry/materials-and-chemical-processing

download licenses and customer support. OpenFOAM[8] is an example of an open-source software under the General Public Licence (GPL). GPL allows for free use, modification and redistribution. In chemical engineering, one can find easy-to-use CAE tools for simulating processes in the energy, gas, chemical, petroleum and pharmaceutical industry (e.g. ProSim[9]).

In the food domain, CAE tools offer great assistance for tasks that can be partially automated such as processing (solving equations), post-processing and coding. However, current CAE solutions are unlikely to efficiently assist the modelling of solid food products (i.e. writing mathematical expressions that capture the physical system, Datta., 2016). Problem formulation requires good modelling skills and good knowledge of food physics and experiments. In the food domain, this evidently limits the pool of potential end-users. Hence, in the food industry the application of physics-based modelling is currently conducted by in-house modellers in big companies, specialist software companies or academic research groups.

Datta (2016) proposes two paths to increase the utility of CAE in the food domain: (*i*) the design of a set of modelling frameworks that address food processing, quality and safety, and (*ii*) an increased use of CAE tools and virtualisation in education, as this is happening already in some university engineering courses. It is also possible to take advantage of the emerging cloud-based technologies that have transformed many industries. It has been argued that running numerical simulations of manufacturing processes on cloud-based platforms could foster a collaborative research environment whilst providing means for research digitalisation and knowledge sharing as well as saving on local computational and data storage resources (Yang et al., 2019). This could be a future trend that would facilitate the optimisation and exploitation of advanced mathematical modelling tools by stakeholders.

2.4. Limitations of current diffusion channels

Current channels for KT with scientific software are limited. Scientific papers generally contain minimal descriptions of the implementation, and even when the code is available, using it effectively requires a serious amount of additional work (Gil et al., 2016). The lack of an harmonized exchange format is particularly limiting, as it is well known that being able to integrate, question and challenge new knowledge is essential for perceiving and accepting its added value (Drechsler et al., 2016). Challenges with software commercialisation are the intensity and duration of the procedure. Only a few scientific software vendors are interested, leaving most of the scientific software of a domain aside. Developing CAE solutions dedicated to the food domain would be beneficial for KT, in particular because it would enable the receiving agent to build their own models, reusing components developed by others. For now, this channel has a relatively small user base in the food sector, although it is expected to grow with the development of commercial software (Saguy, 2016). Still, the CAE tools favour certain types of modelling and require suitable training, as such, they are unlikely to offer a generic solution for transferring scientific software.

[8] https://www.openfoam.com
[9] http://www.prosim.net/en/index.php

3. Towards reusable scientific software

In Europe, guidelines have been issued to incite scientists to adopt development practices that will make their software reusable (Chue Hong., 2014, Fehr et al., 2019). Additionally, sharing research data is well established as a key aspect of open science, which is expected to accelerate innovation in industry. It is typically realised using the European Commission's program European Open Science Cloud[10] that implements the FAIR[11] principles (i.e. Findability, Accessibility, Interoperability, and Reusability), as well as related developments on (research) data management plans and domain protocols to share data. This section reports on initiatives that could encourage the reuse of scientific software in the food domain.

3.1. Information to accompany scientific software

There are several proposals like the Science Code Manifesto[12] aiming at paving the path toward reusable scientific software (Chue-Hong., 2014). Among them, "Software Engineering at Google" (Henderson, 2017) illustrates a gold standard that is unrealistic for academics, yet some of the good practices, frameworks and tools presented could inspire the scientific community. The DLR (German Aerospace Center) Software Engineering Guidelines (Schlauch et al., 2018) are an interesting example of top-down recommendations aiming at supporting scientists in improving the reusability of their software. Another framework for informing about scientific software is proposed by Fehr et al. (2019). It defines a list of requirements for academic software, typically pieces of code written by a PhD student, to support the hand-over to the other scientists (in the group) and the continuation of the project. Another approach for evaluating scientific software in the food domain could be to tailor the Technology Readiness Level (TRL) methodology to food science (Altunok and Cakmak, 2010; Armstrong, 2010).

The multi-level framework for scientific software reuse (Chue-Hong, 2014), is a good starting point for scientists new to this topic. This framework associates end-user benefits with four software information levels that support a researcher in the process of providing information about the software, such that a developer can gradually improve the reusability of the software. The proposed four levels are:

- L1 (Absolute Minimum): requirements that put no barrier on the developer. Should be considered basic requirements for any researcher that publishes results from a self-developed software.
- L2 (Useful Minimum): additional effort to support at least the own use of the software.
- L3 (Pragmatic Minimum): a desired (according to Chue-Hong, 2014) standard level of information that supports the collaboration with external developers.
- L4 (Good Minimum): actively encourages software reuse through the adoption of essential software engineering techniques.

For each level, the requirements are classified in categories. **Table 1** shows the requirements for L1. As scientific editors get increasingly concerned with the traceability of research results, requirements of this kind might become mandatory for submission to peer-reviewed journals, as soon as a new scientific software is involved. Notice that, this framework is sufficient to

[10] https://www.eosc-portal.eu/about/eosc
[11] https://www.go-fair.org/fair-principles/
[12] http://sciencecodemanifesto.org/

support the editing of basic metadata (information describing the software) and the creation of accompanying files. Some of these metadata are required for depositing software into a digital repository for archiving and referencing (e.g. Jackson, 2018). Where dealing with copyright and licensing aspects, which is part of the process, can be troublesome, the REUSE[13] website offers useful support in this regard.

Table 1. Level 1 requirements for informing on software reuse (Chue-Hong, 2014).

Category	L1. Absolute Minimum
License (legal information about the software reuse)	"the software has a license that allows for reuse (this can include non-Open Source licenses...under academic or commercial terms)"
Availability (where and how to get access to the software)	"the software has been published somewhere such that people can find it (this could be as a tar archive on a website)"
Quality (functional and non-functional requirements)	"the software has some minimal indication of what it is supposed to do... normally as part of a README"
Support (ways to contact the developer in charge of support)	"the software indicates some way of contacting the original/current developer (instead of good documentation), normally as part of a README"
Incentive (how to acknowledge the software development)	None (starts at level 2)

3.2. Infrastructures for reuse of scientific software

Sustainable scientific software reuse should be based on a suitable infrastructure for storing, archiving and making the code accessible. Therefore, authors must deposit their software alongside other files (e.g. README, RUNME) into digital repositories and fill in registry forms that allow for curation by other users. Jackson (2018) offers useful recommendations for the deposit of software, such as the delivery of a persistent digital identifier (e.g. Digital Object Identifier, DOI) that assures that the software can be cited and that the author gets credited for the work. Notice that, general purpose code repositories, such a Github, do not automatically provide persistent identifiers, although mitigating procedures exist[14]. Certain repositories are recommended for specific developer communities. For instance, CRAN[15] is well-known among users of R[16] as the repository that stores R packages with their documentation. Similarly, SciPy[17] is well known among Python[18] users. For any scientific software, it is important to consider archiving and referencing the software via registry services alongside the deposit of the code. In fact, registration and indexation might be more important for a scientific community than the code repository hosting service itself (Gil et al., 2016). General purpose digital repositories, such as FigShare and Zenodo, can be used for registering and archiving software (as for any other research products) and for making its title, DOI and licence citable (Jackson, 2018). Finally,

[13] https://reuse.software/
[14] https://guides.github.com/activities/citable-code/
[15] https://cran.r-project.org/
[16] https://www.r-project.org/
[17] https://www.scipy.org/
[18] https://www.python.org/

Software Heritage[19] is a recent international initiative that offers a service for indexing, organizing, making referenceable and accessible all the software that conveys technical and scientific knowledge. Software Heritage archives and assigns an intrinsic and persistent identifier for digital objects (i.e. swh-id).

One can also find domain-specific software repositories, driven by a community of scientists for collecting food safety models in their field, such as the Risk Assessment and Knowledge Integration Platform (RAKIP)[20] (Plaza-Rodrigez et al., 2018; de Alba Aparicio et al., 2018). They enable scientists to register their software via a set of metadata that capture relevant information for the domain. Interestingly, some of these repositories require compliance with a common modelling framework to favour data exchange between various modelling tools and the coupling of models in general (Gil et al., 2016).

FSL-Lab is a graphical modelling platform for the integration of risk assessment models that goes a step further in term of model reusability (de Alba Aparicio et al., 2018). One of the FSK-Lab key features is the support of a markup language for script-based or application-based models (Food Safety Knowledge Markup Language, FSK-ML), that is used to annotate models with metadata. FSK-ML allows for a harmonized writing and reading of mathematical models regardless of their sources, which facilitates greatly their integration and re-use in FSK-Lab. FSK-ML is expected to become a format for exchange of information broadly adopted by the microbial food safety community (i.e. regulatory agencies, food industries, consultancy companies, and food scientists) in order to facilitate the reusability of scientific models to improve risk assessment and decision making by food safety managers (Haberbeck et al., 2018).

Software deposit solutions capture metadata about the software, but sometimes in an unstructured way, e.g. as text in a README file. Additionally, the documentation provided in code repositories mostly focuses on the installation process (Gil et al., 2016). This makes it difficult for potential end-users to find software that matches their needs. Having the metadata captured in a software registry linked to the code makes the software searchable, discoverable and re-usable. This is an essential aspect of software sharing that can be addressed with software ontologies (i.e. controlled vocabularies that specify information about a software). The OntoSoft ontology (Gil et al., 2015) is an example of a general software ontology centred on scientific software sharing. OntoSoft[21] captures six information items that can be queried by a user (Gil et al., 2015): identifying the software, understanding and assessing software, executing the software, getting support, doing research, and updating. This ontology is at the core of a distributed software registry that offers a way to register and discover scientific software.

3.3. Barriers for scientific software reuse

The publication of datasets and software is a growing trend that is likely to become even more pronounced in the near future. This trend is encouraged by scientific publishers, funding agencies and research organisms that promote open science. Despite this, there is a risk that a great deal of datasets and software currently developed by researchers in food science remain unpublished and inaccessible to potential users.

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[19] https://www.softwareheritage.org/
[20] https://foodrisklabs. bfr.bund.de/rakip-model-repository-web-services/
[21] https://www.ontosoft.org/index.html

Main explanations for the limited adoption of practices that favour software reuse reported in other domains (e.g. Gil et al., 2016) also apply to the food modelling community. They can be summarised into three categories, lack of credit, lack of knowledge, lack of suitable "ecosystem", e.g. guidelines and tools. Traditionally, food science does not rely heavily on programming, therefore the lack of knowledge about practices and tools that favour software reuse is natural.

Similarly, while developing an infrastructure to share food science models might be highly beneficial, the community lacks a format for describing simulation models (Plaza-Rodriguez et al., 2015). However, the lack of credit is probably the most critical bottleneck for a large diffusion of food science models. In science, there is a major imbalance between the effort invested in coding, documenting, maintaining and publishing the code, and the credits/benefits that the author can get from it (Chawla, 2016). Initiatives from publishers and communities to measure the impact of a scientific code are currently tackling this imbalance and will probably continue alongside the evolution of scientific publications, see for example the software citation guide (Katz et al., 2021) and the CODECHECK system (Nüst and Eglen, 2021).

4. Collaboration through shared representations

The code developed by researchers in the process of scientific discovery should be shared with the scientific community, like a research paper or a dataset. However, the primary goal behind the development of scientific code is generally not knowledge transfer. This section focuses on collaborative modelling techniques that aim at creating software usable by people other than scientists.

Collaborating with other scientists, domain experts, stakeholders or even consumers, is not uncommon in the food sector. In general, the need to integrate expertise from various domains grows with the system scale and its complexity (van Mil et al., 2014). For instance, modelling the proofing of wheat dough – i.e. the first fermentation operation of the bread-making process – needs only knowledge of the dough rheology and of the leavening agent activity. However, a bakery will probably find modelling the whole bread-making process more useful, which includes, in addition to the knowledge of the physics of the dough, the assessment of the quality of the flour and the prediction of the sensory properties of the bread; both aspects demand domain expertise and are not fully tractable with the current state-of-the-art. Collaborating actively with industry and civil society is a way to improve the relevance of software beyond the scientific community (Sein et al., 2011).

However, where integrating different views of the same system is expected to promote understandability and (re)usability by a diverse audience, working with non-modeller contributors is challenging and calls for specific methods and tools. Potential mechanisms that facilitate collaboration can be found in the knowledge engineering domain. This field includes the acquisition of knowledge from domain experts, participative modelling and the development of controlled vocabularies (e.g. ontologies). This section reports on collaborative modelling initiatives in the food domain, such as the development of standardized food-related ontologies and the crowdsourcing of food data.

4.1. Involving domain experts in creating food software

Involving experts in the creation of software, while keeping these experts away from low-level implementation details, is a prerequisite in the field of knowledge engineering and the development of Knowledge-Based Systems (KBS). KBSs designate a class of software systems (including expert systems and decision-support systems) that implements an automated knowledge source that can be consulted by users to generate valuable results (e.g. complex question answering or supporting decision-making). A KBS generally collates information from different sources, such as domain specialists, literature, and web resources (Aussenac-Gilles and Gandon, 2013). Basic principles of acquiring knowledge from experts include (Schreiber et al., 2000): (*i*) building a shared representation of the domain knowledge sufficient for fulfilling the goal of the software, (*ii*) focusing on capturing the conceptual structure of the knowledge (i.e. the so-called knowledge-level), leaving aside programming considerations, and (*iii*) adopting iterative and incremental development of the software.

Not many papers have addressed this topic in the context of food. Ndiaye et al. (2009) discusses the creation of a KBS for bread-making that captures the reasoning of bread technologists. Additionally, an incremental modelling approach is proposed to spur experts in providing feedback and informative critiques on the model structure (Kansou et al. 2014). Thomopoulos et al. (2013) presents an approach for learning interpretable data-driven models, which was applied to the processing and qualities of cereal foods. They used a domain ontology to select the factors from the dataset (e.g. cooking temperature) that would most likely affect the quality of the products (e.g. vitamin content). Subsequently, they derived decision trees from the data. The experts' feedback on the resulting decision trees were used to enrich the ontology, starting a new cycle, until the experts required no further improvements. In the same vein, the Food Informatics project (Koenderink et al., 2005) developed an approach for supervised construction of food ontologies, in which food experts had to select relevant concepts and properties (relations) within a set curated automatically from web resources.

Eliciting knowledge about food is often delicate when know-how and sensory criteria are involved, because it often involves tacit knowledge that is difficult to put into words. To describe the human evaluation of an ongoing food process, Curt et al. (2004) adapted an observer-trainee technique combining explanation steps, interviews and concrete practical sessions. The principle was to have an expert practitioner, such as a product manager, explain and train a "trainee" (e.g. the modeller) which led to the identification of the indicators (e.g. colour, stickiness, particle size, etc.) and their attributes (e.g. definition, operating conditions, measurement scales, location in the process, etc.). This approach was adapted by Sicard et al. (2011) for monitoring cheese ripening controlled by the cheesemakers in order to develop a Dynamic Bayesian Network (DBN) of this operation (see section 2.2). The knowledge elicitation was carried out as follows. The first phase captured operational know-how about the cheese ripening process with the aim of building an operational representation of the indicators and of the decision rules used by the operators to control the process. In a second phase, food scientists enriched this operational representation with concepts and relations describing the microbiological and biochemical phenomena. The result was an integrated probabilistic model that was able to predict the indicators of the different phases of cheese ripening.

4.2. Participative modelling

Addressing societal issues, the collaborative and integrative aspects of modelling are even more important. Issues addressed at the food system level, especially those involving food security or sustainable production, are complex as they involve several dimensions and stakeholders with different visions of the system (van Mil et al., 2014) and potential conflicts of interest. This requires an appropriate methodology for reconciling these visions and determining the interventions that would most likely be accepted by the actors, and hence most likely succeed. This asks for participatory approaches that support decision-making in a multi-actor context (e.g. using risk-benefit analysis and multi-criteria decision, Bana E Costa, 2001), involving experts from different disciplines (e.g. agronomy, nutrition, environment) and various stakeholders (e.g. consumers, food producers, public authorities, technical centres) in the decision process that reconciles their different points of view (Joerin et al., 2009).

More specifically, participatory modelling involves the actors in the creation of models that will ultimately facilitate the decisions. The field of resource and environmental management is particularly active in participatory modelling (Voinov et al., 2016). Noteworthy developments in the field of participatory modelling address modelling aspects of the actors' dialogue related to the sustainability of food systems. For example, semi-automated argumentative approaches based on Dung's model (1995) allow for formalising arguments and contradictions, analysing conflicts of interest and helping to solve polemics. Thomopoulos et al. (2015) developed a KBS for re-thinking the agri-food chain's organisation with nutritional, safety and organoleptic recommendation arguments. Bisquert et al. (2017) present a multi-criteria computational cognitive model for argument acceptance (applied to the selection of durum wheat) informed with actor arguments, associations and opinions about food product (e.g. pasta, semolina) quality and life-cycle assessment criteria (e.g. dependence to chemical inputs). With the growing concern regarding the sustainability of the food systems, research projects including participatory modelling are bound to gain importance in the near future.

4.3. Crowdsourcing

Collaboration with experts or stakeholders is based on information exchange, during many meetings, either face-to-face, over the phone or through videoconferencing. This approach favours the elicitation of expertise and non-trivial positions on a subject, but it also hampers the involvement of a large number of contributors from different places, hence it allows only for the creation of small scale KBSs. As web-based services become increasingly sophisticated and powerful, it is possible to collect and integrate inputs from a large number of people across the world, aiming at larger scale applications. Consequently, web technologies and crowdsourcing are expected to play a bigger role in participatory modelling in the near future (Voinov et al., 2016). Several web applications to collaboratively build a model are already available, such as ArguBlogging, an application that automatically formalises and structures dialogues posted on a web platform as a computable model (Bex et al., 2014). Kurtz et al. (2021) propose an AI approach, based on the concept of collective attitude, to analyse a large-scale survey on consumers' perception of food, while Taillandier et al. (2021) mix arguments from web debates and agent-based modelling to simulate opinion diffusion on vegetarian diets.

Because food concerns everyone, food issues can spark the interest of many internet users that could provide information about their consumption or about their preferences. Open Food

Facts[22] epitomizes the successful application of crowdsourcing in the food sector. The contributors (>1800) scan the information given on the product package (e.g. nutritional facts, allergens, ingredient list, barcodes) and send it to a server via a smartphone application. The data collected so far covers more than 75000 products from 150 countries and is available to the public as open data. Open Food Facts conveys massive volumes of basic information about commercial food products to a large audience. Notice that, the community driven FSMR discussed above also relies on the internet to promote reuse of the scientific models and simulation tools developed by the food safety modelling community in academia, the food industry and public institutions. The crowdsourcing strategy assumes the creation of an open repository of models and the development of standardized information exchange formats. As a proof of concept, a web-based model repository has been implemented using a Google based infrastructure[23] to inventory existing food safety models (Filter et al., 2016).

4.4. Standardized food-related ontologies

Collecting and structuring information about a relevant part of the world and disseminating this information such that it can be shared with others is a fundamental aspect of KT. An ontology is defined as an explicit and formal specification of a shared conceptualisation (i.e. a mental model) of an aspect of reality (i.e. the domain) (Ushold & Gruninger, 2004). It has a structuring orientation that can help researchers, professionals and citizens to formalise and share expertise in such a way that it can be processed by both humans and computers (Roa et al., 2014).

As a Semantic Web technology, ontologies promote the semantic interoperability between information from different sources, which limits ambiguity and extends the scope of data available for querying by capturing the intended semantics of data (Shadbolt, 2006). Ontologies can be formally specified in specialised languages, such as the RDF Schema and OWL web-standards, which are lightweight knowledge representation languages, in which inferences can be derived from existing information (Krötzsch, 2012). Many formal ontologies are freely available on dedicated portals (e.g. Bioportal[24], Agroportal[25], Ontology Lookup Service[26]), some provide directly valuable resources to professionals (e.g. Gene Ontology[27]), but most of them are used to annotate information exchange between human agents and/or machines (Roa et al., 2014).

In food science, there are several publicly available ontologies, many of them focussing on a specific product (e.g. wine, pizza, beer). Boulos et al. (2015) review larger scope ontologies such as FOODS, AGROVOC[28], FoodOn[29], Open Food Facts[30]. However, not many can be seen as conclusive realisations of KT from the food science community because the focus is often on the non-technological aspects of food such as safety, food security, disease or health profile, nutritional facts, and supply chain elements. This can be illustrated with FoodOn (Dooley et al.,

[22] https://world.openfoodfacts.org
[23] https://sites.google.com/site/openfsmr/
[24] https://bioportal.bioontology.org/ontologies
[25] http://agroportal.lirmm.fr
[26] https://www.ebi.ac.uk/ols/index
[27] http://www.geneontology.org
[28] http://aims.fao.org/vest-registry/vocabularies/agrovoc
[29] https://foodon.org/
[30] https://world.openfoodfacts.org/

2018), which was initially built to be used in collaboration with Genomic Epidemiology Ontology (GenEpiO[31]) to specify foodborne disease risks and not food science or technology. AGROVOC, on the other hand, is a generic multilingual thesaurus developed by the Food and Agriculture Organisation (FAO) with direct interest for KT and covering many fields in agriculture and food (Caracciolo et al., 2013).

4.5. The way forward

Open-source and open access software and data are becoming the norm in research. From this, we may infer that the trend towards KT is about to accelerate. A breakthrough in the annotation of food-related data with ontologies as a standard practice is needed to unleash the power of data networks (i.e. the value of an individual information item increases with the size of the data-pool it is associated with) (De Leenheer and Christiaens, 2018). This data network is a priority for the community working on vocabularies and ontologies in the field of food and agriculture. Agroportal already offers services to store, handle and display the mappings (or alignments) between ontologies; these mappings can be either uploaded or automatically inferred when classes share common properties (Jonquet et al., 2018).

A concern regarding the evolution towards openness is the intellectual property and data protection. The community should strive to avoid data-monopolies, as they lead to an unfair distribution of the wealth generated from data (Mazzucato, 2008) and protect contextual integrity, which should help preserve privacy and competitive advantage in data-sharing environments (Nissenbaum, 2009). The open-source initiative[32] provides resources for further insight.

5. Education and training

A considerable number of well-stablished European universities offer curricula addressing food science and technology, typically focussing on food engineering, microbiology and supply chain management. Several educational programs teach food modelling through learning-by-doing using general-purpose tools such as Matlab or Comsol. However, few institutions seem to put significant emphasis on advanced modelling and simulation techniques and scientific software in general. The availability of web-based course material appears also to be sparse. Instruments such as Massive Open Online Course (MOOCs) and Small Private Online Courses (SPOCs) have the potential to expand KT on to a large audience, while these can also be deployed to educate and train professionals. Below, three initiatives that illustrate this potential are highlighted.

In 2014, a special interest group of the ISEKI Food Association (IFA) started the International School on Modelling and Simulation in Food and Bio Processes (MSFS), which applies a short-term intensive training format. The Cost Action CA15118, FoodMC[33], chose this school as its training school and over 100 scholars, coming from all over the world, have attended it so far. To the best of our knowledge, it is the only attempt to create a transversal community in which food engineers, food technologists and food scientists improve their modelling skills, interacting with each other and embracing the power of numerical techniques and tools for design and

[31] https://genepio.org/
[32] https://opensource.org
[33] https://www6.inrae.fr/foodmc

innovation in the food sector. Datta (2016) agrees that the development of human resources is important to favour a generalised use of modelling tool in the food industry and KT. Yet, there is a relatively small and geographically dispersed student population eager to acquire the required skills. Therefore, the deployment of MOOCs for an international audience would allow for increasing the global outreach of existing and future initiatives.

Physics-based simulators when embedded in virtual tools could be an excellent medium to support KT and training in the food domain. Singh and Erdogdu (2009) developed a set of interactive computer simulations of food processing operations for students to conduct basic virtual experiments, along with a website that offers the resources[34]. Each of their 23 virtual experiments offers contextual information (e.g. industrial procedure, link to related-information on the internet), theory and data analysis information, a description of the experimental procedure and a simulator that mimics the actual experiment and allows for changing its setup by changing input parameters. Similarly, FEPSIM[35] provides a free web-based education tool that offers various physics-based modules (built on Matlab and ANSYS CFX/FLUENT) related to food engineering (Koulouris et al., 2015).

MESTRAL[36] is another example of pedagogical material based on simulators enriched with related information (Suciu et al., 2021). MESTRAL converted actual research results into educational materials and is currently available for master and PhD students in food engineering. The online repository contains 15 modules. Each module is built along the same conceptual framework that includes a (*i*) simulator (that re-uses scientific software from previous research), (*ii*) contextual information, and (*iii*) background knowledge both captured in standardized conceptual maps (Cmaps, Novak & Gowin, 1984) and in “knowledge sheets”. A Cmap is a knowledge modelling technique using diagrams that represent semantic relationships between concepts. Each Cmap in MESTRAL respects a template (i.e. meta-model) that imposes a tree-like organisation, a type of concept and a limitation on the number of concepts, to facilitate assimilation of the content. The digital material is composed of hypermedia that embed links from Cmaps towards (*i*) other Cmaps or the simulator, (*ii*) knowledge sheets that contain text, photos or videos, and (*iii*) external resources via URLs. The simulators run simulations based on case-study datasets that the user can display at will using sliders and plots.

6. Conclusion

This review paper illustrates the challenge of KT in food science through (*i*) a discussion on existing and emerging dissemination channels and (*ii*) arguing the need for an increased collaboration when building food-oriented software. Section 2 discusses the channels for physics-based models and phenomenological models embedded in software. Physics-based models are often transferred to end-users following a learning-by-doing strategy. This strategy can be improved by the development of adequate Computer-Aided-Engineering solutions and by a stronger emphasis on modelling in food science education programmes. For phenomenological models, the traditional diffusion channels for scientific models (i.e. scientific

[34] http://rpaulsingh.com/learning/virtual/virtual.html
[35] http://fepsim.food.teithe.gr/fepsim/default.aspx
[36] https://lms.agreenium.fr/course/index.php?categoryid=27

publication) insufficiently support the reuse of the scientific software by a large audience even though the Ludovic® example shows that KT can be fruitful for both academia and industry.

Section 3 argues that new diffusion channels relying on web-based technologies develop rapidly and become increasingly relevant for KT. Most promising solutions provide tools for archiving, annotating, querying and publishing software, so as to give any user access to the necessary materials and accompanying information regarding a software (e.g. metadata, documents, running example) and also give credit to the authors.

Section 4 reviews the idea that building scientific software from shared knowledge can facilitate KT between miscellaneous stakeholders, including experts and practitioners, in an iterative process. It may even allow for encoding tacit (i.e. unarticulated) knowledge. Collaborative modelling takes this a step further by supporting a multi-user context, while web-based technologies allow for involving a physically dispersed community.

Section 5 notes that the scarcity of modelling skills amongst food engineers currently hampers successful KT. Several educational programs now teach food modelling through learning-by-doing strategies. In parallel, a few resources for teaching modelling online have been developed by food scientists. However, offering online, easily accessible and high-quality educational material is still an outstanding challenge in the food domain.

By highlighting miscellaneous approaches regarding scientific software, this paper aims at promoting KT between and within academia, industry and other stakeholders, and at opening prospects for synergistic efforts that will allow the food community to face the oncoming challenges.

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