



HAL
open science

Some remarks on computational approaches towards sustainable complex agri-food systems

Nathalie Perrot, Hugo de Vries, Evelyne Lutton, Harald G. J. van Mil, Mechthild Donner, Alberto Tonda, Sophie Martin, Isabelle Alvarez, Paul Bourguine, Erik van Der Linden, et al.

► To cite this version:

Nathalie Perrot, Hugo de Vries, Evelyne Lutton, Harald G. J. van Mil, Mechthild Donner, et al.. Some remarks on computational approaches towards sustainable complex agri-food systems. Trends in Food Science and Technology, 2016, 48, pp.88-101. 10.1016/j.tifs.2015.10.003 . hal-01269357

HAL Id: hal-01269357

<https://hal.science/hal-01269357v1>

Submitted on 28 May 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Accepted Manuscript

Nathalie Perrot, Hugo De Vries, Evelyne Lutton, Harald G.J. van Mil, Mechthild Donner, Alberto Tonda, Sophie Martin, Isabelle Alvarez, Paul Bourguine, Erik van der Linden, Monique A.V. Axelos



PII: S0924-2244(15)00218-6

DOI: [10.1016/j.tifs.2015.10.003](https://doi.org/10.1016/j.tifs.2015.10.003)

Reference: TIFS 1710

To appear in: *Trends in Food Science & Technology*

Received Date: 7 April 2014

Revised Date: 15 September 2015

Accepted Date: 3 October 2015

Please cite this article as: Perrot, N., De Vries, H., Lutton, E., van Mil, H.G.J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguine, P., van der Linden, E., Axelos, M.A.V., *Trends in Food Science & Technology* (2015), doi: [10.1016/j.tifs.2015.10.003](https://doi.org/10.1016/j.tifs.2015.10.003).

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguine, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : [10.1016/j.tifs.2015.10.003](https://doi.org/10.1016/j.tifs.2015.10.003)

SOME REMARKS ON COMPUTATIONAL APPROACHES TOWARDS SUSTAINABLE COMPLEX AGRI-FOOD SYSTEMS

Structured Abstract

Background

Agri-food is one of the most important sectors of the industry in Europe and potentially a major contributor to the global warming. Sustainability issues in this context pose a huge challenge for several reasons: the variety of considered scales, the number of disciplines involved, the uncertainties, the out-of-equilibrium states, the complex quantitative and qualitative factors, the normative issues and the availability of data. Although important insight and breakthroughs have been attained in different scientific domains, an overarching and integrated analysis of these complex problems have yet to be realized.

Scope and Approach

This context creates huge opportunities for research in interaction with mathematical programming, integrative models and decision-support tools. The paper propose a computational viewpoint including questions of holistic approach, multiscale reconstruction and optimization. Some directions are discussed.

Key Findings and Conclusions

Several research questions based on a mathematical programming framework are emerging: how can such a framework manage uncertainty, cope with complex qualitative and quantitative information essential for social and environmental considerations, encompass diverse scales in space and time, cope with a multivariable dynamic environment and with scarcity of data. Moreover, how can it deal with different perspectives, types of models, research goals and data produced by conceptually disjoint scientific disciplines, ranging from physics and physiology to sociology and ethics? Building models is essential, but highly difficult; it will need a strong iterative interaction combining computational intensive methods, formal reasoning and the experts of the different fields. Some future research directions are proposed, involving all those dimensions: mathematical resilience, human-machine interactive learning and optimization techniques.

Keywords

Agri-food systems, sustainability, multiscale modeling, optimization, resilience, human-machine interactive learning.

SOME REMARKS ON COMPUTATIONAL APPROACHES TOWARDS SUSTAINABLE COMPLEX AGRI-FOOD SYSTEMS

Authors

Nathalie Perrot^{a,c*1}, Hugo De Vries^b, Evelyne Lutton^{a,c}, Harald G.J. van Mil^h, Mechthild Donner^g,
Alberto Tonda^{a,c}, Sophie Martin^{c,d}, Isabelle Alvarez^{d,e}, Paul Bourguine^c, Erik van der Linden^{h,i}, Monique
A.V. Axelos^f

Affiliations

^a INRA, UMR782 Génie et Microbiologie des Procédés Alimentaires, F-78850 Thiverval-Grignon,
France (Tel.: +33 1-30-81-53-79; fax : +331-30-81-55-97; email: nathalie.perrot@grignon.inra.fr,
evelyne.lutton@grignon.inra.fr, alberto.tonda@grignon.inra.fr)

^b INRA, UMR1208 Ingénierie des Agropolymères et Technologies Emergentes, F-34060 Montpellier,
France (Tél. : +33 4 99 61 28 31) devries@supagro.inra.fr,

^c ISCIPIF (Institut des Systèmes complexes Paris Ile de France, 133 rue Nationale – F 75013 Paris (Tél.
+331 45 52 64 11 - Fax : +331 45 52 64 55)

^d IRSTEA, LISC. 24 avenue des Landais, BP5 0085 631 72 Aubière, France, (Tel/fax: +33 4 73 44 06 00,
sophie.martin@irstea.fr, isabelle.alvarez@irstea.fr)

^e UPMC, Lip6, 104 av. du Président Kennedy, 75016 Paris, France, (Tel/fax: +33 1 44 27 87 38)

^f INRA, UR1268 Biopolymères Interactions et Assemblages, F-44300 Nantes, France (Tel: +33 (0) 2 40
67 50 31 : email : Monique.Axelos@nantes.inra.fr)

¹ Corresponding author : Nathalie Perrot Tel.: +33 1-30-81-53-79; fax : +331-30-81-55-97; email:
nathalie.perrot@grignon.inra.fr)

22 [§] Montpellier SupAgro, UMR MOISA, 2 Place Pierre Viala, 34060 Montpellier Cedex 02, France (Tél. :
23 +33 4 99 61 28 31 ; email : devries@supagro.inra.fr, mecsthild.donner@supagro.inra.fr)

24 h TI Food and Nutrition, Nieuwe Kanaal 9A, 6709 PA Wageningen, The Netherlands, irede@van-
25 mil.net , vanderlinden@tifn.nl

26 ⁱLaboratory of Physics and Physical Chemistry of Foods, Wageningen University and Research Center,
27 Bornse Weiland 9 (building 118) 6708 WG Wageningen, The Netherlands. e-mail:
28 erik.vanderlinden@wur.nl

29 **Abstract**

30
31 Agri-food is one of the most important sectors of the industry in Europe. Sustainability issues in this
32 context pose a huge challenge. This paper gives a computational viewpoint on this problematic in
33 order to develop a more holistic approach, a link between different scales and clear insights in the
34 complexity of agri-food systems. This creates huge opportunities for research in mathematical
35 programming, integrative models and decision-support tools. In this paper we outline some future
36 research directions on mathematical resilience, human-machine interactive learning and
37 optimization techniques.

38 **Keywords**

39 Agri-food systems, sustainability, multiscale modeling, computing complex system, decision support
40 system, optimization, resilience, human expertise, interactive learning.

41 **1. Introduction**

42
43 Food (Lehmann, Reiche & Schiefer, 2012) is one of the most important sectors of the industry (CIAA
44 2009), encompassing chemicals, agriculture, feed, food processing and trade, retail and consumer

45 sectors. Production and consumption of food is the major contributor to the global warming
46 potential in Europe (31%), taking into account all products required by the society. Amongst food
47 products, meat and dairy have been identified as the main contributors to the global environmental
48 impact, with a share of up to 12% in the case of meat, and up to 4% in the case of dairy products.

49 The food industry is fully aware that environmental performances of products and processes need to
50 be improved in the full production-till-consumption chain². In addition, the consumer's needs should
51 be met for food safety, health, convenience, lifestyle and product choice; and at the same time,
52 commercial and financial benefits of the entire value chain must be assured in order to retain
53 competitiveness. The problem to solve is particularly complex, since the management of the
54 sustainability approach requires a multi-scale, multi-disciplinary and multi-factorial approach.

55 Sustainability starts at the farm level with the application of a large set of good farming practices, the
56 preservation of natural resources and biodiversity, the development of specialized skills and
57 capabilities, as well as the respect of farmer's choices in a given social and economic environment.

58 Subsequently, the transformation phase for biomass must be considered. Processes need to use
59 these natural resources in a highly efficient way, developing bio-refineries to transform waste in by-
60 products, and reconsidering the supply chain, currently still organized in a "product chain". Energy
61 saving and water recycling are of course the major challenges in this step: they require development
62 of new technologies through investments in research, increased awareness, especially crucial for
63 SMEs (small and medium enterprises) to integrate innovation and a strong support from regional and
64 (inter-)national policies. The volume of packaging has considerably increased in response to
65 consumer demands for safety and affordability of products; its reduction is a tremendous challenge
66 in the wider context of reducing household food waste while maintaining food quality.

² For further details, see

http://ec.europa.eu/research/bioeconomy/pdf/201202_innovating_sustainable_growth_en.pdf

http://etp.fooddrinkeurope.eu/documents/2012/SRIA_2012/SRIA_ETP_Food4Life_2012.pdf

67 The third part of the equation concerns logistics, in particular when dealing with perishable products.
68 In a world which did not take into account the environmental balance for a long time, road
69 transportation became the major delivery means, with a considerable impact on greenhouse gas
70 emission. Solutions exist, but require strong initiatives at a pan European level from politics, industry,
71 research institutions and NGOs.

72 Finally, consumers should not be overlooked, because they play a major role in the sustainability of
73 the food chain through their home practices, purchasing decisions, trade of shares and stocks,
74 cultural and normative diverse background and requirements, etc.

75 In this context, creativity to reach breakthrough innovations on the one hand, and efficiency and
76 optimization on the other hand, are crucial to obtain sustainable solutions: appropriate strategic
77 visions, organization, transparency and control, assure safety and quality of novel products and
78 ingredients (Lehmann, Reiche & Schiefer, 2012), as well as accessibility and affordability of food.
79 Reaching these objectives requires multi-scale approaches, starting from the nano-scale for products
80 and their ingredients, up to the km-scale for regional and global management issues, including
81 organization and control of factories and food chains.

82 At each scale, one may observe a diversity of complex products and networks of organizations. In
83 highly developed countries, production is characterized by very different types of enterprises,
84 ranging from single-product manufacturers to generalists providing diverse products, technologies,
85 services and logistics (Lehmann, Reiche & Schiefer, 2012). Production organization ranges from local
86 to global, from farm to fork and beyond, from fast-foods to high-end restaurants, from laboratories
87 to factories and supermarkets, from supply to demand and from single entities to full networks.
88 Historically, agriculture and the linked manufacturing industry are considered to be independent
89 sectors (Thompson & Scoones 2009) (Reilly & Willenbockel 2010); this holds today as well for the bio-
90 based non-food sector. If we consider full food value chains as multi-input and multi-output

91 networks (or systems), it is noticeable how they are still poorly developed, when compared to the
92 specific needs of consumers, society and environment at large; but since this vision of food chains
93 has rarely been taken into account, numerous new opportunities and more sustainable solutions
94 have yet to be considered.

95 In order to achieve sustainable approaches, different strategies can be developed by enterprises and
96 societies. These strategies and their underlying models, however, might be synergic, neutral or in
97 conflict with each other. It is thus crucial to carefully choose the strategies to follow, since these
98 decisions are laden with moral, aesthetical and socio-economical values. Many heterogeneous
99 factors, some being dynamical like zeitgeist, availability of information and perceived pressures, are
100 to be taken into account when creating new legislation on sustainability. Normative dimensions of
101 agri-food problems have the property of being heterogeneous, and can even be self-organising (see
102 section 2.1). Indeed, we may view the normative dimensions involved as a stand-alone complex
103 system, one that influences in turn the development of sustainability in many areas. This problem
104 calls for a systematic approach on fair decisions, able to respect different moral, aesthetic and social-
105 economical constraints (e.g. see Rawls, 1999).

106 A transition towards a bio-based society, while maintaining a viable planet and ethically well-
107 accepted conditions, requires addressing various opportunities and devising appropriate solutions.

108 This paper gives a computational viewpoint and guidelines in order to develop (1) a more holistic
109 approach, (2) a link between different scales and (3) clear insights in the complexity of agri-food
110 systems. The rest of the paper is organized as follows: Section 2 considers the most relevant
111 questions in a complex system approach for sustainable food systems. Section 3 reviews possible
112 research directions, while Section 4 details three sources of inspiration for new approaches in the
113 food domain. Sections 5 and 6 draw the conclusions and sketch high-level perspectives for the
114 future.

115 **2. Methodological approach, main questions and predictable** 116 **bottlenecks**

118 **2.1 A holistic approach: an introduction to complex system science**

119
120 A **holistic approach** can be characterized as the process of integrating, through interdisciplinarity and
121 synthesis, cross-scale research and analysis (Thompson & Scoones, 2009). Integrative science
122 provides a means to answer questions about inherent linkages and feedbacks within social-ecological
123 systems, such as sustainable fisheries (Miller et al., 2010) and agricultural value chains (Higgins et al.,
124 2010). Several dimensions should be taken into account: spatial, organizational, temporal scales, and
125 the correlated rates of change; spatial distributions of variables, their scaling, and feedback loops
126 have to be considered, as well as their interpretation within the relevant scientific disciplines.

127 This holistic approach cannot be managed “manually” *ab initio* and there is a clear need for decision-
128 support tools based on different fields of computer science (applied mathematics, artificial
129 intelligence, optimization), see sub-section 2.3 below. One of the most crucial tasks related to the
130 development of such support tools is the design of models (Perrot et al., 2011, Charpentier, 2010,
131 Trystram, 2012). **Modeling complex systems through a holistic approach** is an iterative activity that
132 requires knowledge and comprehension of scientific facts, expert skills and sensory assessments, and
133 relies upon methods allow for cross-overs with new fields in computer science.

134 **CSS (complex system science)** makes it possible to cope with the expanding boundaries of complex
135 adaptability in agri-food systems; there is an increasing focus on interacting economic, social and
136 environmental goals. Emergence of properties from these dynamical interactions should be studied.

137 The 2012-2020 roadmap defined the science of complex systems³ as distinct from any other
138 particular science, because it focuses on the methods of reconstructing the dynamics of
139 heterogeneous systems across traditional domains.

140 Systems can exhibit many properties that make them appear complicated or complex. These include:

- 141 • heterogeneous parts, e.g. a city, agriculture and the climate;
- 142 • complicated transition laws, e.g. agriculture and climate transitions;
- 143 • unexpected or unpredictable emergence, e.g. chemical systems, accidents;
- 144 • sensitive dependence on initial conditions, e.g. weather systems, investments;
- 145 • path-dependent dynamics, e.g. international relations, regional subventions;
- 146 • network connectivity and multiple subsystem dependencies, e.g. ecosystems, multiple
147 industrial sectors;
- 148 • dynamics that emerge from interactions of autonomous agents, e.g. agriculture, traders;
- 149 • self-organization into new structures or behavioral patterns, non-equilibrium and far-from
150 equilibrium dynamics, adaptation to changing environments, e.g. biological systems, manufacturing
151 design.

152 Such properties are vertical, in the sense that they cut across disciplines which are researched
153 horizontally in greater depth, based on the assumption that they can be treated in isolation (to a
154 greater or lesser extent) by other domains. Economists, sociologists, food engineers, plant scientists,
155 etc. traditionally tend to work in isolation from each other, while the science of complex systems
156 aims at using a new methodological perspective. The transdisciplinary nature of CSS makes it unique
157 because it strives to combine the methods, knowledge and theory of other disciplines. The complex
158 system methodology starts from heterogeneous data and knowledge (Figure 1). The objective is to
159 produce an augmented phenomenology where Δ , the statistical difference from observation, is as

³http://roadmaps.csregistry.org/tikiindex.php?page=The+science+of+complex+systems&structure=european_roadmap

160 small as possible but taking care of the danger of overfitting. For example, from the data and
161 knowledge available about the structure-function elaboration of a food product, a phenomenological
162 model encompassing the impact of a change in raw material usage on the food structure, its
163 function, and consumer acceptance, can be created. Coupled to a model expressing the link between
164 the raw material production and the territory scale organization, an agent-based computer
165 simulation can be built to create an augmented phenomenology for this system, spanning from the
166 km-scale to the nano-scale (Figure 1, bottom-center). On the basis of these simulations and
167 knowledge availability, a model of organization covering the various scales is proposed to create
168 another augmented phenomenology and the possibility of conceptual modeling by mathematical
169 means (Figure 1, bottom-right), developed in more detail in (Van Mil et al., 2014).

170

171 [Figure 1 about here]

172

173 These augmented phenomenological holistic models are complex in their own right, and not always
174 easy to interpret on a more general level, nor directly translatable to different contexts or related
175 problems. More general models can be applied to a broader range of systems, but they lack the
176 quantitative precision of augmented phenomenological models: thus, we need different classes of
177 models to deal with complex problems at a deeper conceptual and abstract level. It is almost
178 impossible to deduce models of complex systems *ab initio*: a good research strategy would be to
179 start from empirical or phenomenological models, and then search for invariant structures, see
180 (Stoutemyer, 2013) and, in a slightly different context, (Suppes, 2002). These invariant structures can
181 then be interpreted in the light of overarching theories, or help theory construction. In order to find
182 meaningful model structures, it becomes necessary to use more advanced mathematics and
183 computer science, which allow different models to be mapped onto each other, and uncover the

184 invariant parts (Suppes, 2002; Stoutemyer, 2013). Giving meaning to these invariant structures calls
185 for thorough interdisciplinary knowledge of the subject and the consultation of experts (see below
186 3.2). Such a strategy creates interesting opportunities for fundamental mathematics and logic in the
187 context of computer science: this fact is not yet fully realized, but it can lead to innovations very
188 difficult to obtain otherwise. We will not explore this branch of research further in the publication
189 but will focus more on computational methods.

190 We only would like to note here that augmented phenomenological models and more general
191 models can strengthen each other in terms of research quality. As in physics, analytic models are
192 checked by numerical simulation and vice versa. This abstract process makes it possible to gain
193 insights that would be otherwise very difficult to reach, and shows the necessity of a pragmatic
194 pluralistic approach, as defined by (Suppes, 2002). No matter how complex, a holistic approach
195 should have internal checks and balances, and create a well defined link between study design, data
196 and models of different types, precision and abstraction.

197

198 **2.2 A multi-scale approach**

199

200 A major challenge is to crossover and to connect the scales, from the resource-structure level to the
201 territory scale, and even beyond. While individual farmers or food companies at particular locations
202 may be our empirical focus, their options and opportunities must be understood in relation to
203 processes interacting across scales (Thompson & Scoones 2009), from the very local to the global
204 ones. A pathway being pursued at one level may interact – positively or negatively – with options at
205 another level, thus interconnections between individual, household, institution, regional clusters on
206 one hand and (sub-)molecules, cells, plants and ecosystems on the other hand are all critical. Too
207 often, analyses begin and end at the same scale, failing to explore larger effects. It is thus necessary

208 to step out of “disciplinary boundaries”, the comfort zone, which define and frame traditional
209 analyses, in order to establish more useful interdisciplinary connections.

210 Problems that are non-linear in nature, cross-scale in time and space, and dynamic in character
211 require a systemic perspective (Thompson & Scoones 2009). Interdisciplinary and integrated modes
212 of inquiry are necessary for understanding and designing effective responses to human-environment
213 interactions, related to food and agriculture, in a dynamic world.

214 Nevertheless, bio-based sciences emerged from traditional experimental sciences, the latter having
215 procedures that often to narrow down the focus in order to pose specific questions, set hypotheses,
216 collect data and design critical tests for hypothesis rejection. The goal has been to reduce uncertainty
217 up to the point where acceptance of an interpretation among scientific peers is essentially
218 unanimous. A drawback of this traditional “trial & error” approach is the limited knowledge it
219 provides on the entire systems (Thompson & Scoones 2009) (Walker *et al.*, 2006).

220 Recent work on resilience suggests that many of the observed shifts, crises, or nonlinearities in
221 ecological systems arise from processes and structures interacting across scales (Holling, 2001); and
222 in fact, disruptions at different scales at the same time push the full system into another attractor
223 more easily than a single perturbation on a single scale. For instance, resilience has been studied and
224 extensively discussed for sustainable fisheries (Miller *et al.*, 2010). A possible trap experts can fall
225 into is to try to understand the single parts and, consequently, lose the global perspective of the
226 system (Walker *et al.*, 2006). Complexity, diversity and opportunity in complex (local) systems
227 emerge from a handful of critical variables and processes that operate over distinctly different scales
228 in space and time. There is a strong need for integrative frameworks that bridge disciplines and
229 scales (Van Mil *et al.*, 2014).

230

231

232 2.3 Decision making issues and quantitative sociodynamics

233

234 Decision support tools and argumentation based models are built and used in a limited number of
235 areas. These areas are often well described, possess reliable data sources (e.g. processing line
236 characteristics) and are single-step oriented (Matser *et al.*, 2010). When dealing with chains of
237 operations, the tools and models become more complex (Bourguet *et al.*, 2013). For complex multi-
238 scale systems, we need to further develop sound argumentation and decision support systems
239 integrating a considerable number of variables and interactions; here, one should face the following
240 key elements:

- 241 • Surprises: as defined by (Thompson & Scoones 2009), are the qualitative gaps between
242 perceived reality and expectation in ecological systems. Taking them into account, as well as
243 the so-called technological surprises (Reilly & Willenbockel 2010) is a major challenge for
244 agri-food systems. These unpredictable events must be considered in management practices
245 besides other social and institutional mechanisms, in order to reduce poverty and increase
246 resilience.
- 247 • Uncertainties: many variables are influenced by uncertainties, namely environmental
248 regulations, demand, supply, initial capital cost, technological, biological effects like
249 structure/function relationships, impact of processes and ingredients on quality (Perrot *et*
250 *al.*, 2011). Interesting reviews and examples related to uncertainties in the biofuel Supply
251 Chain Management can be found for instance in (Doukas, 2013) and (Awudu & Zhang, 2012).
252 Additionally, if we consider uncertainty in energy sustainability, vague and complex concepts
253 and their implications as a policy objective are difficult to define and measure (Grossman &
254 Guillén-Gosálbez, 2010).

- 255 • Complex, qualitative and quantitative information sources, uncertain and incomplete data
256 (Higgins et *al.*, 2010), non-harmonized data acquisition⁴, availability and accessibility of
257 information (Perrot et *al.*,2011).
- 258 • Sustainability metrics: currently available sustainability metrics are mostly devoted to
259 individual organizations, only (Hassini, Surti, Searcy 2012).
- 260 • Dynamic adaptive behaviour: a reductionist vision is not enough to understand complex
261 adaptive networks (Surana, Kumara, Greaves & Raghavan, 2013).
- 262 • Heterogeneous problems: market values, environmental, social, legal issues with some
263 indicator measurements difficult to quantify (Meulen, 2013), due to the lack of numerical or
264 probabilistic assessments.
- 265 The emerging field of quantitative sociodynamics, an offspring of econophysics, provides some
266 interesting results in dealing with the problems discussed above; using theory and models developed
267 in physics, but reinterpreting them with concepts from the sociology domain (Helbing 2010a, Helbing
268 2010b).

270 **2.4 Summary of relevant questions**

271

272 In the synthesis of model and real agri-food systems lies a huge research opportunity for
273 mathematical programming, integrative models and decision-support tools (Gupta & Palsule-Desai,
274 2011).

275 Several research questions based on a mathematical programming framework are emerging: how
276 can such a framework manage uncertainty, cope with complex qualitative and quantitative
277 information essential for social and environmental considerations, encompass diverse scales in space
278 and time, cope with a multivariable dynamic environment, and with scarcity of data. Moreover, how

⁴ <http://www.globalharmonizationinitiative.net>

279 can it deal with different perspectives, types of models, research goals and data produced by
280 conceptually disjoint scientific disciplines, ranging from physics and physiology to sociology and
281 ethics?

282 These questions are generally addressed separately by laboratories working in fundamental
283 mathematics or computer science, and focus on theoretical, “simple” systems of various disciplines.
284 These approaches should now be integrated and adapted to with regards to sustainability in real-
285 world problems.

286 A new science corpus should be developed at the frontier of theoretical sciences and agri-food
287 science, where these topics can be addressed. Some directions for building this corpus from the
288 computational perspective are proposed in the next section.

289 **3. Directions for future research in sustainability**

290
291 Some directions are proposed in this section to face the challenge of sustainability in agri-food
292 systems:

- 293 • Defining an overarching conceptual scheme: e.g. mathematical resilience,
- 294 • Sharing knowledge and expertise: man-machine interactions
- 295 • Augmented phenomenology: model construction and decision making.

297 **3.1 Mathematical resilience perspectives**

298
299 When integrating research that spans a number of scales and disciplines, its expedient to introduce
300 an overarching principle or concept. The term “resilience” is often used when the sustainability of a
301 system is analyzed. Resilience is an emergent property of interactions within a system. Quantifying it
302 remains a key scientific challenge (Carpenter et *a.l.*, 2001). The word resilience was first used at the

303 end of the nineteenth century in Material Physics to refer to the quality of some metals to resist to
304 stresses and to return to their original shape after a blow. During the 20th century, its use has
305 extended to several other domains, in ecology, economics, social sciences, etc. While the objects
306 change, the underlying idea remains the same: resilience is defined as the capacity of the system
307 under study to keep or restore some properties despite disruptions caused by perturbations
308 (Carpenter *et al.* 2001). In ecology, the conceptual definition of Pimm (Pimm, 1984), considers
309 resilience as the ability of a system to resist disturbance and the rate at which it returns to its steady
310 state following a disturbance. For Gunderson and Holling (Gunderson & Holling, 2002), resilience is
311 the capacity of a system to undergo disturbance and maintain its functions and controls and is
312 therefore related to the concept of robustness in control theory (Carlson & Doyle, 2000). As far as
313 operational definitions in the context of ecosystem models are concerned, the main mathematical
314 definitions of resilience are based on dynamical systems theory, and more specifically on attractors
315 and attraction basins (see (Pimm & Lawton 1977), (van Coller, 1997)). More recently, the viability-
316 based measure of resilience (Martin 2004) focuses on the desired properties of the system that do
317 not necessarily correspond to attraction basins, but to an evolutionary development. Moreover, this
318 general definition makes it possible to consider different management actions, and allows the
319 experts to interact with the system and appropriately respond to disturbances (Alvarez, De Aldama,
320 Martin & Reuillon, 2013). In economics, Martinet and Doyen have been the first to link sustainability
321 with viability concepts. An intergenerational equity feature is naturally integrated within this
322 framework (Martinet & Doyen, 2007). Moreover, the definition of a set of constraints bringing
323 together desirable sustainable situations makes it possible to address sustainability as the possibility
324 of finding a path that is an acceptable compromise for all parties (Fuentes, 1993). Since then, (Wei,
325 Alvarez & Martin, 2013) have shown how the concepts of viability kernels and capture basins allow
326 researchers to take into account spatial and time factors of a sustainability analysis with transient
327 dynamic features. Several sustainability studies using mathematical viability tools have been

328 performed, for example in fisheries management (Martinet, Thebaud & Doyen 2007), (De Lara &
329 Martinet 2009), and in forest preservation (Bernard & Martin 2013).

330 The main characteristic of the viability theory approach is to emphasize the definition of the
331 constraints and means of actions before applying any optimization concerns. This is a powerful
332 source of innovation, as illustrated, for example, by an application on the Camembert cheese
333 ripening process (Sicard *et al.*, 2012)(Mesmoudi *et al.*, 2014).

334 The viability framework is used to compute the set of possible states and controls from which it is
335 possible to reach a predefined quality target of Camembert cheese (figure 2 presents a result of the
336 computation described in (Mesmoudi *et al.*, 2014)). This procedure makes it possible to evaluate that
337 some ripening times are more crucial for the viable pathways of the state variables than others; at
338 the beginning, for example, few values are admissible; and after 10 days, irreversible phenomena
339 have taken place. This set of possible states contains trajectories that have never been considered by
340 experts so far (Sicard *et al.*, 2012). The exploration of this set makes it possible to find ripening
341 trajectories one-third shorter than the standard procedure, which had never even been
342 contemplated at the beginning of the project, contrary to more traditional criteria such as energy or
343 raw material quantity. In parallel, quality was maintained.

344 Moreover the knowledge of this set of viable states allows to take into account the distance to the
345 boundary and to define in this way the robustness to perturbation. This approach was validated by
346 experiments at the pilot scale.

347 [Figure 2 about here]

348 When the key variables, constraints (including sustainable ones) and possible controls of an agri-food
349 systems can be identified, the viability approach can establish whether present practices and
350 sustainable objectives are compatible and how.

351 Assume we look at a small local Camembert factory that caters a small connoisseurs market of
352 Camembert devotees. Then we can combine two sustainability targets, environmental and cultural;
353 two value systems that have always been intertwined and each of their own form an example of a
354 complex problem, and as a combination. By
355 including environmental/sustainability parameters/variables/targets to decrease of environmentally
356 unfriendly output or increasing environmentally positive output, the model built could optimize
357 sustainability targets if combined with optimizing computing tools (cf. chapter 3.3). One of the
358 reasons to use the augmented phenomenology is to effectively optimize the process using the local
359 Camembert expert to safeguard the cultural and uniqueness of the product and the knowledge of
360 environmental experts in the process optimization using the augmented phenomenology as a third
361 party. In this way the process also includes cultural values of the food product that relates the
362 product to the cultural heritage of the region that is essential of its unique taste and structure so
363 recognizable and enjoyed by the connoisseurs (cultural sustainability target) and the environmental
364 sustainability target. Moreover, as culture is not a static phenomenon but a balance result between a
365 conservative cultural dogmas and new innovations, it fits well in the culture development allowing
366 for the evolution of new products out of old ones within the cultural same context; e.g a new variety
367 of Camembert with a distinct taste, structure and smell, a triumph of the "man-
368 machine cooperation". The main limit of the approach is the complexity of the computation which is
369 exponential with the number of state variables. This presently limits practical nonlinear applications
370 to less than 10 variables. Research work is currently performed to overcome this limitation (with the
371 use of classification functions or test methods)

372

373 The trade-off between efficiency and resilience remains obvious (Walker et al., 2006, , Carlson &
374 Doyle, 2000 and ref). Optimizing performance by increasing efficiency in a nonlinear adaptive system
375 is a complex task. Experts have indeed gained the skills to cope with the complexity of their

376 environment while keeping the sense of the whole. For example, pilots are able to steer their aircraft
377 in complex environments without losing control. Drawing a parallel with sustainability purposes can
378 be relevant: however, the major bottleneck of these approaches remains the acquisition of
379 knowledge (Hoffman, Shadbolt, Burton, & Klein, 1995), which is often a difficult and time consuming
380 step (Sicard *et al.*, 2011). Interactive approaches coupling autonomous computations and human
381 expertise thus represent an attractive perspective.

382

383 **3. 2 Interactions with human knowledge and expertise**

384

385 Another question, addressed by several authors, concerns the place of experts and human
386 knowledge in mathematical approaches applied to sustainability. Although several studies analyze
387 expertise both in psychology and artificial intelligence, it is not possible to provide a consensual and
388 operational definition of this notion (Shanteau, 1992). Expertise may include skills, knowledge or
389 abilities in tasks, jobs, games or sports, and is domain-specific (Chi, Feltovich, & Glaser, 1981). In spite
390 of the diversity of task domains and of expert definitions, literature reports three criteria to define
391 experts: they are better at producing inference, at anticipating dynamics, and have a more functional
392 view of the process (Cellier, Eyrolle, & Marine, 1997). Finally, experts are characterized by a large
393 number of automatisms and knowledge acquired during practice (Raufaste, Neves, & Marine, 2003).
394 In human cognition, perceptive processes are an automatic and continuous form of learning (Gibson,
395 1969). Perception learning is based more on experience (so called SB, for sensory based) than on
396 rules (so called RB, for rules based) (Ballester, Patris, Symoneaux, & Valentin, 2008), (Valentin,
397 Chollet and Abdi, 2003) show that experts have an advantage in recognition memory: they illustrate
398 that these higher performances are likely derived from more efficient coding and retrieval of long-
399 term memories. One of the efficient coding mechanisms used by experts is the cognitive “chunk”
400 recognition (Chase & Simon, 1973). A “chunk” is a grouped set of variables, taken from a situation,

401 that are closely related to each other. These variables are acquired through experts' sensorial
402 perceptions.

403 Operational research is a discipline that deals with the application of advanced analytical methods to
404 help make better decisions. This is an active field in the domain of sustainability, where expertise has
405 an important role. Higgins et al. (Higgins et al. 2010) have underlined the following key elements:

406 • Mathematical representation of the problems (integer or linear programming) is not
407 generally consistent with the way in which the decision maker understands the problem
408 when constructing the solution. Approaches should take into account this dimension and
409 integrate it iteratively, for instance through an interface with the decision makers (figure 3,
410 from Miller et al., 2010), where authors propose a structure where a participatory process is
411 embedded iteratively in the loop of an algorithm. Integration is performed at the validation
412 level.

413 [Figure 3 about here]

- 414 • Quantifying factors considered by experts when generating a desired solution is hard; often
415 solutions are found through extensive exploration, and not focusing on efficiency and
416 inclusion of feedback loops.
- 417 • Data requirements and uncertainties may be huge.
- 418 • Whole-of-chain system understanding of practical problems, particularly when social and
419 environmental drivers are concerned, is difficult to reach for the industry and practitioners.

420

421 Another element is given by (Melnik, 2009): with the increasing complexity of technological systems
422 that operate in dynamically changing environments, the relative share of human errors is increasing
423 across all applications. This means that human errors can no longer be ignored (or eliminated easily

424 by conventional formal statistical methodologies) but should be integrated into the modeling
425 framework.

426 Reilly and Willenbockel (2010) propose to consider uncertainty, complexity and diversity as means to
427 enhance adaptability of agri-food systems; by contrast, current policies and practices aspire to
428 maintain the status quo or to control change in systems assumed to be stable. In other words, this
429 implies a radical change from reactive to proactive system approaches. Improving the process of
430 innovation via knowledge sharing is strongly linked to the ability of models to capture not only the
431 planned but also the unplanned outputs of knowledge sharing (Miles & Snow, 2007; Zwart et al,
432 2006). Computer aided design must help the person or group to communicate easily and generate
433 more and richer ideas (encourage generation of diverse even inept ideas that carry potential for new
434 ideas), while maintaining their diversity.

435 Applied to manufacturing processes, where generally the assessment of alternative solutions is based
436 on life cycle assessment, (LCA), some contributions have been developed at the frontier of artificial
437 intelligence, to take into account expert knowledge. Authors like (Giovannini *et al.*, 2012) used for
438 example ontologies that implement a support to sustainable manufacturing. The authors' main
439 statement is that a cultural shift is required that involves in-depth software and hardware insights in
440 manufacturing processes. They propose to design a KBS (knowledge based system) simulating the
441 role of a sustainable manufacturing expert, who is able to automatically identify change
442 opportunities and to propose alternatives. The human dimension is thus included and considered in
443 the cost function evaluation. The next step is to integrate not only the external evaluator role within
444 a more or less balanced system but in a full network that link local connections and from which
445 global properties emerge.

446 For instance, a tool that is currently available to explore multi-dimensional data sets is EvoGraphDice.
447 It is based on the EVE framework (Evolutionary Visual Exploration) (Boukhelifa et al., 2013). This

448 approach for data exploration combines a classic interactive visualization technique (a scatterplot
449 matrix with linked views) with evolutionary stochastic optimization. The EvoGraphDice prototype
450 extends the concept of principal component analysis of scatter plots by using interactive optimization
451 to evolve a population of secondary axes of observations as linear or nonlinear combinations, thus
452 providing users with nontrivial views on their data.

453 However, current projection axes are not defined from the mathematical structure of the model in
454 hand; rather they are dynamically generated to favor views showing an interesting visual pattern to
455 the user where the notion of “interesting” is defined dynamically using an image-based metric and
456 subjective user ranking of views.

457 The EVE framework could be further extended to take into account different types of knowledge,
458 both quantitative and qualitative (e.g. mathematical structures, statistical information, or confidence
459 level), to better guide the exploration to pertinent areas of the search space. The uncertainty itself
460 could be fed into the interactive evolutionary algorithm such that user exploration is driven towards
461 more certain (or informative) areas of the search space. Whereas Scatterplot Matrices (SPLOMs) are
462 effective for visualizing small to medium-sized static multidimensional data sets, new scalable
463 visualization techniques need to be investigated to better visualize time-varying scale-dependent
464 relationships between a large number of dimensions (e.g. using dynamic networks instead of or
465 linked to the SPLOM). In this new context, new navigation techniques are also required to allow for
466 the smooth transitioning between the different scales and types of data (e.g. using appropriate
467 animated transitions).

468

469 3.3 Optimization

470

471 Optimization in the context of complex adaptive systems is far more difficult than when dealing with
472 plain systems based on sequences of static configurations; the latter has been extensively
473 elaborated, for example in chemical engineering (Grossmann & Guillén-Gosálbez, 2010; Lainez &
474 Puigjaner, 2012).

475 Optimization is used for various purposes: in this work, we are mainly interested in (a) building
476 models, learning their parameters and structures from available data and knowledge; and (b) using
477 such models in decision-making processes.

478 Optimizing the efficiency and resilience of an entire industry, as a network of business partners and
479 competitors, is fundamentally different from optimizing each individual business unit within the
480 context of that industry (Miller et al., 2010). However, contemporary management is based almost
481 entirely on the optimization of individual business units for static “average” conditions. Influences
482 arising from states and dynamics above and below the scale of interest are ignored, but affect the
483 ability of the system to reorganize and resist after some disturbance (Walker et al,2006).
484 Furthermore it should be noticed that integer or linear program optimization strategies can have a
485 small spatial or temporal range in terms of predicting the effects of an action if the system exhibit
486 strong nonlinear properties. Depending on the point in parameter space, the variable underlying
487 distributions or phase space can change, leading to different dynamics and equilibriums or steady
488 state solutions. Moreover, these systems evolve; intervention, control mechanism and innovations
489 introduce new objects and relations, affecting the fitness landscape of the function to be sustained
490 or other seemingly unrelated important processes. Therefore optimization should be viewed as a
491 continuing dynamic and adaptive process.

492 As said above, the implication of single human users or groups of users in optimization processes is a
493 challenging question (for dealing with expertise on model building, decision making, control,
494 monitoring, data gathering, tacit knowledge, etc.). Techniques involving human expertise in
495 optimization processes are sometimes referred to as *humanized optimization* (Takagi, 2008).

496 While potentially very effective, humanized optimization has several important limitations, the major
497 one being *user fatigue*, the tendency of human users to lower the quality of their assessment as the
498 time spent interacting with an algorithm increases. There is a considerable amount of literature on
499 compensating or limiting user fatigue (Lam, 2008): concerning model building, a possible approach is
500 to let the user itself set the pace of the procedure. (Tonda *et al.*, 2014), for instance, proposes a
501 framework for Bayesian network structure learning, capable of producing probabilistic graphical
502 models with a semi-supervised approach. The framework is tested by two experts in food science,
503 using datasets from food processing, and while the results are satisfying, further limitations are
504 uncovered: given the choice between multiple learning algorithms, users show a predominant
505 preference for quick and sub-optimal algorithms, with respect to slower, more effective ones. Thus,
506 it seems that the expert would rather see the immediate result of his/her ideas, more than obtain
507 the best possible approximation. Another limit of this approach concerns the number of variables
508 that a human can manage: even when interacting with a graphical model, users cannot successfully
509 analyze more than a few tens of nodes. This limit is also true for the advanced visualization methods
510 discussed in paragraph 3.2. These are non-trivial insights that should be taken into account for
511 devising further methods combining human expertise and machine learning.

512 Even more difficult but strategic issues are related to optimization for decision making in a
513 hierarchical environment with a variety of business functionalities (Lainez & Puigjaner, 2012), where
514 the behaviour of the system and the available knowledge at different scales has to be considered.

515 In order to design efficient optimization algorithms, various points need to be addressed: structure of
516 the search space (for instance with mixed variables), constraints, and optimisation aims (mono- or
517 multi-criteria objectives) (Pavone and Coello Coello, 2012). The question of multiple conflicting aims
518 can be tackled using multi-objective optimization tools (Miettinen and Sayin, 2013), providing the
519 user with a full range of optimal compromises, called Pareto front. Even if the Pareto front might be
520 large and hard to understand for a human user, efficient decision tools and ad-hoc visualization
521 techniques can help the user to efficiently explore the set of proposed solutions, and finally take a
522 decision (Coello Coello, 2009).

523 **4. Examples**

524

525 **4.1 Multi-scale analysis in the chemical industry**

526

527 Sustainability is indeed largely addressed by the chemical industry, in particular in process synthesis.
528 A review about this topic can be found in (Nicopoulou and Lerapetritou, 2012). Several scales can be
529 considered as depicted by (Lainez & Puigjaner, 2012). An example among others is related to a
530 biofuel chemical plant (You, Tao and Snyder, 2011), where several configurations at the equilibrium
531 are tested. The focus of this work is not only on the manufacturing process but also on the supply
532 chain. Numerical approaches like MILP (multiperiod, mixed integer linear programming) and MOO
533 (multiobjective optimization) are widely used to reduce costs in process synthesis by choosing the
534 best organisation at the equilibrium. The strategy is based on the following steps (Grossmann &
535 Guillén-Gosálbez, 2010): (1) development of a representation of alternatives, (2) formulation of a
536 mathematical program for the selection of the configuration and operating levels that involve
537 discrete and continuous variables, (3) the solution of the optimization from which the optimal
538 solution is selected. Several optimization methods have been tested in literature, from gradient
539 search to global ones, as tabu-search or evolutionary algorithms.

540 The drawback of system dynamics models (type MILP) is that the structure has to be defined before
541 the simulation starts. Another drawback of these chemical engineering applications is that
542 optimization is achieved on solutions at the equilibrium of the system, and transient dynamics are
543 disregarded. Queuing theory has primarily been used to address the steady-state operation of a
544 typical network. Mathematical programming has also been used to solve the problem of resource
545 allocation in networks. This is meaningful when dynamic transients can be disregarded, which is not
546 always relevant with regards to the problem tackled. A useful paradigm for modelling a supply chain,
547 taking into consideration the detailed patterns of interaction, is to view the process as a network
548 involving interacting agents: (Surana, Kurava, Greanes & Raghavan, 2013) propose an approach
549 originating from complexity theory: an agent-based model, or 'bottom-up approach', simulates the
550 underlying processes that yields a global pattern. This makes it possible to evaluate which
551 mechanisms are the most influential in producing the emergent pattern. Networks are inherently
552 difficult to understand due to their structural complexity, evolving structure, connection diversity,
553 dynamical complexity of nodes, node diversity and meta-complication where all these factors
554 influence each other.

555 If we translate this to agri-food systems, it becomes even more crucial to consider many agents and
556 scales, and especially their reciprocal interconnections. Embodying scales in this domain means also
557 taking simultaneously into account structure, function, preferences, acceptance, perception and
558 needs. If this viewpoint is shared with the chemical industry (Charpentier, 2010) (see figure 4) there
559 is an increased complexity due to the nature of living phenomena and their environmental impact on
560 the entire system. As a consequence, sustainability approaches include the molecular level (even
561 down to sub-atomic levels), i.e. the scale guiding the dynamics of structure-function relationships
562 and biological processes around equilibrium, up to the factory level and beyond. Territory mega scale
563 level may even be considered when sustainability purposes are investigated. In this context,

564 sustainable solutions emerge from transient states and not only at equilibrium. This makes it possible
565 to include human interventions, both locally and globally.

566 [Figure 4 about here]

567 **4.2 Multi-scale analysis in biological processes**

568

569 An interesting example of multiscale challenge is the management of the ecosystems in agri-food
570 systems. Microbial ecosystems are present everywhere (e.g. in soil, animal gut, food products and
571 marine sediments). Understanding their multi-scale properties to be able to make predictions is of
572 major importance to life sciences (Faust and Raes, 2012). The assessment of microbial ecosystems
573 mechanisms, from gene expression to emergence of functional properties is a challenging issue for
574 several reasons, including the presence of many scales, uncertainties, out of equilibrium (instability),
575 and complex quantitative (generally big data) and qualitative information (a long scientific
576 descriptive expertise).

577 Ecosystems are involved in a large variety of food systems. For example one typical microbial
578 ecosystem widely studied is cheese. Cheese is one of the oldest dairy products and, nowadays,
579 constitutes the most diverse group of dairy products with several hundreds of distinct varieties. It
580 involves a dairy industry that plays a key role in the French economy with 27.7 billion income and 3.6
581 billions trade surplus in 2013, representing over 250000 jobs.

582 Cheese ripening is a complex process involving a range of microbiological and biochemical reactions.
583 During this process, three major biochemical events occur: lactose consumption, lipolysis, and
584 proteolysis. These catabolic reactions are responsible for the production of various compounds
585 including volatile aroma compounds which play an important role in flavor perception.

586 The cheese microflora is characterized by a high cell density, as it can reach more than one billion
587 cells per gram of cheese. It is composed of both aerobic members, i.e. those developing on the

588 cheese surface such as microorganisms found in the rind of soft cheeses, and anaerobic, i.e. those
589 growing inside the curd like species found in the middle of hard cheeses. The main technological
590 activities sustained by the microbial community regard the matrix biodegradation which lead to the
591 development of interesting organoleptic properties (cheese sensory quality), and the potential
592 protection effect against spoilage microorganisms and pathogens (cheese safety).

593 A large microbial diversity has already been isolated from cheese products, providing an important
594 resource of cultivable microbes for microbiological, biochemical and molecular analyses. It mainly
595 contains Firmicutes (lactic acid bacteria, staphylococci), Actinobacteria (coryneform bacteria),
596 Proteobacteria, Bacteroidetes, yeasts and moulds. Recent inventories of the cheese microbial
597 diversity allowed estimating that almost three hundred different species might inhabit cheese
598 products. For example, microbial interactions between ripening microorganisms have been
599 highlighted by co-culturing isolated strains in experimental cheeses providing key knowledge on
600 competitions or growth inhibitions occurring in cheese (Mounier et al., 2008) but not completely
601 explained. In parallel, meta-omics analyses were conducted on a reduced ecosystem composed of
602 nine microorganisms in which keystone species omissions were experimented. This project
603 generated > 300 GB of meta-transcriptomic data corresponding to the expression level of 37,923
604 individual genes as well as numerous associated physico-chemical, biochemical and metabolomic
605 data. The classification of the expression data from those genes into functional classes made possible
606 to obtain an overview of the metabolic activities of the nine microorganisms composing the
607 ecosystem (Figure 5). Nevertheless from those study to the mathematical prediction and simulation
608 of the system, there is a gap not yet filled in.

609 In such a complexity (limited in comparison to the intestinal microbiota!), there is still a gap that
610 needs to be bridged between the molecular scale information (genetic, expression, compounds
611 detection) and the macroscopic properties (e.g. flavor for a cheese) (Landaud, Helinck & Bonnarme,
612 2008). Several reasons can explain this fact.

613 First, the chemical compounds, particularly the products that are secondary metabolites for well-
614 known metabolic functions are often not connected to metabolic models due to the lack of genetic
615 information. Emergence of macroscopic properties from genome expression using classical
616 bioinformatics tools is then still limited. If knowledge can be found in several descriptive studies
617 about microbial communities, it is not often exploited because it generally needs a huge work of
618 extraction and formalization (Liu et al., 2014).

619 A second reason is related to the scale of observation of the mechanisms involved. Indeed, if several
620 works are achieved regarding a single organism based on genome-scale metabolic network (see
621 Bordbar et al., 2012 and Wodke et al., 2015 for examples), few have proposed to manage an in situ
622 metabolic activity of a microbial community (Bowen et al., 2014). Generally the focus of such studies
623 is on the description, sometimes the modelling of the metabolic detailed pathways and their
624 associated chemical compounds.

625 It is not at all easy to manage a balance between (1) a detailed description of each compound of the
626 metabolism pathways for one microorganism and (2) an ability to cut across the individual scale to go
627 through an in situ expression of a community. Computing problems arise as well as an uncertainty on
628 the scales needed to extract a synthetic architecture able to predict the emergence of macroscopic
629 functionalities. Moreover, reconstructing multiscale dynamics of the in situ community, involves
630 finding a mathematical structure able to organize in a relevant way the links between the scales and
631 variables. Nevertheless, the optimal way to structure and aggregate the knowledge embedded in the
632 big database available and in the heuristics manipulated by experts is not an easy task to achieve.
633 This is why we have to work on how to develop optimal mathematical structures (cf. chapter 3.3);

634 [Figure 5 about here]

635 As stated the gap between micro-scale information and macroscopic properties (e.g. flavour profiles
636 and macro-structures) should be bridged. Even more, the bridge needs to be extended towards the

637 flavour and structure perceptions of consumers. Even though those perceptions are individual - and
638 highly dependent on the environmental conditions during consumptions, cultural values, etc - one
639 needs to (1) abstract collective information in order to efficiently adapt products offers with
640 demands and (2) understand the underlying consumer preferences. Concerning the latter,
641 quantitative sociodynamics could help in better understanding those preferences. The first requires
642 handling of complex data sources and optimization processes in order to let emerge collective
643 properties.

644

645 **4.3 Sustainability of networks by collective regional branding.**

646

647 France is characterized by strong regional forces and relevant connected activities. Their “pôles de
648 compétitivité” (“competitive clusters”) are recognized by the European Commission as a source of
649 innovation and employment, while maintaining and enforcing traditional values (EC report on
650 regional policy for sustainable growth, see below). Linked to local cultural values, these clusters show
651 a diversity of multi-scale characteristics, dynamical patterns (Porter, 2000), resilience, (intuitive and
652 strategic) decision making and optimization steps, either by a ‘hierarchic leader’ or by the
653 stakeholders within the cluster. Two key examples are the collective regional food marketing
654 initiatives “Produit en Bretagne” (North-West of France; region Brittany) and “Sud de France” (South
655 of France, region Languedoc-Roussillon).

656

657 The first is a private, entrepreneurial-driven network of food companies that have developed a
658 common regional brand for typical products. It has slowly evolved into a strong business network of
659 nearly 300 companies in Bretagne, sharing not only a common commercial ambition, but also
660 cultural values and ethical principles as solidarity and sustainability. It is a key example of a self-
661 organized complex system in which the stakeholders and their interactions – either intuitively or via
662 joint strategic actions – result in resilience accompanied by periodically renewed emerging properties

663 showing the diverse quality characteristics of their products. “Produit en Bretagne” is one of the
664 oldest European regional brands.

665
666 The second example, “Sud de France”, is a public policy-driven initiative to promote products of the
667 Languedoc-Roussillon; the major reason to create the brand in 2006 was the decline in sales of
668 regional wines, due to an increasing worldwide competition and low appreciation of their origin. As
669 the largest region of wine production worldwide, this tendency should be counteracted according to
670 policy makers. Step by step, wine producers have been persuaded to use the “Sud de France” label;
671 later on, the brand has been extended to other food producers and to sustainable tourism. The
672 brand is even used as institutional tool, labeling other sectors, as logistics, sport, culture, research
673 etc., raising its complexity. Wine export has been rising afterwards, and over 3000 companies have
674 joined the initiative, which currently brings 9.400 different agricultural products and 850 quality
675 tourism services under the banner “Sud de France”. However, it is not adopted by the companies in a
676 sense that they have fully taken over the investment and running costs of this joint marketing action;
677 it is still a publicly funded marketing offensive (Donner *et al.*, 2014). Thus, one could conclude that
678 involved stakeholders of “Sud de France” are not yet fully embedded in a regional cluster (Uzzi,
679 1996), neither the brand has evolved in a dynamic, self-organised, network.

680 Here, the full complexity of the regional food system is recognized, as well as its players (agents) and
681 their interactions, the diversity of products – and their overall quality and functional properties –
682 and production chains (including local and global resources), its (historical) development, emerging
683 properties and new perspectives at local and global scale for a wide range of consumers. Boundary
684 conditions also impact the system as a whole, including regional branding restricted usage,
685 protection of origin labels, global trade regulations, protective measures, global price volatility,
686 political changes, public and/or private investments, etc. A key feature is the leading role of the
687 Region Languedoc Roussillon, with periodically large investments and extensive marketing initiatives
688 trying to optimize the overall output of the Sud-de-France region. Hence, the various regional

689 activities show a multitude of patterns, from periodical but rather static, up to highly chaotic. The
690 activities in between seem to balance well at the edge of order and chaos, and would most likely
691 reveal resilience and a high level of self-organization, in this case supervised by the Region LR who is
692 major decision maker, at all scales from molecular level (recognized functional properties of their
693 products) up to global scales (recognized marketing related to a well-appreciated country of origin
694 cluster).

695 As stated by the Santa Fé institute (Kaufmann, 1995) (self-organization in complex systems) and by
696 Helmsing and Vellema (Helmsing & Vellema, 2011) (socio-technological innovations and embedding),
697 the design of a full technological-socio-economical food system deserves to be a major research line.
698 A multi-disciplinary approach for qualitatively and quantitatively analyzing complex regional branding
699 for high quality and diverse products, combining several disciplines such as economics, mathematics,
700 marketing, politics, sociology or geography (Dinnie, 2004), together with engineering, agri-food and
701 bio-based sciences, is needed in order to better understand the success and failures of regional
702 clusters.

703 Practically, we propose the following strategy to achieve those new insights and to give sound
704 recommendations. Step 1 concerns painting a picture in time (including thus its history) of a territory
705 marketed via a common brand, including products and their distinct values locally and globally,
706 stakeholders involved and their interactions, regional characteristics, boundary conditions and
707 incentives, ... Step 2 considers the different scales all along the chain from resources and product
708 quality characteristics towards final characteristics appreciated by target groups of consumers. Step
709 3 addresses a first complex system model in which the rigidity, resilience and chaos situations of the
710 territorial cluster(s) are incorporated. Step 4 analyzes in more detail the emergent properties of the
711 cluster in which new products are (co-)developed, marketed, ... Step 5 focuses on which optimization
712 steps are carried out and by whom as decision makers in order to better position a competitive

713 cluster. Step 6 includes a repetitive procedure to further optimize the complex system approach to
714 better adapt the complex system to the realistic conditions.

715 **5. Conclusions**

716 To conclude, even if some approaches -- agent-based approaches among the most representative
717 ones -- are already available and applied to some fields of research like embryogenesis (Olivier et al.,
718 2010) and urban simulations (Irwin, 2010), there is a clear need for efficient, intensive and parallel
719 computational methods for the agri-food domain (Reuillon, Traore, Passerat-Palmbach and Hill,
720 2012).

721 At present, several issues remain unanswered:

- 722 • Find the right level(s) of description to simulate the system. The answer will generally be
723 strongly connected to the objective of the study and at present a methodology to find the
724 right level(s) does not exist and should be rediscovered for each application without any
725 guarantee of relevance.
- 726 • Multiscale reconstruction limitations: progress has been done on computational tools to
727 manage uncertainty, for example Bayesian formalisms, theory of possibility on heuristics
728 manipulated by humans, stochastic approaches applied to different mathematical
729 representation ie on individual based models, ontology-based data access. Nevertheless,
730 used independently these solutions require lots of knowledge or data at each scale while
731 only some of them are available (cf. example chapter 4.2). Moreover, even with a big data
732 basis, without any oriented structured approach, a part of the knowledge is lost or unusable.
733 In this sense there is a necessity to propose tools for coupling heterogeneous model and
734 knowledge and connect different computing communities (see the smart data tendency).
- 735 • Parameters tuning limitations: another limitation is linked to the necessity for those
736 approaches to tune empirically some parameters: graph and discretization for the DBN;

737 indexation for the data mining; parameters of the stochastic laws, far more complex to be
738 tuned than parameters of known physical laws; parameters of the optimization algorithms or
739 other AI algorithms. Some new research focusses on this point at present (interactive
740 learning, visualization).

- 741 • Computational limitations: if stochastic approaches are really well adapted to the multiscale
742 reconstruction in an uncertain context, it relies on a high capacity of computation. Even if
743 now the computational power is largely increased, with clusters of computers, the number of
744 variables that could be manipulated by some approaches is still limited: for example, less
745 than 10 for the viability theory (cf. chapter 3.1), 5 variables for the approaches of
746 optimization coupled to visualization (cf. chapter 3.3),....
- 747 • Visualization and user fatigue limits: all methods based on machine-man interaction impose
748 a consistent exertion on the expert (Lem, 2008), often referred to as user fatigue. While
749 semi-supervised learning of models through graphical user interfaces can be very effective,
750 combining the best aspects of machine learning and expert knowledge, the strain imposed
751 on the user severely limits the effectiveness of these approaches.

752 Decision making in sustainability management of agri-food systems will require building a science
753 able to cope with uncertainty, emergence of properties, multi-scale reconstruction, optimization of
754 non-linear systems in dynamic environments, interactive learning and human expert knowledge,
755 non-equilibrium exploration and dynamical behavior at the edge between order and chaos. Building
756 models is essential, but highly difficult and allows for plenty opportunities for the mathematical and
757 computational sciences; it will need a strong iterative interaction combining computational intensive
758 methods, formal reasoning and the experts of the different fields.

759 Although generic methods are still not available and relevant expert knowledge dispersed, complex
760 system science and associated fields already provide the first answers to basic, well-defined and
761 context-oriented problems. Nevertheless, the tools of complex science need to be extended to

762 especially in-depth research at interfaces of previously considered separated scales, as illustrated
763 here. The key building blocks of efficient methods have been addressed, as well as the way they
764 potentially could contribute to a generic complex system approach. Table 1 is a synthesis of the steps
765 required for an approach of the complex problem of sustainability of food systems, the work realized
766 in this direction, reachable or more difficult to achieve, and a list of mathematical or computing tools
767 already available or under study at present. As a next step, we need to enter a technological-socio-
768 economical regime in which scales are interlinked in order to develop a flexible but rigorous concept
769 for the complex system approach. Then, this would make it possible to come up with practical tools
770 for decision makers who are facing challenges on sustainability.

771

772

[Table 1 about here]

773

774 **6. Perspectives**

775

776 We need to come up with more radical innovations and solutions integrating all (linked) scales, with
777 the help of a generic approach as proposed here, in order to maintain a viable planet; if not, our
778 current innovations may only extend the “expiration date” of our planet. We are convinced that a
779 creative, multi-scale, multi-discipline and complex system approach is able to provide tools that are
780 needed to tackle the current challenges in research, development and business strategies.

781 Our society is facing challenges that have to be approached with new strategies. The review of
782 current trends for the obesity, growth of world population, atmospheric levels of greenhouse gases,
783 national debt of countries, all exhibit a common feature, that is a (near) exponential growth. This
784 growth is incompatible with balanced systems. These systems show periodic changes but always

785 return to an attractor or a stable position after a given period. The optimization of such out-of-the-
 786 equilibrium systems should rely on the stochasticity of the signal during a significant time.
 787 Innovations relying on integrated and deep knowledge, may help in trying to level off exponential
 788 curves.

789 Acknowledgements

790
 791 The authors would like to thank all participants of the duALIne project, and in particular Dr C. Esnouf
 792 for her help; Acknowledgement for the financial support of government (French ANR project
 793 INCALIN). Acknowledgment for the funding received from the European Community's Seventh
 794 Framework Program (FP7/2009–2013) under grant agreement DREAM No. 222654-2.

795 References

- 796
 797 Alvarez, I., de Aldama, R., Martin, S., Reuillon, R., Aug. 2013. Assessing the resilience of bilingual societies:
 798 coupling viability and active learning with kd-tree. application to bilingual societies. In: IJCAI 2013 AI and
 799 Computational Sustainability Track. Beijing, China, pp. 2776–2782.
- 800 Alvarez, I., de Aldama, R., Martin, S., Reuillon, R., 2013. Assessing the resilience of socio-ecosystems: Coupling
 801 viability theory and active learning with kd-trees. In: IJCAI 2013, Proc. of the 23rd International Joint
 802 Conference on Artificial Intelligence pp. 2776-2782.
- 803 Aubin, J., 1991. Viability Theory. Birkhauser, Basel.
- 804 Awudu, I., Zhang, J., 2012. Uncertainties and sustainability concepts in biofuel supply chain management: A
 805 review. Renewable and Sustainable Energy Reviews 16, 1359–1368.
- 806 Baudrit C., Wuillemain, P.H., Perrot, N. (2013). Parameter elicitation in probabilistic graphical models for
 807 modelling multi-scale food complex systems" Journal of food engineering, 115(1), 1-10.
- 808 Bernard, C., Martin, S., 2013. Comparing the sustainability of different action policy possibilities: Application to
 809 the issue of both household survival and forest preservation in the corridor of fianarantsoa. Mathematical
 810 Biosciences 245 (2), 322–330.
- 811 Bordbar, A., Mo, M.L., Nakayasu, E.S., Schrimpe-Rutledge, A.C., Kim, Y.M., Metz, T.O., et al. Model-driven multi-
 812 omic data analysis elucidates metabolic immunomodulators of macrophage activation. Mol Syst Biol. 2012;8.
 813 doi:10.1038/msb.2012.21
- 814 Boukhelifa, N., Cancino, W., Bezerianos, A. and Lutton, E., 2013. Evolutionary Visual Exploration: Evaluation
 815 With Expert Users. Computer Graphics Forum (EuroVis 2013, June 17–21, 2013, Leipzig, Germany),
 816 Eurographics Association, 32 (3).

- 817 Bowen, J.L., Babbin, A.R., Kearns, P.J., Ward, B.B., 2014. Connecting the dots: linking nitrogen cycle gene
818 expression to nitrogen fluxes in marine sediment mesocosms. *Aquat Microbiol*, 5, 429.
819 doi:10.3389/fmicb.2014.00429.
- 820 Bourguet, J.R., Thomopoulos, R., Mugnier, M.L., Abecassis, J. 2013. An Artificial Intelligence-Based Approach to
821 Deal with Argumentation Applied to Food Quality in a Public Health Policy. *Expert Systems with Applications*, 40
822 (11): 4539–4546.
- 823 Bousson, K., Steyer, J.P., Travé-Massuyès, L. Monitoring and diagnosis of fermentation processes, in *Issues of*
824 *Fault Diagnosis for Dynamic Systems*, (Ed. Patton, Franck and Clark), Springer-Verlag, 2000, ISBN 3-540-19968-
825 3.
- 826 Carlson, J., & Doyle, J. (2000). Highly Optimized Tolerance: Robustness and Design in Complex Systems. *Physical*
827 *Review Letters*, 84(11), 2529–2532.
- 828 Carpenter, S., Walker, B., Anderies, J., Abel, N., 2001. From metaphor to measurement: resilience of what to
829 what? *Ecosystems* 4, 765–781.
- 830 Charpentier, J., 2010. Among the trends for a modern chemical engineering, the third paradigm: The time and
831 length multiscale approach as an efficient tool for process intensification and product design and engineering.
832 *chemical engineering research and design* 88, 248–254.
- 833 Coello Coello, C. A., 2009. Evolutionary multi-objective optimization: some current research trends and topics
834 that remain to be explored. *Frontiers of Computer Science in China* 3 (1), 18–30. URL
835 <http://dx.doi.org/10.1007/s11704-009-0005-7>
- 836 De Lara, M., Martinet, V., 2009. Multi-criteria dynamic decision under uncertainty: A stochastic viability analysis
837 and an application to sustainable fishery management. *Math. Biosci.* 217 (2), 118–124.
- 838 Dinnie, K., 2004. Place branding: overview of an emerging literature. *Place Branding*, 1, 106-110.
- 839 Donner, M., Fort, F., Vellema S., 2014. How to capture place brand equity? The case of Sud de France. *Place*
840 *branding and public diplomacy* (forthcoming).
- 841 Doukas, H., 2013. Modelling of linguistic variables in multicriteria energy policy support. *European Journal of*
842 *Operational Research* 227 (2), 227–238.
- 843 Dovers, S. R., Handmer, J. W., 9 1993. Contradictions in sustainability. *Environmental Conservation* 20, 217–
844 222. URL http://journals.cambridge.org/articleS_0376892900022992
- 845 Dugat-Bony, E., Straub, C., Teissandier, A., Onésime, D., Loux, V., Monnet, C. et al. (In Press). Overview of a
846 surface-ripened cheese community functioning by meta-omics analyses. *PLoS ONE*. In press.
- 847 EC Document, 2011 Regional Policy contributing to sustainable growth in Europe ; ISBN: 978-92-79-20333-6;
848 doi:10.2776/39448 published by European Commission, Directorate-General for Regional Policy
- 849 Edwards, M., 2006. Product engineering: some challenges for chemical engineering. *Chemical Engineering.*
850 *Research and Design, TranslCheme* 84, 255–260.
- 851 Faust, K., Raes, J., 2012. Microbial interactions: from networks to models. *Nat Rev Microbiol.* 10, 538–550.
852 doi:10.1038/nrmicro2832

- 853 Fengqi You, F., Tao, L., Graziano, D., Snyder, S., 2012. Optimal design of sustainable cellulosic biofuel supply
854 chains: Multiobjective optimization coupled with life cycle assessment and inputoutput analysis. *AIChE Journal*
855 58(4), 1157–1180.
- 856 Fuentes, R. E., 1993. Scientific research and sustainable development. *Ecol. Appl.* 3, 576–577.
- 857 Giovannini, A., Aubry, A., Panetto, A., Dassisti, M., Haouzi, H., 2012. Ontology-based system for
858 supporting manufacturing sustainability. *Annual Reviews in Control* 36, 309317.
- 859 Grossmann, I., Guilln-Goslbez, G., 2010. Scope for the application of mathematical programming techniques in
860 the synthesis and planning of sustainable processes. *Computers and Chemical Engineering* 34, 13651376.
- 861 Gunderson, L., Holling, C. S., 2002. *Panarchy : understanding transformations in human and natural systems.*
862 Island Press, Washington, D.C., USA.
- 863 Gupta, S., Palsule-Desai, O., 2011. Sustainable supply chain management: Review and research opportunities.
864 *IIMB Management Review* 23, 234–245.
- 865 Hassini, E., Surti, C., Searcy, C., 2012. A literature review and a case study of sustainable supply chains with a
866 focus on metrics. *Int. J. Production Economics* 140, 69–82.
- 867 Helbing, D., 2010a Pluralistic Modeling of Complex Systems CCSS-10-009,
868 <http://ssrn.com/abstract=1646314>.
- 869 Helbing, D., 2010b. *Quantitative Sociodynamics*, Springer Berlin Heidelberg.
- 870 Helmsing, A.H.J., Vellema, S., 2011. Value Chains Governance and Inclusive Endogenous Development: Towards
871 a Knowledge Agenda. Development policy review network (DPRN), 2011.
- 872 Higgins, A., Miller, C. J., Archer, A., Ton, T., Fletcher, C., McAllister, R., 2010. Challenges of operations research
873 practice in agricultural value chains. *Journal of the Operational Research Society* 61, 964–973.
- 874 Holling, C., 1973. Resilience and stability of ecological systems. *Annual Review of Ecology and Systematics* 4, 1–
875 24.
- 876 Holling, C. S., 2001. Understanding the complexity of economic, ecological, and social systems. *Ecosystems* 4,
877 390–405.
- 878 Kauffman, S., 1995. *At Home in the Universe, The Search for the Laws of Self-Organization and Complexity.*
879 Oxford University Press.
- 880 Lainez, J., Puigjaner, L., 2012. Prospective and perspective review in integrated supply chain modeling for the
881 chemical process industry. *Current Opinion in Chemical Engineering* 1, 430–445.
- 882 Lam, Heidi, 2008. A framework of interaction costs in information visualization. *Visualization and Computer*
883 *Graphics, IEEE Transactions on* 14.6, 1149-1156.
- 884 Landaud, S., Helinck, S., Bonnarme, P., 2008. *Applied Microbiology and Biotechnology* 77, 1191 (Jan, 2008).
- 885 Lehmann, R., Reiche, R., Schiefer, G., 2012. Future internet and the agri-food sector: State-of-the-art in
886 literature and research. *Computers and Electronics in Agriculture* 89, 158–174.

- 887 Liu, M., Bienfait, B., Sacher, O., Gasteiger, J., Siezen, R.J., Nauta, A., et al., (2014). Combining Chemoinformatics
888 with Bioinformatics: In Silico Prediction of Bacterial Flavor-Forming Pathways by a Chemical Systems Biology
889 Approach "Reverse Pathway Engineering." PLoS ONE, 9: e84769. doi:10.1371/journal.pone.0084769
- 890 Martin, S., 2004. The cost of restoration as a way of defining resilience: a viability approach applied to a model
891 of lake eutrophication. *Ecology and Society* 9 (2). URL <http://www.ecologyandsociety.org/vol9/iss2/art8>.
- 892 Martin, S., Deffuant, G., Calabrese, J., Gilbert, N., 2011. Defining resilience mathematically: from attractors to
893 viability. *Understanding complex systems*. Springer. URL <http://cemadoc.cemagref.fr/cemoa/PUB00033173>.
- 894 Martinet, V., Doyen, L., 2007. Sustainability of an economy with an exhaustible resource: A viable control
895 approach. *Resour. Energy Econ.* 29 (1), 17–39.
- 896 Martinet, V., Thebaut, O., Doyen, L., 2007. Defining viable recovery paths toward sustainable fisheries. *Ecol.*
897 *Econ.* 62 (2), 411–422.
- 898 Matser, A., Quataert M., Hamoen R., de Vries HSM, 2010. Decision Support System. *New Food*, Issue 5, P. 65 –
899 69
- 900 Melnik, R., 2009. Coupling control and human factors in mathematical models of complex systems. *Engineering*
901 *Applications of Artificial Intelligence* 22, 351–362.
- 902 Meulen, B., 2013. The structure of european food law. *Laws* 2, 69–98. 2.
- 903 Mesmoudi, S., Perrot, N., Reuillon, R., Bourguine, P., Lutton, E., 2010. Optimal viable path search for a cheese
904 ripening process using a multi-objective ea. (2010). ICEC 2010. International conference on evolutionary
905 computation. 24-26 October Valencia (Spain).
- 906 Mesmoudi, S., Alvarez, I., Martin, S., Reuillon, R., Sicard, M., Perrot, N., 2014. Coupling geometric analysis and
907 viability theory for system exploration: Application to a living food system. *Journal of Process Control*, 24, 18-
908 28.
- 909 Miettinen, K., Sayin, S., 2013. Special issue: 21st international conference on multiple criteria decision making;
910 articles on multiobjective optimization. *Journal of Global Optimization* 57 (2), 279–280. URL
911 <http://dx.doi.org/10.1007/s10898-013-0041-6>.
- 912 Miles, R., Snow, C., 2007. Organization theory and supply chain management: An evolving research perspective.
913 *Journal of Operations Management* 25, 459–463.
- 914 Miller, K., Charles, A., Barange, M., Brander, K., Gallucci, V., Gasalla, M., Khan, A., Munro, G., Murtugudde, R.,
915 Ommerj, R., Perry, R., 2010. Climate change, uncertainty, and resilient fisheries: Institutional responses through
916 integrative science. *Progress in Oceanography* 87, 338–346.
- 917 Mounier, J., Monnet, C., Vallaey, T., Arditi, R., Sarthou, A-S., Helias, A. et al. (2008). Microbial Interactions
918 within a Cheese Microbial Community. *Appl Environ Microbiol.* 74: 172–181. doi:10.1128/AEM.01338-07.
- 919 Mouzé-Amady, M., Raufaste, E., Prade, H., & Meyer, J.P. (2013). Fuzzy-TLX: using fuzzy integrals for evaluating
920 human mental workload with NASA-Task Load index in laboratory and field studies. *Ergonomics*, 56 (5), 752-
921 763.
- 922 Neubert, M., Caswell, H., 1997. Alternatives to resilience for measuring the responses of ecological systems to
923 perturbations. *Ecology* 78 (3), 653–665.

- 924 Nikolopoulou, A., Ierapetritou, M., 2012. Optimal design of sustainable chemical processes and supply chains:
925 A review. *Computers and Chemical Engineering* 44, 94–103.
- 926 Olivier, N., Luengo-Oroz, M., Duloquin, L., Faure, E., Savy, T., Veilleux, I., e. a., 2010. Cell lineage reconstruction
927 of early zebrafish embryos using label-free nonlinear microscopy. *Science* 329, 967–971.
- 928 Pavone, M., Coello Coello, C. A., 2012. Optimization on complex systems. *Memetic Computing*, 1–2.
- 929 Perrot, N. (2006). Fuzzy concepts applied to food product quality control. Editorial. *Fuzzy Sets and Systems*,
930 157, 1143-1144.
- 931 Perrot, N., Trelea, I. C., Baudrit, C., Trystram, G., Bourgine, P., 2011. Modelling and analysis of complex food
932 systems: State of the art and new trends. *Trends in Food Science & Technology* 22 (6), 304–314.
- 933 Pimm, S., 1984. The complexity and stability of ecosystems. *Nature* 327, 321–326.
- 934 Pimm, S., Lawton, J., 1977. Number of trophic levels in ecological communities. *Nature* 268, 329–331.
- 935 Porter, M.E., 2000. Location, competition, and economic development: Local clusters in a global economy.
936 *Economic development quarterly*, 14, 15-34.
- 937 Rawles, 1999, *A theory of justice*. Belknap press, Cambridge Massachusetts.
- 938 Reilly, M., Willenbockel, D., 2010. Managing uncertainty: a review of food system scenario analysis and
939 modelling. *Philosophical transactions of the royal society* 365, 3049–3063.
- 940 Sebag, M., 2014. *A tour of Machine learning: an AI perspective*. AI communications, IOS Press, 27(1), 11-23.
- 941 Sicard, M., Baudrit, C., Leclerc-Perlat, M.N., Wuillemin, P.H., Perrot, N., 2011. Expert knowledge integration to
942 model complex food processes. Application on the camembert cheese ripening process. *Expert Systems with*
943 *Applications*, 38(9), 11804-11812.
- 944 Sicard, M., Perrot, N., Reuillon, R., Mesmoudi, S., Alvarez, I., Martin, S. 2012. A viability approach to control
945 food processes: Application to a Camembert cheese ripening process. *Food Control*, 23, 312-319.
- 946 Stoutemyer, D. R., 2013, Can the Eureka Symbolic Regression Program, Computer Algebra, and Numerical
947 Analysis Help Each Other? *Notices of the AMS* (60), 713-724.
- 948 Suppes, P., 2002. *Representation and Invariance of Scientific Structures*, University of Chicago publications.
- 949 Surana, A., Kumara, S., Greaves, M., Nandini, C., Raghavan, U., 2013. Supply-chain networks: a complex
950 adaptive systems perspective. *International Journal of Production Research* 43(20), 4235–4265.
- 951 Takagi, H., 2008. New topics from recent interactive evolutionary computation researches. In: *Knowledge-*
952 *Based Intelligent Information and Engineering Systems*. p. 14.
- 953 Thompson, J., Scoones, I., 2009. Addressing the dynamics of agri-food systems: an emerging agenda for social
954 science research. *Environmental science & policy* 12, 386–397.
- 955 Tonda, A., Spritzer, A., and Lutton, E., 2014. Balancing User Interaction and Control in BNSL. In *Artificial*
956 *Evolution* (pp. 211-223). Springer International Publishing.
- 957 Trystram, G., 2012. Modelling of food and food processes. *Journal of Food Engineering* 110, 269277.

- 958 Uzzi, B., 1996. The sources and consequences of embeddedness for the economic performance of
959 organizations: The network effect. *American sociological review*, 674-698.
- 960 Van Coller, L., 1997. Automated techniques for the qualitative analysis of ecological models : Continuous
961 models. *Conservation Ecology* 1 (1), 5.
- 962 Van Mil, H.G.J. , Foegeding, A.E. , Windhab, E.J. , Perrot, N., Van der Linden, E. (2014). A complex system
963 approach to address world challenges in food and agriculture. *Trends in Food Science and Technology*, 40 (1),
964 20-32.
- 965 Walker, B., Gunderson, L., Kinzig, A., Folke, K., Carpenter, S., Schultz, L., 2006. A handful of heuristics and some
966 propositions for understanding resilience in social-ecological systems. *Ecology and Society* 11, 1–13.
- 967 Wei, W., Alvarez, I., Martin, S., 2013. Sustainability analysis: Viability concepts to consider transient and
968 asymptotical dynamics in socio-ecological tourism-based systems. *Ecological Modelling* 251, 103–113.
- 969 Wodke, J.A.H, Alibés, A., Cozzuto, L., Hermoso, A., Yus, E., Lluch-Senar, M., et al., 2015. MyMpn: a database for
970 the systems biology model organism *Mycoplasma pneumoniae*. *Nucleic Acids Res.* 2015;43: D618–D623.
971 doi:10.1093/nar/gku1105
- 972 Zwart, Sjoerd D., Ibo van de Poel, Harald van Mil, and Michiel Brumsen. 2006. A Network Approach for
973 Distinguishing Ethical Issues in Research and Development. *Science and Engineering Ethics* 12 (4):663-684.

974

975 **Figure captions**

976

977 Figure 1: Complex system approach inspired from the CS roadmap 2012-2020

978 Figure 2: A viability kernel recalculated for the cheese ripening application described in (Sicard *et al.*,
979 2012) (Mesmoudi *et al.*, 2014). The First 8 days of the 12-days viability tube of the ripening process of
980 Camembert Cheese are represented. The color shows the robustness (square distance to the
981 boundary of the viability day-section) with blue points less robust than red ones. The target in black
982 is reached in 12 days but at day 8 some robust states are already in the target.

983 Figure 3: Integrated assessment and policy-development process indicating key ingredients, flows,
984 and interactions between analytical and participatory components of the process. Inspired and
985 redrawn from Miller *et al.*, 2010

986 Figure 4: Length scales in the manufacture and supply structured products.

987 Figure 5: Example of Functional classification of the metatranscriptome during surface-ripened
988 cheese maturation (from Dugat-Bony *et al.*, In press).

989

990 **Table caption**

991 Table 1: A synthesis of methodologies and computing tools, already available or in development, for
992 sustainable food systems. For each point, we provide examples taken from subsection 4.3, as this
993 case study addresses issues spanning all the considered elements.

994

995

ACCEPTED MANUSCRIPT

Table 1

		Partly realized	Reachable	To achieve
Step 1: Systemic analysis, or 'painting the picture'	Description	Description of concepts and factual information.	Gathering human and expert knowledge. This step is sometimes performed, but there is no generic methodology yet.	Linking knowledge from different sources.
	Computing paradigms	Ontologies and conceptual graphs, mathematical descriptions mediated by cognitive science approaches (Sicard et al., 2011)	Fuzzy logic (Perrot, 2006), qualitative physics (Bousson et al., 2000), mathematical graphs (Baudrit, Willemin & Perrot, 2013), cognitive science. Concepts from cognitive science, however, are not easy to link to mathematical concepts (Mouzé-Amady, Raufaste, Prade & Meyer, 2013)	Intelligent systems, able to treat different sources of information into a homogeneous framework.

<p>Step 2: reconstructing different scales in a mathematical frame</p>	<p>Description</p>	<p>Characterization of separate elements, at different levels of detail and complexity.</p>	<p>Linking separate elements into a systemic approach.</p> <p>Inter-cluster operations and dynamics are sometimes already described, but usually the focus is one part, while the rest of the system is treated as constraints.</p>	<p>A multi-scale approach is needed (cf. chapter 2.2). Too many variables may hinder a consistent model showing emergent properties of the entire system.</p> <p>The difficulty is to select the right scales bringing a good representation of the whole.</p> <p>Managing uncertainty is fundamental.</p>
	<p>Computing paradigms</p>	<p>Depending on the case study and the available data: differential equations, neural networks, fuzzy logic, ...</p>	<p>Model coupling, Bayesian networks, probabilistic approaches (Sicard et al., 2011). However, these techniques are rarely connected and used in conjunction with each other, even</p>	<p>Complex system science, coupling stochastic (roadmap) and deterministic approaches, individual-based models, interactive learning. These techniques have</p>

			when the final application could benefit from such an integration (see Perrot et al., 2011, Van der Linden et al., 2014)	been already successfully applied, but not in the food science domain (see Van Mil et al., 2014)(Sebag, 2014)
	Example (from 4.3)	Description of separate food chains and characteristics of products. Some regional clusters are described in detail regarding actors and the competitive force (Porter, 2000)	Valorize not only the grapes for wine, but also all remaining plant parts, for non-food applications, energy, etc.	The translation of consumer demands to the various scales, namely interaction between actors, characteristics of products, functionality of ingredients.
Step 3: uncovering emerging properties	Description	Knowledge engineering approaches allow having factual information about emerging properties of a system under study.	Human and expert knowledge approaches may allow to get explicit and implicit knowledge.	Consistent interpretation of the different knowledge sources and their 'real' contributions to emergent properties in a multi-dimensional

				landscape.
	Computing paradigms	Visualization techniques (Boukhelifa et al. 2013), especially interactive ones, can be efficiently used to uncover emerging trends.	Interactive learning (Tonda et al., 2014), interactions between machine learning systems and human experts (Sebag, 2014). These approaches still exist as prototypes, and are mainly used in research.	Existing interactive approaches cannot still overcome user fatigue (Lem, 2008); machine learning, despite recent improvements, cannot automatically detect all emerging trends.
	Example (from 4.3)	Once a model of a regional cluster is prepared, it is executed, and the results of the in-silico experiments are analyzed for emerging properties.	Working with experts of each company inside a cluster, trying to encode the implicit knowledge they possess about the network into explicit knowledge.	Build a homogeneous framework of expert knowledge, encompassing all aspects of a regional cluster.

<p>Step 4: system optimization and resilience</p>	<p>Description</p>	<p>The various actors could be easily identified including their decisive power at all scales and their constraints and decision criteria. Formalization of their constraints and choices is possible.</p>	<p>The necessity is to learn from a large benchmark of simulations in interaction with the experts. The expression of the mathematical function to optimize, the tuning of the algorithms are not trivial (Sebag, 2014).</p>	<p>The value of optimization may be rather complicated to establish, because the appropriate definition of the highly complex and diverse environmental context would require taking into account feedback and feedforward effects. In practice, these factors cannot yet be practically implemented, as the non-linearity of the system increases.</p>
--	---------------------------	--	--	---

	Computing paradigms	Evolutionary computation, memetic algorithms, viability theory.	For all optimization methods, computation is very heavy: the target models are stochastic in nature, and several repetitions are needed to obtain reliable results. This issue can be addressed by clusters, grids and computing clouds; as well as by surrogate functions (computationally lighter).	Another way to optimize is to be able to cluster the search space, using formalized expertise and interactive optimization; these techniques might solve some of the issues, but research in the field is still far from producing tools that are usable out-of-the-box. See (Lam, 2008) for a discussion on the costs of human-machine interaction.
	Example (from 4.3)	Regional clusters with a long history could be analysed in terms of repetitive actions taken to optimize a local cluster.	Example: resilience of the systems may be well tested in real life as a consequence of decisive actions, e.g. improved international sales, faster adaptation	Example: optimizing logistics of a whole network of regional clusters, taking into account their reciprocal interaction, and

			to external changes by enterprises, ...	their influence on the environment and other existing structures.
--	--	--	---	---

ACCEPTED MANUSCRIPT

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguin, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : 10.1016/j.tifs.2015.10.003

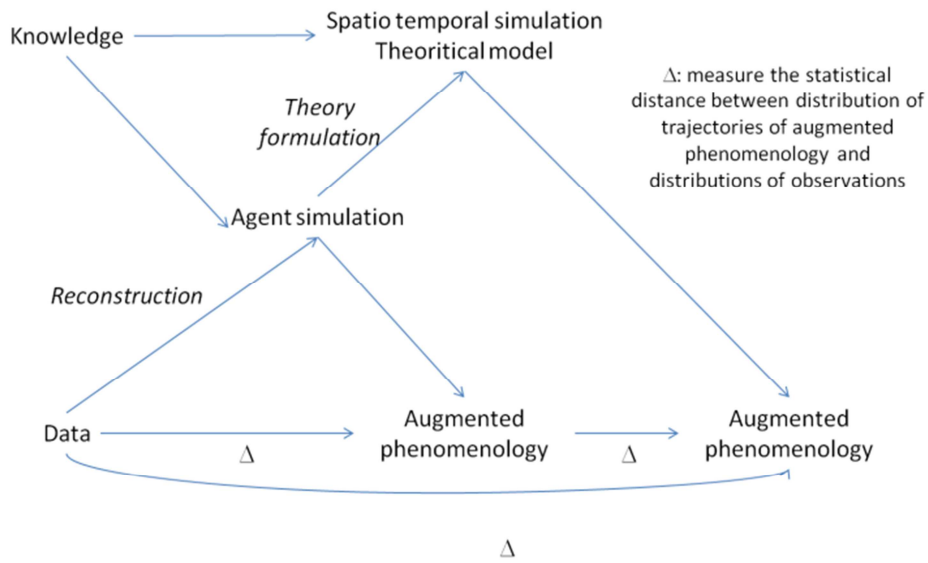


Figure 1

ACCEPTED MANUSCRIPT

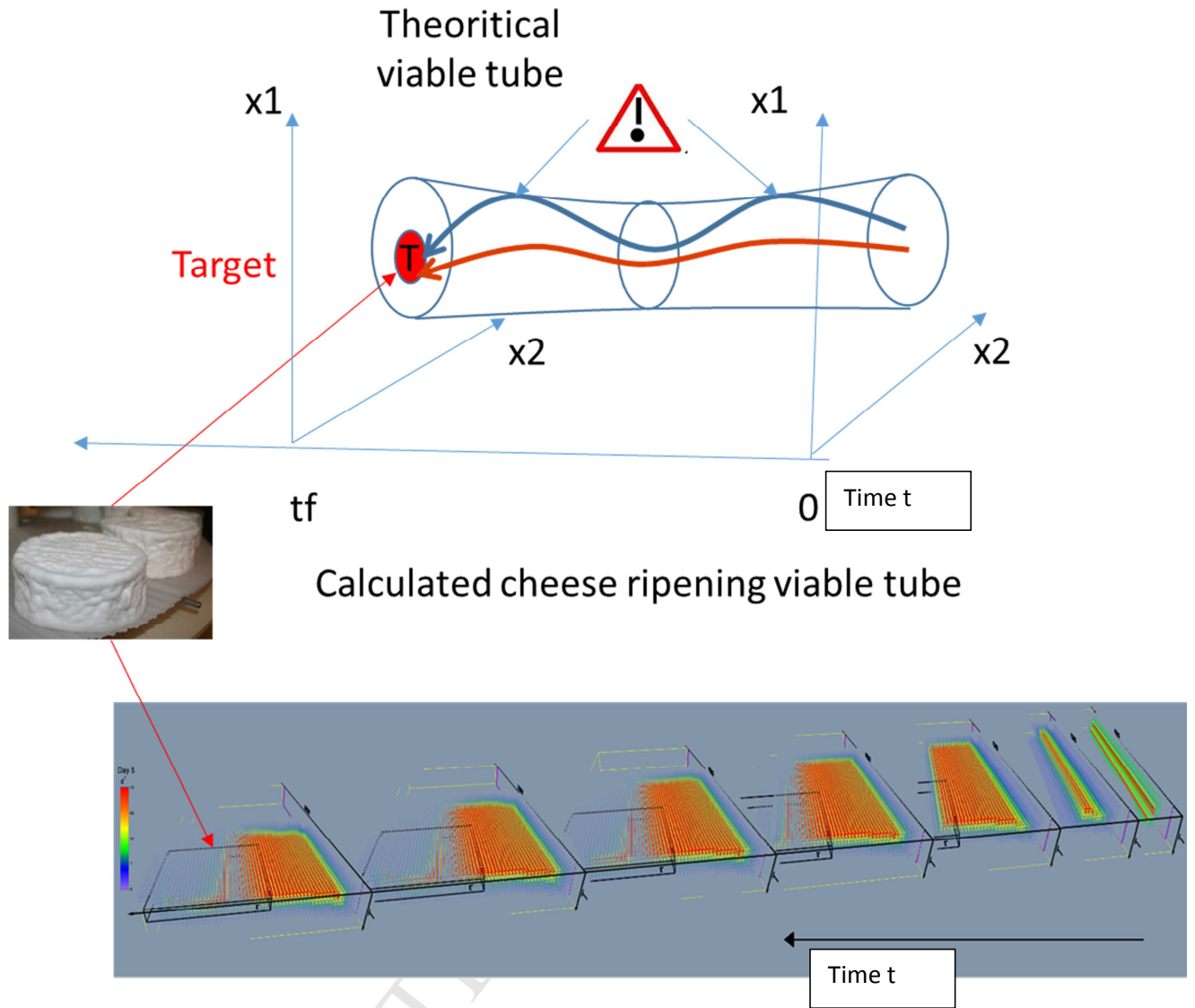


Figure 2

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguin, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : 10.1016/j.tifs.2015.10.003

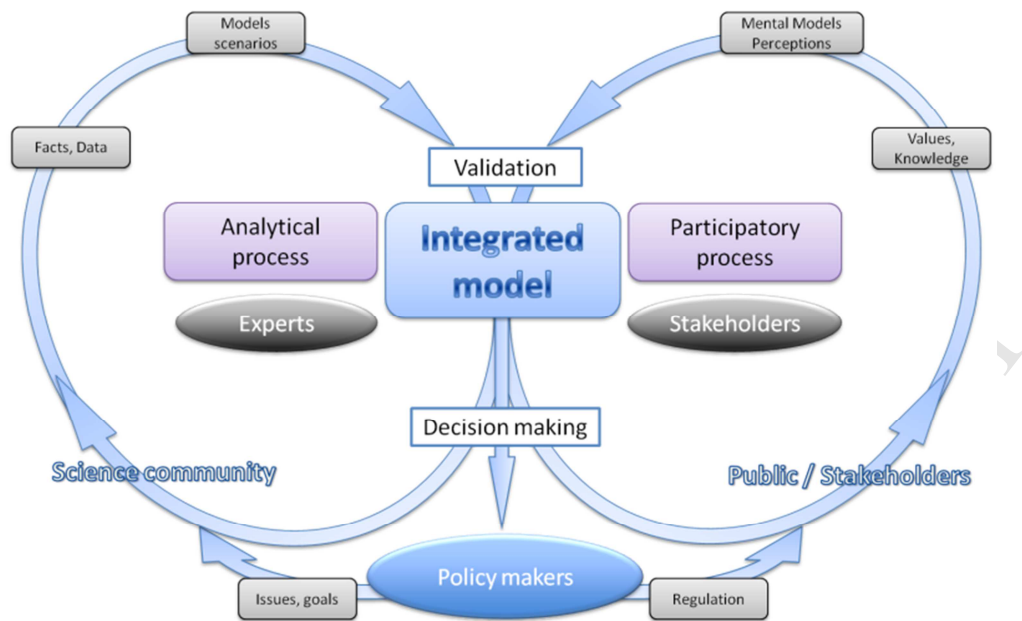


Figure 3

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguin, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : 10.1016/j.tifs.2015.10.003

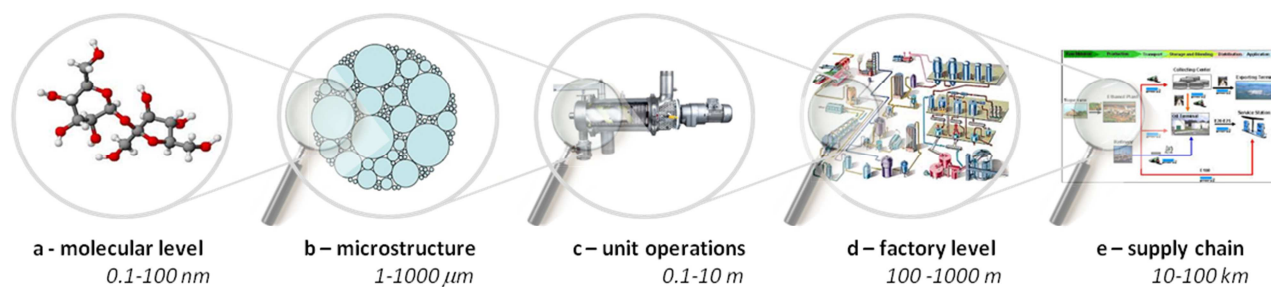


Figure 4

ACCEPTED MANUSCRIPT

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguin, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : 10.1016/j.tifs.2015.10.003

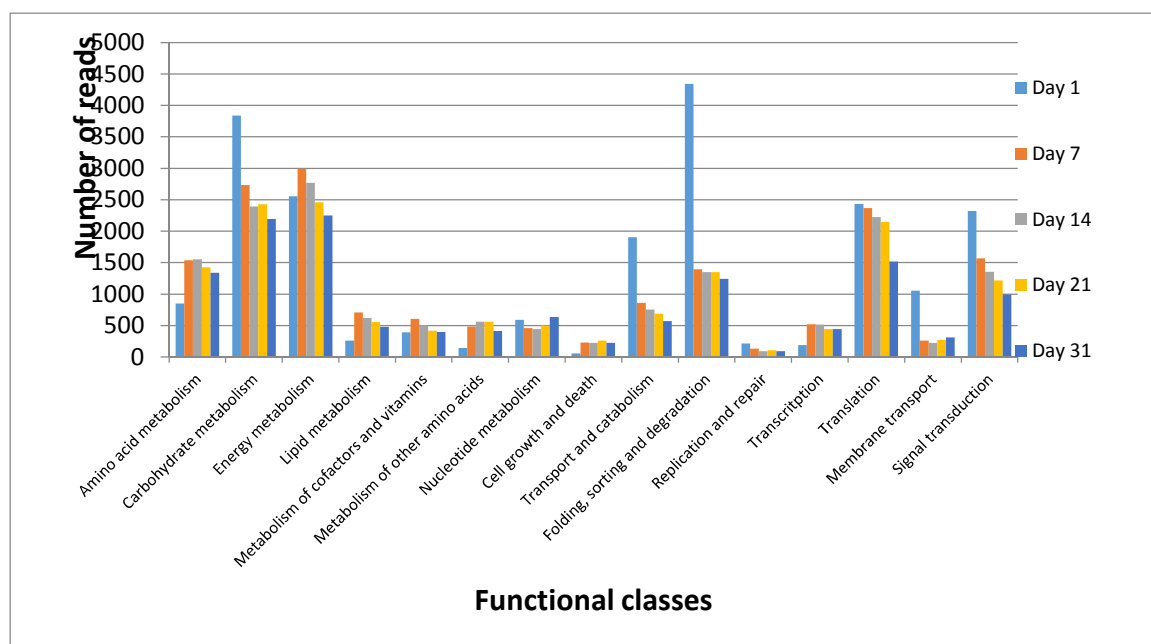


Figure 5

Highlights :

The agri-food sector is one of the most important sectors of the industry

Dealing with sustainability issues in this sector, is a enormous and difficult challenge.

Here lies a huge opportunity at the frontier of agri-food and computing science.

New mathematical tools are proposed to address sustainability of food systems.

Key examples are developed.

ACCEPTED MANUSCRIPT

Comment citer ce document :

Perrot, N., De Vries, H., Lutton, E., van Mil, H. G. J., Donner, M., Tonda, A., Martin, S., Alvarez, I., Bourguin, P., van der Linden, E., Axelos, M. (2016). Some remarks on computational approaches towards sustainable complex agri-food systems. *Trends in Food Science and Technology*, 48, 88-101. DOI : 10.1016/i.tifs.2015.10.003