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
Bourgine, Erik van Der Linden, et al.

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

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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.

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4 **Authors**

5 Nathalie Perrot[a,c*1], Hugo De Vries[b], Evelyne Lutton[a,c], Harald G.J. van Mil[h], , Mechthild Donner[g],

6 Alberto Tonda[a,c], Sophie Martin[c,d], Isabelle Alvarez[d,e], Paul Bourgine[c], Erik van der Linden[h,i], Monique

7 A.V. Axelos[f]

8

9 **Affiliations**

10 [a] INRA, UMR782 Génie et Microbiologie des Procédés Alimentaires, F-78850 Thiverval-Grignon,

11 France (Tel.: +33 1-30-81-53-79; fax : +331-30-81-55-97; email: nathalie.perrot@grignon.inra.fr,

12 evelyne.lutton@grignon.inra.fr, alberto.tonda@grignon.inra.fr)

13 [b] INRA, UMR1208 Ingénierie des Agropolymères et Technologies Emergentes, F-34060 Montpellier,

14 France (Tél. : +33 4 99 61 28 31) devries@supagro.inra.fr,

15 [c] ISCPIF (Institut des Systèmes complexes Paris Ile de France, 133 rue Nationale – F 75013 Paris (Tél.

16 +331 45 52 64 11 - Fax : +331 45 52 64 55)

17 [d] IRSTEA, LISC. 24 avenue des Landais, BP5 0085 631 72 Aubière, France, (Tel/fax: +33 4 73 44 06 00,

18 sophie.martin@irstea.fr, isabelle.alvarez@irstea.fr)

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

20 [f] INRA, UR1268 Biopolymères Interactions et Assemblages, F-44300 Nantes, France (Tel: +33 (0) 2 40

21 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)

1

22   [g] 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, mechthild.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   [i]Laboratory of Physics and Physical Chemistry of Foods, Wageningen University and Research Center,

27   Bornse Weilanden 9 (building 118) 6708 WG Wageningen, The Netherlands. e-mail:

28   erik.vanderlinden@wur.nl

Abstract

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.

Keywords

39   Agri-food systems, sustainability, multiscale modeling, computing complex system, decision support

40   system, optimization, resilience, human expertise, interactive learning.

1. Introduction

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

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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 chain[2]. 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.

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[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

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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

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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.

5

2. Methodological approach, main questions and predictable bottlenecks

2.1 A holistic approach: an introduction to complex system science

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

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

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

6

137 The 2012-2020 roadmap defined the science of complex systems[3] 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

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

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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

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

9

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).

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10

2.3 Decision making issues and quantitative sociodynamics

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

- Surprises: as defined by (Thompson & Scoones 2009), are the qualitative gaps between perceived reality and expectation in ecological systems. Taking them into account, as well as the so-called technological surprises (Reilly & Willenbockel 2010) is a major challenge for agri-food systems. These unpredictable events must be considered in management practices besides other social and institutional mechanisms, in order to reduce poverty and increase resilience.

- Uncertainties: many variables are influenced by uncertainties, namely environmental regulations, demand, supply, initial capital cost, technological, biological effects like structure/function relationships, impact of processes and ingredients on quality (Perrot et *al.*, 2011). Interesting reviews and examples related to uncertainties in the biofuel Supply Chain Management can be found for instance in (Doukas, 2013) and (Awudu & Zhang, 2012). Additionally, if we consider uncertainty in energy sustainability, vague and complex concepts and their implications as a policy objective are difficult to define and measure (Grossman & Guillén-Gosálbez, 2010).

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255   ● Complex, qualitative and quantitative information sources, uncertain and incomplete data

256   (Higgins et *al.*, 2010), non-harmonized data acquisition[4], 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).

269

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

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[4] http://www.globalharmonizationinitiative.net

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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.

296

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

13

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, 200). 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 constraintsbringing

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

14

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.

15

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

3. 2 Interactions with human knowledge and expertise

383
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,

17

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

18

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

19

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

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3.3 Optimization

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

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

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

21

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.

23

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,

24

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]

4.2 Multi-scale analysis in biological processes
567
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

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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.

26

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

4.3 Sustainability of networks by collective regional branding.

645

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

28

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

30

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.

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;

31

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

33

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.

Acknowledgements

790

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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

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, Wuillemin & 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.

| Step 2: reconstructing different scales in a mathematical frame | Description | Characterization of separate elements, at different levels of detail and complexity. | Linking separate elements into a systemic approach. 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. | 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. The difficulty is to select the right scales bringing a good representation of the whole. Managing uncertainty is fundamental. |
| | Computing paradigms | Depending on the case study and the available data: differential equations, neural networks, fuzzy logic, … | Model coupling, Bayesian networks, probabilistic approaches (Sicard et al., 2011). However, these techniques are rarely connected and used in conjunction with each other, even | Complex system science, coupling stochastic (roadmap) and deterministic approaches, individual-based models, interactive learning. These techniques have |

			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.

Step 4: system optimization and resilience	Description	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.	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).	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.

	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.
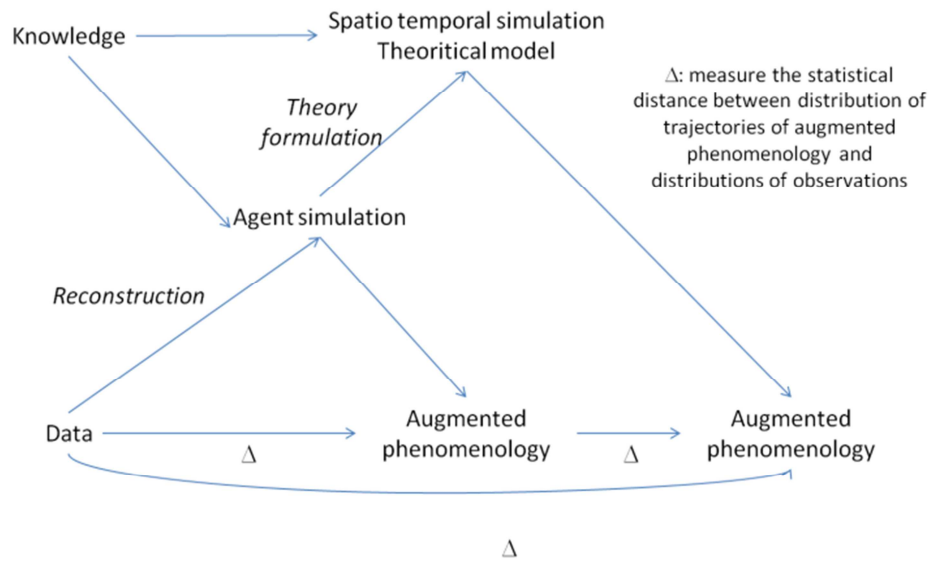
Figure 1

Figure 2

Figure 3

| a - molecular level | b – microstructure | c – unit operations | d – factory level | e – supply chain |
| *0.1-100 nm* | *1-1000 μm* | *0.1-10 m* | *100 -1000 m* | *10-100 km* |
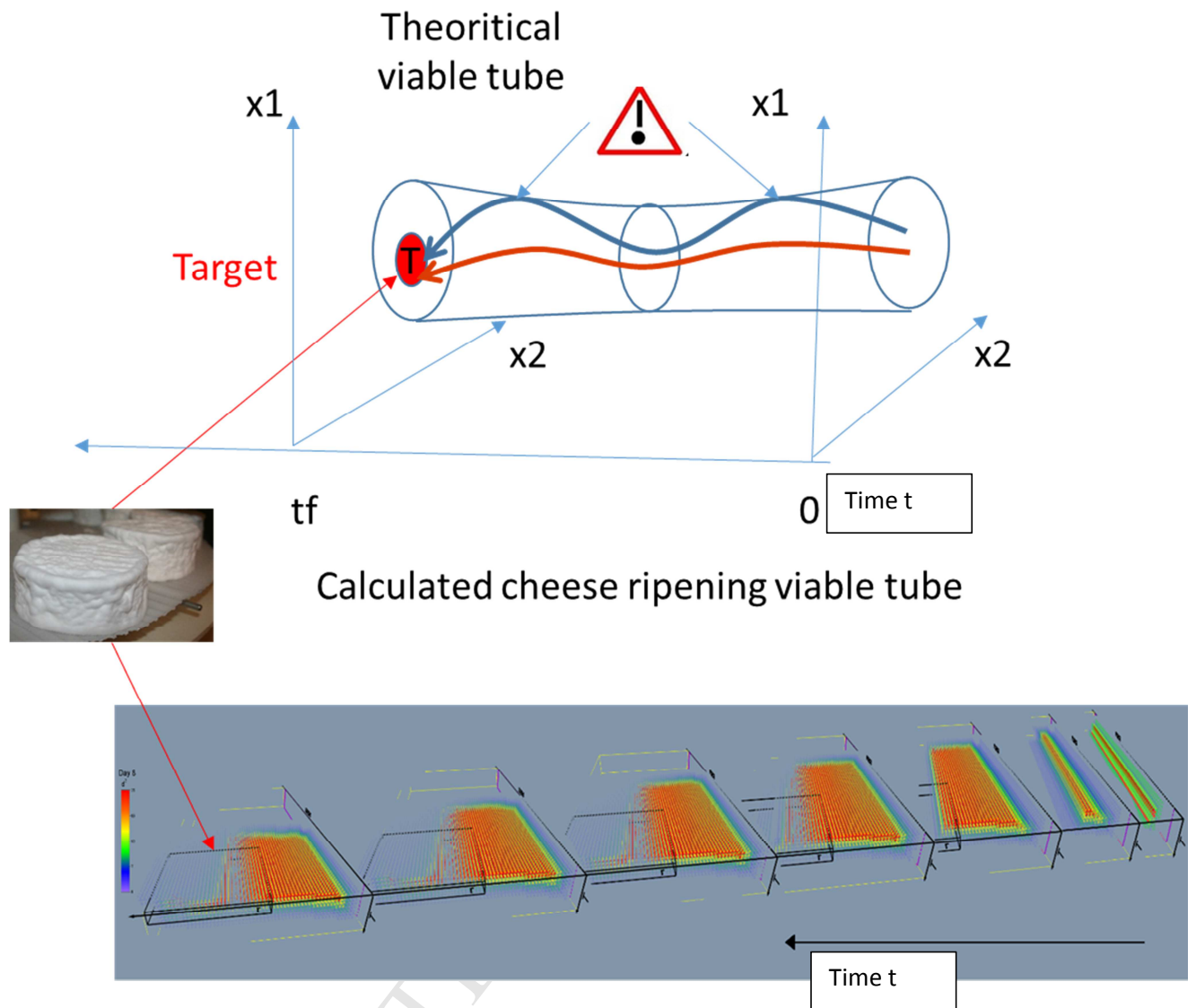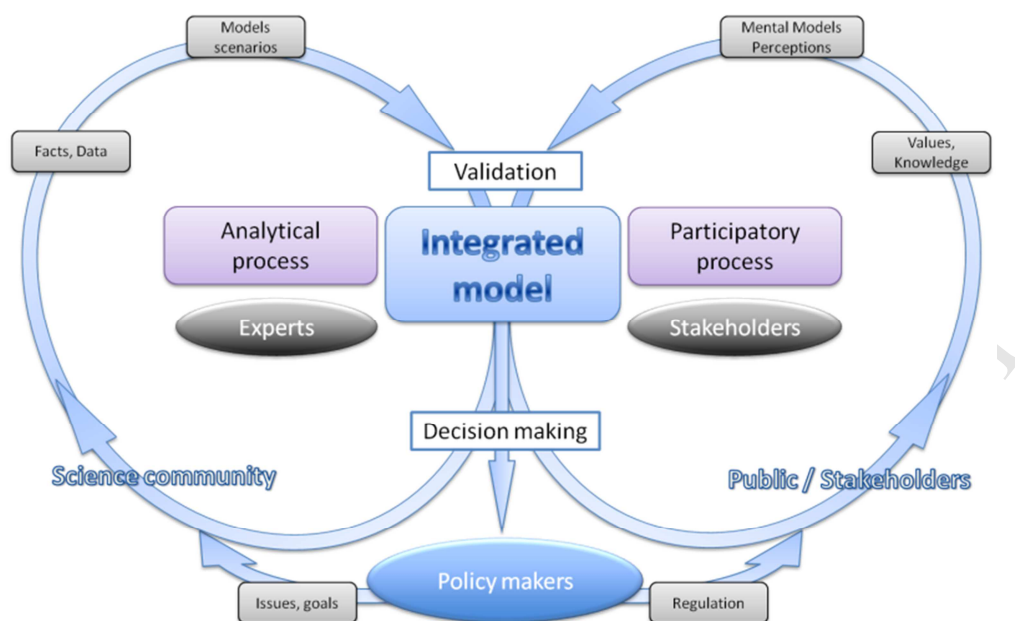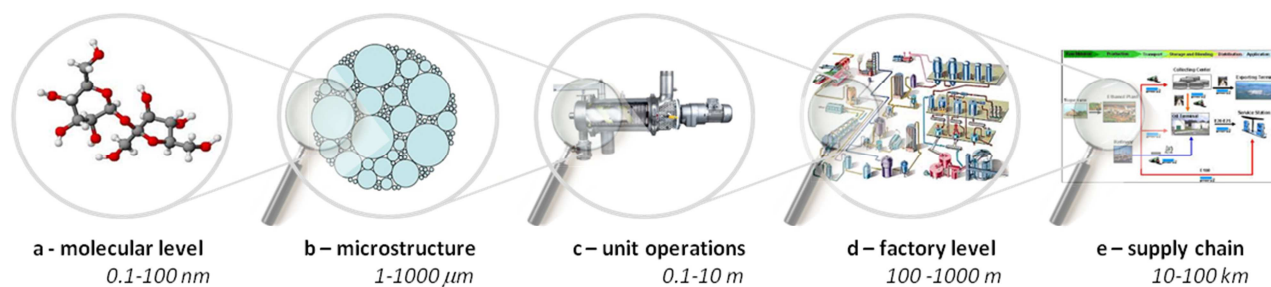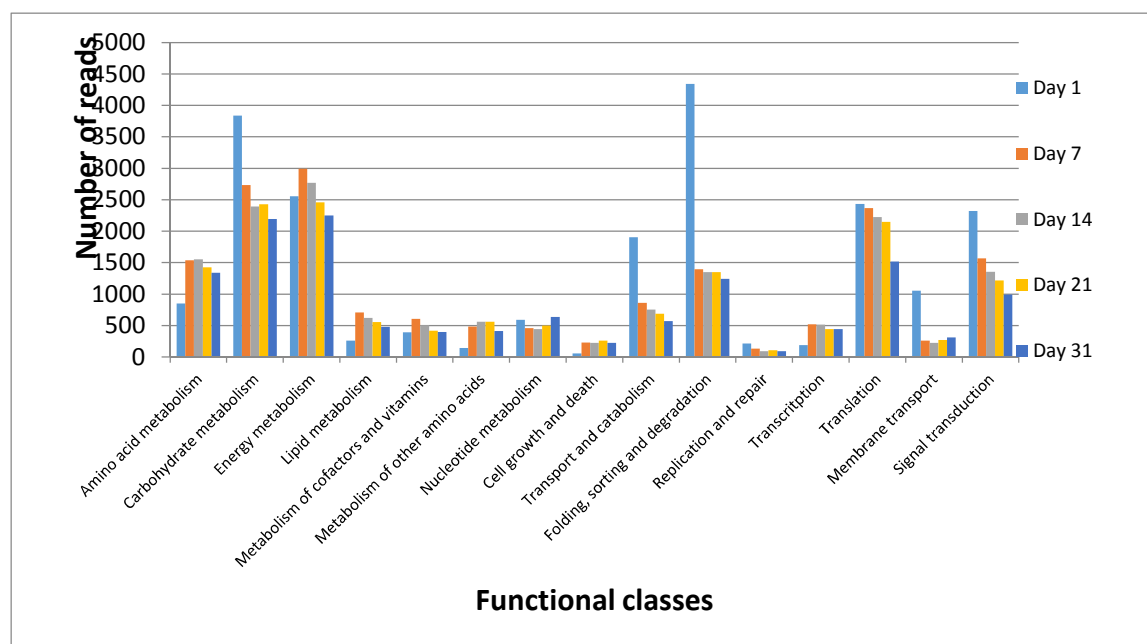
Figure 4

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.