

Smart Agriculture and Sustainable Development in Agro-Ecosystems: Innovative Computational Modeling for Digital Twins

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Abstract: - By boosting yields, improving efficiency, and reducing costs (while managing resources), digital technologies have driven innovation in agro-ecosystems in recent years. As a means to overcome ever-limited resources, Smart Agriculture – sometimes also referred to as Agriculture 4.0 – has increasingly leveraged digital solutions to achieve efficiency and sustainability. Digital twins in rural systems perform as computational (*in silico*) replicas of food production lines, which can drive innovation by enabling real-time optimization as well as predictive decision-making. Considering that both non-human and human actors are directly involved, this paper discusses (from a strategic alignment viewpoint) a prospective symbiotic ethos that farmers and ranchers may pursue when it comes to integrated, participatory and efficient transfer and usage of digital technology in rural activities. Bearing particularly in mind smallholders, challenges and opportunities for Smart Agriculture include: (i) implementation of hybrid in-house simulators of agro-ecosystems by suitably combining mechanistic modeling with data-driven simulation; (ii) use of dimensionless mathematical modeling to expedite scale-up, optimization, and translation of innovative digital technologies; and (iii) validating as well as transferring novel digital solutions in consideration of strategic issues identified by rural end-users.

Key-Words: - Sustainable Development Goals, Agro-Ecosystems, Agriculture 4.0, Mathematical Modeling, Numerical Simulation, Technology Transfer, Rural Systems

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1 Introduction

In order to uphold humanity's well-being and our planet's resources, on September 2015 the member states of the United Nations adopted 17 Sustainable Development Goals (SDGs) – comprising 169 targets altogether – to help thinkers as well as leaders in decision-making for sustainability [1]. In view of SDG-2 Zero Hunger, Smart Agriculture – sometimes equally referred to as Agriculture 4.0 – closely aligns with specific targets such as Target 2.3 Double the productivity and incomes of small-scale food producers, Target 2.4 Sustainable food production and resilient agricultural practices, and Target 2.6 Invest in agricultural research, technology, gene banks, rural infrastructure [2].

As the global population continues to expand, food production at enough levels (while concurrently reducing its environmental footprint) has become a worldwide challenge [3]. To overcome ever-limited resources, Smart Agriculture has increasingly leveraged digital tools as a means to achieve efficiency and sustainability of rural systems [4]. By reducing costs, boosting yields and improving efficiency, digital technologies have fostered the

development as well as driven innovation in agro-ecosystems in recent years [5].

Digital twins are dynamic *in silico* (i.e., virtual) replicas of real-world objects, systems or processes [6]. By staying synchronized through live data from sensors, digital twins are designed to numerically simulate the behavior and performance of physical counterparts [7]. In regard to agro-ecosystems, digital twins can rely on real-time information from drones (besides sensors) to support Smart Agriculture [8]. In rural systems, digital twins can support and improve data-driven decision-making by creating and keeping digital-physical interlinks among farming assets and resources such as crops, livestock, energy, water, machinery, and workforce [9].

Comprehensive computational modeling is a stepping-stone for conceiving and implementing digital twins [10], and such a rule of thumb should be equally pursued in Smart Agriculture. However, as agro-ecosystems usually invoke intricate relations [11], the resultant all-inclusive digital twins are prone to entail complex governing equations.

Agro-ecosystems behavior changes in line with (for example) biodiversity, composition variability, and assorted (bio)chemical kinetics [12]. As a result,

a stochastic feature can be assigned to not only model parameters but also to boundary / initial conditions for governing differential equations [13].

As mutual interactions are expected among key variables mathematically depicting agro-ecosystems such as pressure, temperature, and concentrations of chemical species (including pH or moisture content) [14], governing equations tend to become coupled to each other. Also, constitutive equations are generally required to mathematically close the model [15]. Equally known as closure equations, they are data-driven empirical correlations with limited application scope as they rely on specific observations rather than fundamental laws [16].

2 Problem Statement

Instead of pursuing a generic method, computational models (and thus digital twins) in Smart Agriculture should be customized for local development and sustainability [17]. Food production systems overlap ecological limits, resource availability, local politics, and socioeconomic issues [18]. Further sources of complexity refer to context-specific dynamics, path dependencies, power relations, multiple temporal-spatial scales, and unpredictability [19].

When conceiving simulation codes, this inherent complexity of food production systems is prone to render forward and backward reasoning. Each model assumption should be regularly re-examined to avoid either over-complicating or over-simplifying a given approach to the detriment of another [20]. Care must be exercised to prevent, for instance: incomplete causality, biased questioning, or improper underlying ideas and/or data [21].

At this point, interdisciplinary and collaborative approaches become strategic. While the development and implementation of the digital twin is undoubtedly under the computational modelers' responsibility, farmers' and ranchers' expertise and experience play a foremost role in tailoring the computational model to their needs and production scenarios [22]. All-inclusive computational models of agro-ecosystems require specialist-oriented features possibly absent in general-purpose (off-the-shelf) software [23]. Hence, user-defined code lines must be externally conceived and programmed by trained computational modelers to accurately address – and simulate – the prevailing agro-ecological scenario.

Last but not least, commercial software costs can be exorbitant for non-academic end-users [24], which can create a barrier for smallholder farmers, ranchers, or food producers. Therefore, in-house – relatively cheaper – simulation software comes forward as a feasible solution.

In view of research, development, and innovation (RD&I) in rural systems supported by virtualization (i.e., digital) tools, possible strategies for in-house computational modeling (and consequential digital twins) are discussed next. A compromise (trade-off) between comprehensiveness and applicability is then envisaged by tackling agro-ecosystems concurrently from diverse fronts with respect to their mathematical modeling and numerical simulation.

3 Solution Strategy and Discussion

Agro-ecosystems nexus encompasses exact, life and social sciences, thus its all-inclusive computational modeling becomes inherently interdisciplinary [25]. In view of taking several agro-ecological dimensions into account [26], an inventive mathematical model can be envisaged by relying on multiple generalized coordinates, ultimately generating an One Health hyperspace. Agro-ecological models certainly invoke numerous variables and parameters, so dimensionless modeling can mitigate the mathematical complexity while expediting translation, optimization, and scale-up [27].

With regard to the computational implementation, simulation techniques should empower in-house software development [28]. With large potential for computational parallelism while simplifying in-house simulation development, the lattice Boltzmann method (LBM) arises as a compelling alternative for agro-ecological applications [29].

Finally, in-house simulators of food-production systems can be implemented by suitably combining first-principles modeling with data-driven methods, thus rendering hybrid simulators suitable for digital twins [30]. In what follows, such a combined solution strategy is conceptually addressed and discussed.

3.1 Transport Phenomena and One Health

Unifying frameworks of natural phenomena are not only among the pursuits of agro-ecological sciences [31] but also can trigger paradigm shifts. Driven and upheld by gradients of intensive quantities such as pressure, temperature, and species concentration, transport phenomena are ubiquitous in nature since momentum, energy, mass transfers always take place among humans, animals, plants, and the environment [32]. Besides conceptually underlying computational fluid dynamics (CFD) in agriculture [33], transport phenomena can confer novel insights for all-inclusive modeling of agro-ecosystems.

As far as matter, energy, and species balances are concerned, compartmental models in agro-ecology mathematically divide bio-ecosystems into a number

of discrete clusters [34]. Compartments are linked to each other so that “flows” of nutrients, biomass, or infectious diseases between them are modeled via ordinary differential equations (ODEs), which are – thus – coupled to each other [35]. By contrasting with a unifying framework (if this approach is pursued), raising the number of compartments greatly amplifies possible arrangements of exchanged “flows”, thus overloading the system of coupled ODEs [36]. By modeling all-inclusiveness with the help of several interconnected compartments, either mathematical or numerical instabilities raise further concerns [37].

Transcendental rationales of transport phenomena can indeed push the boundaries of agro-ecology [38]. In line with transport-phenomena-inspired *in silico* epidemiology [39], a reductionist model for dynamic and interlinked agro-ecosystems can rely on a single partial differential equation (PDE), expressed with the help of generalized One Health coordinates.

In a far-reaching agro-ecological model rationale, transport phenomena balances can entail diffusive transfer due to “disordered” interactions involving the transported entity (which is an intensive quantity) and the host medium as well as convective transfer from “ordered” external actions – if any – onto the “flowing” medium [32]. By taking either source or sink rates into account, basic conservation principles render a governing PDE, which can be referred to as “agro-ecosystem transport equation”, namely:

$$\frac{\partial(\rho\varphi)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \varphi) = \nabla \cdot (\rho D \nabla \varphi) + S_{\varphi} \quad (1)$$

where φ is the transported quantity, ρ and $\mathbf{v}$ are the host medium density and velocity (for an allegedly “flowing” medium), D is the diffusivity, S_{φ} includes either source or sink rates of entity φ , and t is time. By treating the host medium as a continuum, Eq. (1) can simulate the local dynamic behavior $\partial(\rho\varphi)/\partial t$ of agro-ecological quantity φ by modeling its “ordered” transport $\nabla \cdot (\rho \mathbf{v} \varphi)$ via convection, its “disordered” transport $\nabla \cdot (\rho D \nabla \varphi)$ through diffusion, and its local generation and/or consumption rates.

In “canonical” transport phenomena, the nabla operator ∇ is restricted to 3D spatial coordinates [32]. Likewise the paradigm shift in [39], transcending Eq. (1) to agro-ecosystems is also a matter of allocating as many generalized coordinates x_i (i.e., independent variables in One Health hyperspace) as the number of agro-ecological dimensions mathematically invoked in the model framework. Time t can be identified as coordinate x_0 , if convenient.

Accordingly, rather than a (perhaps large) system of coupled governing ODEs, Eq. (1) is a reductionist PDE in holistic One Health hyperspace. Instead of a sequence of interconnected compartments (clusters),

each one assigned to a governing ODE, generalized coordinates can be used to categorize agro-ecological features, apart from time dependence. In the quest for a unifying description, Eq. (1) is a single differential equation modeling the spatial-temporal behavior of a multidisciplinary – but single – host medium.

For both isotropism and isomorphism reasons, the generalized coordinates x_i must be cast dimensionless with the help of suitably identified reference scales. The same applies to time t , which always remains as an independent variable in One Health hyperspace (i.e., for dynamic systems modeling).

3.2 Dimensionless modeling

Phenomenological (i.e., mechanistic) models usually start with primitive variables, since they are directly measurable. Regardless of being ‘ready-to-use’, such a mathematical formulation may overload sensitivity analyses while making scale-up awkward, mainly if the model relies on several variables [40].

Agro-ecosystems models do not require primitive variables or parameters to be cast into dimensionless form. However, this practice is advisable whenever possible [41], in view of the following rationale:

- Primitive parameters can be lumped into fewer dimensionless quotients (ratios), which shrinks the number of tests (experimental asset), condenses influencing effects into fewer plots (mathematical asset), and helps interpreting their mutual interplay (engineering asset);
- Results become independent from the system of units, for both exchange and translation;
- Solutions achieved in a particular scenario can be applied to others, even those not connected to the scenario originally solved, given they are set up at the same dimensionless form;
- Non-tested scenarios (even disallowed ones) may become achievable while boundary and/or initial conditions can be easily handled.

Having Buckingham-Vaschy (Π ’s) theorem as its cornerstone [42], dimensionless modeling is a tool to rationalize engineering research [43]. This powerful theorem allows dimensionless modeling to cluster primitive parameters into fewer dimensionless ratios (quotients) [44], which radically reduces the amount of parameters to be studied (whether experimentally or numerically), thus expediting optimization, scale-up, and translation.

In the Smart Agriculture context, dimensionless modeling may rationalize the simultaneous influence of agro-ecological variables due to (for example):

- Inclusion of as many generalized coordinates as the ontology features in the model (e.g., assorted aspect ratios of solution domain extensions);

- Modeling non-uniform agro-ecosystems with different diffusive spread among compartments;
- Modeling agro-ecological rheology (e.g., assorted convective spread or latency mechanisms);
- Unbalancing source (i.e., generation) and sink (i.e., consumption) terms in agro-ecosystems;
- Imposing mixed boundary conditions to model different agro-ecological (rural system) scenarios;
- Modeling agro-ecosystems as multicomponent-multiphase media as well as porous media (e.g., porosity as a measure of crowding trends and/or permeability as a measure of connectivity).

3.3 In-House Computational Method

When developing and implementing in-house digital twins for agro-ecosystems, the transport-phenomena-inspired governing PDE, Eq. (1), can be numerically solved via lattice Boltzmann method (LBM). LBM can be applied to computationally model biosystems and bioprocesses using dimensionless variables [45].

Envisaged in 1988 [46], LBM is more recent than customary discretization methods like finite elements (FEM) or finite volumes (FVM). LBM has become a powerful method to numerically simulate biosystems and bioprocesses at different scales [47]. In the agro-ecological context, LBM has tackled flows through fibrous materials [48], particle-fluid suspensions [49], agrochemical transport within soil [50], liquid-vapor interface [51], and agroindustrial wastewater treatment in bioreactors [52].

LBM separates itself from macroscale methods (i.e., FEM or FVM) or microscale simulation (e.g., molecular dynamics – MD) as it treats any system (whether solid or fluid) as a collection of fictitious constituent particles in a discrete space, namely, a fictitious lattice structure. Those particles follow two courses of action in discrete time steps. During the ‘collision’ step, fictitious particles bump into each other at lattice sites as they arrive from pre-defined lattice links, so their velocities (momenta) become rearranged. In the ‘streaming’ step, particles resume their motion along lattice links toward neighboring sites, consistent with rearranged streaming velocities. By imposing conservation principles to this particle dynamics, the behavior of macroscopic medium can be numerically simulated [53].

As its notable feature, LBM can simulate transport phenomena and fluid flow without directly solving Navier-Stokes equations [53]. As a result, LBM lays off computational-demanding Galerkin formulations in FEM [54] as well as pressure-velocity coupling in FVM [55]. LBM thus yields simpler computational codes if compared to in-house numerical simulators

implemented by means of traditional discretization methods (e.g., FEM or FVM) [56].

Furthermore, LBM forthrightly deals with either moving boundaries or multiphase-multicomponent systems of agro-ecological interest [57]. Allied to its large potential for computational parallelism, LBM is attractive (from the code-developer’s perspective) to numerically solve governing PDEs similar to Eq. (1). In other words, LBM comes forward as a prospective route for in-house digital twins of agro-ecosystems with spatial-temporal dependence.

3.4 Hybrid Simulation

Inclusiveness in computational modeling is pursued by grasping complexity while excluding unrelated information [58]. In view of the complexity of agro-ecosystems, the development of digital twins should appropriately integrate physics-based (also referred to as mechanistic or deterministic) modeling with data-driven (equally known as empirical or heuristic) techniques, thus rendering hybrid simulation [59].

Rather than fully relying on each approach alone, with limited scope when used separately [60], hybrid simulation can breed both fundamental research and on-farm technology [61]. If “data is the new gold” (famous quote), then hybrid computational modeling is the best pickaxe. Furthermore, hybrid simulators must be implemented as knowledge repositories to be continuously improved and extended by up-to-date or more accurate information.

Thinking-enhancement in agro-ecosystems can be achieved through an advantageous benefit-cost ratio between realistic virtualization and applicability [62]. For instance, machine learning has been coupled to LBM to simulate complex multiphase flow occurring in natural systems [63].

3.5 On-Farm Adoption Challenges

Computational modeling is a helpful and powerful tool not only when mathematical difficulties prevent analytical solutions from being deduced but also if attaining either laboratory or on-farm data becomes awkward – perhaps unfeasible – due to technological, environmental, economic, safety, and/or even ethical issues [64]. In view of costs to carry out either *in vivo* or *in vitro* experiments, *in silico* (i.e., computational) testing can save valuable human, material, energetic, and human resources for research, development, and innovation (RD&I) in agro-ecosystems [65].

Smallholder farmers tend to be reluctant to adopt new technologies, principally digital ones [66]. To overcome those barriers, a sociotechnical approach must consider both non-human (e.g., soil, water, plants, animals, sensors, drones, software, and digital twins) and human actors (e.g., food producers, rural

workers, extensionists, policymakers, researchers, and traders) in the agro-ecosystem network [67].

A possible roadmap could start from mapping and depicting potential digital technologies to compose a portfolio of viable solutions to smallholder farmers. Then, field diagnoses could be carried out to grasp current usage panorama, together with bottlenecks in implementing digital technologies in rural production processes. Based on data collected, a next step could envisage technology transfer procedures in view of – usually non-trivial – interactions between non-human and human actors. A final step could then focus on proposing and implementing pilot actions (e.g., in selected smallholder farmers) so as to test, validate, and adjust the extension procedure for the prevailing agro-ecosystem scenario.

4 Conclusion

Digital technologies can help smallholder farmers to tackle issues related to sustainable agriculture such as energy availability, treatment of contaminated soil, and groundwater supply. In those applications, either fluid flow or transport phenomena play an influential role, whose comprehensive computational modeling can underlie the development of digital twins to assist rural technology innovation.

Thinking-enhancement in Smart Agriculture (i.e., Agriculture 4.0) confers challenges and opportunities to be tackled by an integrated (i.e., holist) approach bearing in mind:

- Implementation of hybrid in-house simulators of agro-ecosystems by suitably merging mechanistic modeling with data-driven simulation;
- Use of dimensionless modeling to expedite scale-up, optimization, and translation of novel digital technologies;
- Validating and transferring the innovative digital technologies (and solutions) in view of strategic issues identified by rural communities.

Smart Agriculture thus bestows broad niches for strategic cross-collaboration among non-human and human actors. A symbiotic ethos must be pursued in view of integrated, participatory and efficient digital technology transfer for smallholder farmers. Ultimate goal is to increase productivity, sustainability, and resilience of agro-ecosystems, therefore upholding the Sustainable Development Goals (SDGs), such as SDG-2 ‘Zero Hunger’, SDG-3 ‘Good Health and Well-Being’, SDG-6 ‘Clean Water and Sanitation’, SDG 9 ‘Industry, Innovation, and Infrastructure’, and SDG-15 ‘Life on Land’.

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