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Modelling Water-Energy-Food nexus by a network of Agents

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1. Introduction

There has been growing scientific discussion around the complexity of the Water, Energy and Food (WEF) systems and their inter-connections such that traditional "vertical" planning and decision making about these essential commodities is challenged when also dealing with the growing pressures of urbanization, population growth and climate change. The term "WEF nexus" was coined to describe the multiple aspects and cross-disciplinary nature of the research required to model Water, Energy and Food interconnections on macrosocial (countries or regions) [1],[2],[3] as well as on microsocial (local settlements or households) [4] levels.

One of the common issues mentioned by WEF nexus researchers [5] is the inadequacy of the existing—sometimes quite elaborate—models for energy, water and food sectors that may be very good for macro-level and long-term projections used to inform strategic decision making [6], but those same elaborate models are less applicable at local or household levels which are often, and rightly so, a focus of WEF nexus research. Overall, the problem of upstream and downstream planning and policy making for the WEF nexus, ideally supported by the same or similar class of models for all scales of aggregation, has not yet found a practicable and suitable resolution.

One of the reasons for the lack of suitable universal cross-scale models is conceptual: modellers tend to think about WEF nexus as a complex system with certain rules or laws to discover and formalize, then the resulting model is handed over to planners and decision makers. There is typically a certain effort in WEF nexus projects to engage with various Agents (stakeholders) directly involved in daily nexus operations [7] but when it comes to modelling, these "grassroots" Agents are perceived at best as suppliers of measures and indicators for a complex model that will eventually do all the magic. In short, a WEF nexus model is typically handled as a big complex machine with no or only borderline Agents' involvement.

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We suggest an alternative approach to WEF nexus modelling with all the Agents clearly identified and combined in a well-defined network of interactions. We suggest that each Agent (who is not necessarily an individual—it may be e.g. a local administration managing a certain territory, or a business managing an industrial unit—should be modelled as a WEF nexus in its own right. In that sense, our approach focuses on a "nexus of nexuses" as already highlighted from previous studies [8], but from an Agent perspective.

Different kinds of Agents characterized by their specific WEF nexus can be connected in a network with certain internal and external exchange rates of Water, Energy and Food. We demonstrate that such a network of Agents, each of them being represented as a WEF nexus, is conceptually suitable for its application in modelling at different aggregation scales, and can be used in *in silico* experiments (computer simulations).

This work, first, details our conceptualization of a WEF nexus as a network of Agents, then illustrates how this approach can be applied to the known problems of defining nexus boundaries and aggregation. We also suggest a generic mathematical formalization of the suggested Agents-based nexus model that is suitable for the design and implementation of computer simulations. We outline high-level business requirements in the form of plausible research questions that such a model simulation could address.

2. Introducing Agents in the nexus definition

Implicitly, Agents—be they families, businesses, local administrations or national authorities—have always been present in the WEF nexus research discussions; we make their presence explicit, and usable in nexus models. We define a nexus Agent as a self-governing entity with a certain level of autonomy that, on one hand, consumes a variety of Water, Energy and Food resources from the environment or other Agents and on the other hand, produces a (different) variety of Water, Energy and Food resources, which may also be consumed within the Agent's realm.

The explicit introduction of autonomous Agents may at a first glance complicate modelling , but in fact, introducing Agents that look after their respective WEF nexuses makes conceptualization and practical modelling of the nexus more natural and more complete. Specifically, impact studies of how a specific policy or policy change affects the nexus behaviour, as well as "what-if" scenario-based planning will become much clearer with the explicit introduction of Agents. The alternative is an artificial parametrization of the WEF models in order to take into account behavioural influences from a variety of interconnected stakeholders.

We suggest in this work how to model an Agent-specific nexus and provide a mathematical formulation which offers, a balance between simplicity and conceptual richness. .

We consider how the WEF conceptual framework modified by the addition of autonomous Agents can help to solve the known challenges of defining a nexus boundary and having appropriate up/downscaling between granularity and aggregation.

We then propose research questions that could be addressed by computer simulation based on the network of Agents.

3. Modelling WEF nexus for a particular Agent and its possible mathematical expression

There are conceptually two major approaches to Agent-centric WEF modelling: either having considered “impacts” of the Agent behaviour on Water, Energy and Food production and consumption, or having considered “balances” of Water, Energy and Food associated with a particular Agent. We deliberately follow the latter approach based on “balances” as it allows better quantification based on available data.

We suggest considering each Agent as an autonomous system with certain flows of Water, Energy and Food during four defined stages: ingestion, production, consumption, loss and supply. For the sake of simplicity and estimability, we will combine in-nexus internal consumption and loss in one conceptual unit.

Our suggested model of an Agent-centric WEF nexus is represented by Figure 1 with the following variables (each of which has to be thought of as a vector rather than a scalar value):

W_in ¬ water resource(s) ingested by the Agent; this concerns interaction with the environment or other Agents (water suppliers),

W_out – water resource(s) supplied by the Agent; this concerns interaction with the environment or other Agents (water consumers),

WtW – water resource(s) conversion to other water resource(s), e.g. making a certain share of circulating water for drinking water,

WtF – a share of water resource(s) consumed by Food production within the nexus,

WtE – a share of water resource(s) consumed by Energy production within the nexus,

Wcl – a share of water resource(s) consumed or lost by the Agent within the nexus,

and we use similar designations for the flows of Food and Energy.

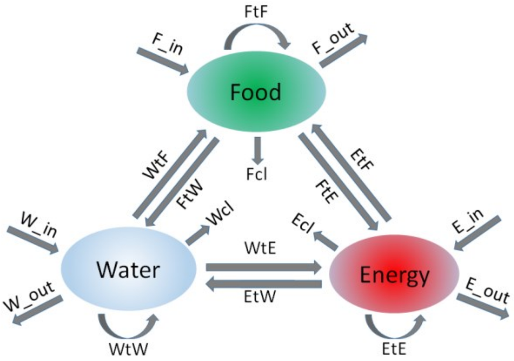

Fig. 1. Water-Energy-Food nexus for a particular Agent.
All *_in and *_out parameters are potential connections to other similarly modelled Agents.

Depending on the context of the WEF research, this diagram could be thought of either as a “snapshot” of the nexus state at a particular moment in time, then each parameter introduced can be interpreted as the flow of a particular resource, or in certain research contexts they could be thought of as integral values measured over a certain period. We expect that, owing to the dependency on available data for estimation of the nexus models, the initial interpretation would be typically integral with possible extrapolations and normalizations in order to obtain “snapshot” derived values when required. For this agent then, the model is a compartmental model.

In addition to the introduced parameters—many, if not all of which can be measured directly or with only a small recalculation from the available directly measured indicators—it will be conceptually useful to consider the flows of Water, Energy and Food that are produced by the Agent within its nexus; let us designate them as **W_p**, **E_p** and **F_p**. These can be considered measures of the nexus productivity in respect to Water, Energy and Food; having these measures explicit is conceptually useful as the nexus productivity, and models of it are both practically important, and are often a concern for WEF nexus research. We then can compile a simultaneous system of balance-based equations as follows:

$$\begin{aligned} W\_in + W\_p &= WtE + WtF + WtW + Wcl + W\_out \\ E\_in + E\_p &= EtF + EtW + EtE + Ecl + E\_out \qquad (1) \\ F\_in + F\_p &= FtE + FtW + FtF + Fcl + F\_out \end{aligned}$$

The physical meaning of these equations is that the total of the respective resource used by or produced by the Agent (LHS of equation 1) should be equal to the total of conversions of other nexus resources , as well as with the output (yield) of the resource that can be used by other Agents or contributed to the surrounding socioeconomic or natural environment (RHS equation 1).

These fairly simple balance equations can be in fact a useful instrument for discovering gaps in data; if available data is lacking for any of these measures then they cannot be reliably estimated, we do not have enough knowledge about the nexus in question. Identifying and measuring these gaps may not be straightforward as the required Agent-specific data may not be available or may have been collected over different periods, with different granularity and using different indicators and measurement units. Harmonizing such data and applying them to balance equations even for one Agent / nexus, or one class of Agents / nexuses may constitute a dedicated research project of its own. However, these balance equations have a clear potential to offer a sound framework for such a gap analysis and for constructive feedback to policy makers. This feedback can provide evidence and argument why, in some cases, the amendments to statistical reporting and to data collection procedures by the Agents are required in order to support the WEF nexus research, planning and decision-making.

Agent-specific data such as resource conversion rates for energy-to-food, water-to-food and similar ones in the balance equations cannot entirely rely on official or administrative statistics; the collection and normalization of such data requires a dedicated research effort. An example of this is the research required for water and energy consumption in agriculture, broken down by a particular crop in a particular climate [9]. As seen on Figure 1, we have introduced the rates of conversion for energy-to-energy, water-to-water and food-to-food,. Another example of when such conversions would be applicable is a transformation of one form of energy into another, e.g. using an electricity generator working on liquid fuel; another example will be crops fed to the cattle. As is frequently the case in modelling, the intensity of these conversions can be negligible in some cases and then these components of the overall balance can be disregarded but for some types of Agents, such energy-to-energy, water-to-water and food-to-food conversions may be the Agents’ core business.

In addition to having modelling balances, we also need models of the nexus productivity. It is reasonable to suggest that the nexus productivity in respect to a particular resource depends on the resource consumption by the Agent, on the consumption of the other two resources, and on the conversion rates from every available resource into the resource in question. In a generalized form, this functional dependency can be expressed as follows:

W_p = W_p (W_in, E_in, F_in, E_p, F_p, EtW, FtW, WtW)
E_p = E_p (W_in, E_in, F_in, F_p, W_p, FtE, WtE, EtE) (2)
F_p = F_p (W_in, E_in, F_in, W_p, E_p, WtF, EtF, FtF)

where W_p, E_p and F_p denote the nexus productivity in respect to Water, Energy and Food.

Linear dependencies may be sufficient approximations in some cases, so that, as an example, Energy production by the nexus might look like:

E_p = E_in*EtE + (W_in+W_p)*WtE + (F_in+F_p)*FtE (3)

but in reality, the functions may be more complex, and there may be inequalities to express the (absolute or conventional or economy-driven) limits of the availability of a certain resource, e.g. the economically or ecologically practical availability of Water for the Agent’s nexus.

The direct consumption (by the Agent) and loss of resource within the Agent’s nexus has been a topic of some WEF nexus research, although often of a qualitative rather than quantitative nature. As an example, researchers can explore the consumption of Energy within a household that is driven to some extent by the consumption of Food and the associated social elements (such as it is more comfortable having a family dinner in a large room that requires heating and lighting). Modelling these consumption-and-loss interdependencies can be the main topic of some detailed WEF nexus research with a socioeconomic or cultural flavour. However, it is not a focus of this work, so for the time being, we offer a placeholder for this aspect of WEF nexus modelling related to direct resource consumption and loss by the Agent, with generally expressed functional dependencies as follows:

Wcl = Wcl (Ecl, Fcl)
Ecl = Ecl (Wcl, Fcl) (4)
Fcl = Fcl (Ecl, Wcl)

From the model implementation and validation perspectives, the system of “balance” equations (1) can be supported by the available administrative data, with the system of equations serving to identify gaps in the available data.

The part of the model that is represented by the system of equations (2) is best served by fitting using methods from “data science”. This is likely to require sufficient data collected with the modelling in mind (as a research exercise) directly from the nexus / Agent in question; those data collected by national and international bodies in aggregated form will not be sufficient for model fitting or inference.

Data for fitting the functions in (4) can be again obtained only directly from a particular Agent, , and the advent of ubiquitous sensors and smart meters will facilitate the collection of such data.

4. Nexus boundaries and nexus aggregations

The problem of defining the WEF nexus boundaries and a related problem of aggregation of local/granular nexus models into a scaled up model, e.g. for a certain region, are challenges that face many WEF nexus research projects, but they can be avoided if we consistently apply the Agent-based approach to nexus modelling. The boundary of the nexus then is the Agent itself with its interfaces with other Agents or environment illustrated in Figure 1 which suggest this interface is just a tuple of six parameters (W_in, E_in, F_in, W_out, E_out, F_out).

It is straightforward to introduce different kinds of Agents in a newly aggregated nexus where outputs of some Agents are the inputs for the others. Figure 2 illustrates a possible aggregated nexus for two farms, a co-located food processing facility, as well as energy (fuel and electricity) and water suppliers for them. Additional inputs and outputs can be added as required, e.g., energy and water inputs from nature. The interconnected inputs and outputs cease to be a boundary in this example; the new boundary for an aggregated nexus is represented by "external" inputs and outputs, and all the "internal" (interconnected) inputs and outputs remain essential only for the functioning of the aggregated nexus model itself but not for the definition of its boundary or its interfaces with other Agents or environment.

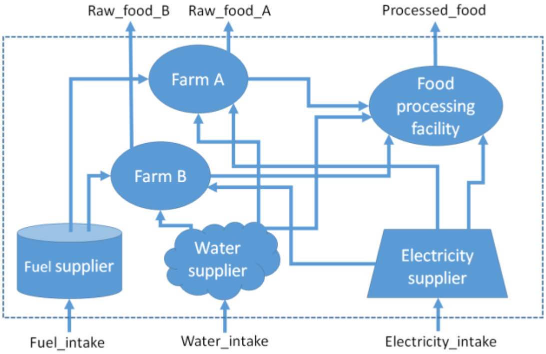

Fig. 2. An aggregated WEF nexus with a newly defined boundary. Each Agent within the aggregation owns a WEF nexus characterized by inputs, outputs and conversions as illustrated by Figure 1; certain outputs for some Agents are inputs for the others hence do no contribute to the definition of the aggregated nexus boundary.

There are conceptual difficulties with this sort of aggregation, as an example not every watt of electricity supplied to the food processing facility is of interest here but only the amount of electricity involved in processing the food supply from Farm A and Farm B. However, in this and other similar cases, reliable estimates are often possible (driven by economic requirements such as calculating and charging a food processing fee), so these moderate conceptual difficulties can be overcome and are likely to be insignificant compared to conceptual gains from the flexibility of boundaries definition. Any Agent and its nexus can be sensibly connected with any other Agent and its nexus, resulting in setting the nexus boundaries as required by the objectives of a particular research focus or planning or decision making exercise. Using the Agents' connection-in-network technique, the nexus boundaries can be effectively and unambiguously defined on a territorial basis, or represent a slice of a certain industry, e.g. food processing, or be entirely ad-hoc as in the example illustrated by Figure 2.

5. Using the network-based model in computer simulation

One real challenge to this modelling framework is, as mentioned, data gaps make it hard to fit the "balance" equations (1) and very specific data are required to fit the functions in (2) and (3). However as a simulation tool, it is possible to model a network of Agents and their nexuses using plausible values e.g., simulated from a distribution, where prior distributions are defined based on available knowledge. The better the simulated distributions relate to real data, then the more realistic the simulations become. This is likely to rapidly become computationally intensive for substantial networks of Agents (potentially, millions of them with thousands of different parameters). Fitting the models to data may present a computational challenge, too. To realise our modelling framework, there needs to be further consideration given to the engineering of data pipelines to support the modelling. Having the data pipelines well engineered and traceable is essential for the credibility of the entire model. What is required is not just "data stories" and visualizations that are often the publically delivered outcomes of a narrowly understood subject of data science, but a credible computer simulation framework supported by configurable data supply and data harmonization.

We have compiled a short list of essential research questions that the WEF nexus computer simulation based on the network of Agents should be able to address in order to make it applicable in the actual planning and decision-making:

- What are the limits of productivity of a particular WEF nexus in terms of Water, or/and Energy, or/and Food if supplied with enough external resource?
- How the addition or removal of certain Agents—either numbers or classes of them—affect the productivity of a particular WEF nexus? (Let us bear in mind that the actual operational goal may not be to increase the WEF nexus productivity but also to reduce it, e.g. to alleviate a pressure on a scarce natural resource)
- Whether changing the configuration of the Agents network (without changing the numbers or classes of them) allows a more efficient use of a certain resource, or affects the nexus productivity?
- How the Agents network model can relate to available socioeconomic models? (To allow for these cross-connections between models, the Agents network model will require clearly defined interfaces for their use by the third parties)
- What are the relative strengths and weaknesses of computer simulation based on the Agent network model compared to the universal computer simulation models [10] that are currently being modified [11] for use in a WEF nexus research?
- Whether results of Environmentally-Extended Input-Output Analysis (IEEIO) [12], [13] can be used in an Agents network model, say for model adjustment or validation using the aggregated WEF flows in cases where enough statistical data is available?

This short list of research questions can be considered, at the same time as, generic requirements for a computer simulation platform to model a WEF nexus s a network of interconnected Agents, each of them being defined as a WEF nexus of its own.

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