A framework for modelling the complexities of food and water security under globalisation

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Abstract

We present a new framework for modelling the complexities of food and water security under globalisation. The framework sets out a method to capture regional and sectoral interdependencies and cross scale feedbacks within the global food system that contribute to emergent water use patterns. The framework integrates aspects of existing models and approaches in the fields of hydrology and Integrated Assessment Modelling. The core of the framework is a multi-agent network of city agents connected by infrastructural trade networks. Agents receive socioeconomic and environmental constraint information from IAMs and hydrological models respectively and simulate complex, socioenvironmental dynamics that operate within those constraints. The emergent changes in food and water resources are aggregated and fed back to the original models with minimal modification of the structure of those models. It is our conviction that the framework presented can form the basis for a new wave of decision tools that capture complex socioenvironmental change within our globalised world. In doing so they will contribute to illuminating pathways towards a sustainable future for humans, ecosystems and the water they share.

Keywords: food and water security, globalisation, urbanization, complex systems, hydrology, integrated-assessment models

1 Introduction

Ensuring sustainable food and water security is an urgent and complex challenge (Shiklomanov, 2000; United Nations Water, 2015). The magnitude of the challenge is outlined in the Sustainable Development Goals, which set a target of zero hunger globally whilst at the same time drastically reducing impacts of food production on aquatic and terrestrial ecosystems as well as the climate system (United Nations, 2015). Food security and water security are inextricably intertwined, with variability in agricultural production impacting water resource use and vice versa (Liu and Savenije, 2008). Trade, both international and domestic, plays a central role in determining water use, because when we trade food, we are also trading the water embedded in the production of that food (Fader et al., 2013; Hoekstra and Mekonnen, 2012). The global system of food production and trade is complex and drives interdependency among heterogeneous regions, meaning that socioeconomic or environmental changes in one part of the globe can have cascading impacts for food and water security throughout (Fig. 1b) (D'Odorico et al., 2010; J. Liu et al., 2015; Marchand et al., 2016; Young et al., 2006). Equally, there is interdependency across sectors with the mechanisation of agriculture leading to a tighter coupling of the food, water and energy sectors in recent years, often referred as the food-water-energy nexus (Fig. 1a) (Bazilian et al., 2011). Within this interdependent system, interactions occur across spatial and temporal scales (d'Amour et al., 2016; Sivapalan and Blöschl, 2015) (Fig. 1c). For example, the combined effect of small-scale abstraction of ground and surface water to secure short-term food and water security can lead to large scale and long-term depletion of water resources, which ultimately undermines food and water security (Sivapalan and Blöschl, 2015; Sophocleous, 2012).

Given the complexity of the food system, it is challenging to develop effective food and water management strategies because policies can leak across regions, sectors and scales (Eakin et al., 2009; Hejazi et al., 2015; Meyfroidt et al., 2013). Models and decision tools exist to inform policy makers on these issues. For example, Integrated Assessment Models have made significant progress in capturing sectoral interdependencies with the food-water-energy nexus (Bazilian et al., 2011; Lotze-Campen et al., 2008; Stehfest et al., 2014). In the hydrological sciences, water footprint studies capture regional interdependence whilst sociohydrological studies capture cross-scale sociohydrological interactions (Hoekstra and Chapagain, 2006; Sivapalan, 2012). However to our knowledge, regional and sectoral interdependencies and cross-scale feedbacks associated with food and water security have not been captured in a single modelling framework. As a result, existing approaches miss important dynamics (Konar et al., 2016a; Srinivasan et al., 2017). It is urgent that we develop decision tools that capture these complexities to assist decision makers in navigating the increasingly complex global food system and help ensure that we stay within the natural limits of our planet's boundaries for water resources (Steffen et al., 2015; Wagener et al., 2010).

Figure 1. Complex dynamics within the global food system that lead to emergent water use patterns.

In this paper, we present a modelling framework for capturing regional and sectoral interdependencies and cross-scale feedbacks in the global food system that contribute to emergent water use patterns. The framework builds upon existing approaches in the fields of Integrated Assessment and hydrology and combines them via a multi-agent network of city agents and infrastructural trade links. We focus on cities because they are centres of food and water demand and important agents of change within the global food system, with 54% of the world's

population urbanised, consuming a disproportionately large, 75% of the world's resources (United Nations, 2012; UNEP, 2013).

Cities play a key role in driving regional interdependency via trade. In fact, cities and trade coevolved, with demand from cities determining the location of physical trade networks that constrain our ability to extract food and water resources from the environment and redistribute them around the globe to meet demand (Barber et al., 2014; Barredo and Demicheli, 2003; Friedmann and Wolff, 1982; Fujita et al., 2001; Rees and Wackernagel, 2008) As city populations grow, infrastructural networks continue to upgrade capacity and extend further into natural systems, increasing our ability to extract natural resources, but also increasing regional interdependence (Ibisch et al., 2016; Laurance et al., 2015). The infrastructural networks that radiate from cities, serve to link environmental resources in city hinterlands to global food markets, thus playing a key role in facilitating cross-scale socioenvironmental feedbacks within the global food system (Brenner, 1999; Güneralp et al., 2013; Harvey, 1990).

Cities are also crucibles for cross-sectoral socioeconomic interactions. Socioeconomic conditions across different sectors of the economy constrain cities demand for, and capacity to produce food (Stehfest, 2014; UNEP, 2013). Socioeconomic conditions also constrain the ability of cities to trade food on regional and global markets (FAO, 2015). Trade cannot occur directly between two cities unless the socioeconomic links exist and not at all if the infrastructural links are missing (De Benedictis and Tajoli, 2011). Of course, physical infrastructural and socioeconomic networks cannot be disentangled. Strengthening of socioeconomic ties invariably leads to strengthening of infrastructural links, whilst the cost of investment in that infrastructure serves to stabilise those socioeconomic ties (Khanna, 2016).

In the following section 2, we present an overview of existing models and approaches to understand food and water security. We highlight some important knowledge gaps in these approaches that our framework aims to fill. In section 3 we present our framework in detail, outlining how we aim to capture regional and sectoral interdependencies and cross-scale feedbacks in a single framework. In section 4 we outline potential applications of a realised version of the framework. In section 5 we outline steps required to make this ambitious vision a reality.

2. Challenges to capturing the complexity of food and water security using existing models
2.1 Regional Interdependence

As the food system becomes increasingly globalised and urbanised, trade, both domestic and international, drives interdependency for food and water security among trading regions (FAO, 2015; Sartori and Schiavo, 2015). Water footprint studies have played an important role in quantifying the volume of water used in food production and embedded in traded food, known as virtual water trade (Allan, 1998; Fader et al., 2011; Hanasaki et al., 2010; Konar et al., 2016b). These studies apply hydrological models to estimate the amount of green (recently precipitated, rapidly replenished water in the upper soil layer) or blue water (slowly replenished ground and surface water resources) used in food production (Fader et al., 2011; Hoff et al., 2010). At a global scale, 84% of food production relies on green water, which has generally less negative impacts on the environment compared with blue water. In terms of internationally traded food, 16% of traded food comes from green water resources and 6% from blue water resources (Fader et al. 2011). As a result, at a global scale, international trade saves water (de Fraiture et al., 2004; Hanasaki et al., 2010; Konar et al., 2011). However, recent studies have revealed that an

increasing proportion of traded food is produced from unsustainably abstracted blue water resources (Dalin et al., 2017; Wada et al., 2012, 2010). Owing to regional interdependency of the food system, these unsustainable practices threaten the future food and water security of trading regions (Gleeson et al., 2012; Wada and Bierkens, 2014) (Fig. 2a). The increase in unsustainable water abstraction is principally owing to increased demand arising

5 from population growth, with climate change projected to exacerbate stress on food and water resources in the future (Gerten et al., 2011).

A knowledge gap in these water footprint studies is that there tends to be a focus on international bilateral trade, meaning the much larger domestic trade fluxes are often neglected (Konar et al., 2016). In the developed world, almost all food reaches consumers through trade whilst in the developing world, trade is also increasing in

10 importance as people move to cities and the numbers of people involved in subsistence agriculture decreases (Chen, 2007; IFPRI, 2017; Seto and Reenberg, 2014; United Nations, 2012). The lack of studies on domestic trade is in large part owing to the lack of data. However, increasingly there are attempts to quantify virtual water flows within countries (Fig. 2b) (Dalin et al., 2014; Dang et al., 2015) and the water footprints of cities (Hoff et al., 2014). Identifying the fine-scale networks that constrain where water resources are extracted from the

15 environment to meet remote demand is essential for managing water under globalisation. This will improve our ability to diagnose the remote drivers of water resource use and understand how local water resource use may be teleconnected with socioenvironmental change in another part of the global food system (d'Amour et al., 2016). Thus, the first knowledge gap our framework seeks to fill is to capture the fine-scale networks that constrain water resource extraction and virtual water trade.

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Figure 2. Water footprint studies.

2.2 Sectoral Interdependence

Owing to the increased mechanisation of agriculture and the development of more diverse energy sources, the

25 interdependencies among the food, water energy sectors are stronger than ever (Bazilian et al., 2011; Kraucunas et al., 2015; United Nations Water, 2015). Currently 30% of energy produced is used within the food sector, with fluctuations in energy costs having direct impacts on agriculture and thus water resources (Frieler et al., 2015). Next to this, the energy sector itself requires considerable water resources (Bijl et al., 2016). Fossil fuel extraction such as coal mining and shale gas fracking are highly water intensive, whilst biofuel production competes with

30 food production for land and water resources (Bonsch et al., 2016; Hejazi et al., 2015). Failure to capture sectoral interdependencies means we may fail to identify synergistic solutions, or worse still, policies in one sector may have unintended negative consequences in another. For example, investment in climate change mitigation measures such as biofuel production may lead to increased competition for water between the food and energy sectors and exacerbate unsustainable water use (Hejazi et al., 2015).

35 Integrated Assessment Models (IAMs) are powerful tools to explore sectoral interdependencies (Bazilian et al., 2011). Until now, IAMs have principally been focused on projecting greenhouse gas emissions, however increasingly, the agricultural sector is being captured within IAMs (Stehfest et al., 2013; Stehfest and Bouwman, 2006; Wise et al., 2009). For example, the IMAGE IAM contains an agriculture and land module which is internally coupled with an energy supply and demand module. IMAGE calculates changes in agriculture based on

40 two-way interactions between the agriculture and energy sectors (Stehfest et al., 2014). IMAGE has also been

coupled with the MAGNET agro-economic model, a Computable General Equilibrium (CGE) model that uses information from IMAGE on land availability and suitability, labour supply and technological change to estimate international food trade, demand and supply (Stehfest et al., 2013; von Lampe et al., 2014; Woltjer et al., 2014). An integrated approach has also been applied by Bonsch et al. (2016) using MAgPIE (Lotze-Campen et al., 2008), a global land and water-use allocation model, to understand the trade-off between agricultural expansion and intensification via water abstraction to meet biofuel targets. Similarly to Hejazi et al. (2015), their integrated approach showed that changes in the energy sector can lead to competition for water resources within the food sector. The MAgPIE approach also underlined the importance of capturing dynamic vegetation and hydrological processes in the same modelling framework as the two are intrinsically intertwined with changes in vegetation impacting water resources and vice versa (Fader et al., 2011; Konar et al., 2013; Lotze-Campen et al., 2008).

Although IAM approaches capture important sectoral interdependencies, they cannot provide a representation of non-linear transformative change typical of socioenvironmental systems and the dynamics associated with it (Filatova et al., 2013; Folke, 2006; Rockström et al., 2017). Incorporating these processes in IAMs would risk including too much complexity, possibly leading to a trade-off with transparency (van Vuuren et al., 2016). An alternative approach is to couple IAMs with models that capture these important processes, without changing the internal structure of IAMs. Some progress has already been made in this direction by coupling land use models with IAMs, where the IAM set regional socioeconomic constraints for the land use model. Based on these constraints, the emergent fine-scale patterns from the land use model are aggregated at the regional scale captured in the IAM. This approach has resulted in improved regional projections in IAMs as land allocation models capture important within-region heterogeneity (Hasegawa et al., 2017; Stehfest et al., 2013).

In order to model the complexity of socioenvironmental systems, it is necessary to capture dynamics such as agency, emergence, non-linearities and feedbacks (Berger, 2001; Brown et al., 2005; Farmer and Foley, 2009; Farmer and Geanakoplos, 2009; Folke, 2006; Helbing, 2013; Sivapalan et al., 2012). However, the pathway to capturing these dynamics at a global scale is not obvious (Verburg et al., 2016). For example, it is not practical from a computational or data perspective to represent farmers as agents at a global scale. Thus, the second knowledge gap our framework aims to fill is to incorporate the complex dynamics associated with socioenvironmental systems at a global scale within the IAM framework. We aim to achieve this by focusing on cities and infrastructural networks. As stated, cities are key agents of change and lie at the intersection of scales within the global food system, whilst infrastructural networks constrain our ability to extract resources from the environment and redistribute them to meet demand (Brenner, 1999; Khanna, 2016; United Nations Water, 2015). An advantage of using cities as agents is that they have a number of important features which are generalisable. Firstly, all cities, irrespective of where or when they existed, have a common utility function, which is to sustain the import of resources to maintain growth (Batty, 2008). Secondly, cities competitively interact for resources and services irrespective of whether they are in the same administrative region or not (Begg, 1999). Thirdly, the investment in infrastructure, which is a defining characteristic of cities, makes them highly path dependent (Khanna, 2016). This path dependency provides opportunities for narrowing the possibility space of future projections (Brown et al., 2005).

2.3 Cross-scale socioenvironmental feedbacks

Cross-scale socioenvironmental feedbacks describe a broad range of processes where small-scale or short-term actions bring about large-scale or long-term emergent change (Sivapalan and Blöschl, 2015). These emergent higher-level changes may feedback at the finer scale. In terms of water resources, sociohydrological studies have played an important role in helping to understand emergent water use patterns by capturing cross-scale socioenvironmental feedbacks (Di Baldassarre et al., 2013b, 2013a; Montanari et al., 2013; Sivapalan et al., 2012; Troy et al., 2015). They have done so by explicitly considering bi-directional feedbacks between humans and the environment in hydrological basins. An example of emergent dynamics is a "pendulum swing", in communities that have alternated between water extraction for agriculture in the early stages of development, followed by subsequent efforts to mitigate or reverse the consequent degradation of the riparian ecosystems (Kandasamy et al., 2014; Liu et al., 2014). This has been explained by counteracting productive and restorative forces, mediated via technology, environmental awareness and the intervention of governance institutions (Elshafei et al., 2015; Liu et al., 2015; van Emmerik et al., 2014).

However, sociohydrological studies maintain a disciplinary focus on water, failing to capture important sectoral interdependencies as IAMs do (Troy et al., 2015). Equally, they have so far assumed the systems of concern are isolated entities in space, e.g., an agricultural river basin, whereas in a globalised world, many different such entities may be linked through trade as demonstrated in water footprint studies (Konar et al., 2016a). Capturing linkages to regional and global markets is critical to understanding cross-scale feedbacks, because the more connected water resources are to markets via trade, the more sensitive they are to cross-scale feedbacks (Eakin et al., 2009; Pande and Sivapalan, 2016). For example, the 2010 drought in Russia and Kazakhstan led to a spike in the price of wheat on global markets (Nelson et al., 2014). Food producers in other wheat producing regions of the world that were well connected to global markets via physical and socioeconomic trade links were impacted by this price rise as they could sell their products to global markets at increased profit. Thus, environmental change in Russia impacted global markets which drove local water resource use in other parts of the world. There has been a recognition of the important role trade plays in facilitating cross-scale feedbacks in literature related to land use change (Geist and Lambin, 2002; Lambin and Geist, 2008). These studies have highlighted that distant market demand drives local land use change and in order to predict land use change we need to model land as an open system with flows of resources coming in and out (Lambin and Meyfroidt, 2011). However, modelling of these issues in relation to water resources is still in its infancy (Konar et al., 2016a). Thus, the third challenge is to capture the crucial role of trade networks in facilitating cross-scale feedbacks between local water resources and regional and global markets.

3. Modelling Framework

3.1 The City Agent

3.1.1 City agent attributes

The core structure of our framework is a multi-agent network of city nodes and trade links (Fig. 3). In our framework, cities are agents and comprise of an urban area and associated hinterland. City agents sit at the intersection of scales between ecohydrological resources in their hinterlands and global markets via radiating trade networks. The ecohydrological conditions in hinterlands of city agents are determined from a coupled hydrological-vegetation model for natural and managed land. Socioeconomic conditions in the hinterlands of cities are determined from an IAM and CGE. Socioeconomic conditions constrain agent's ability to exploit

environmental conditions within their hinterland for food production. City agents have a common utility function: to satisfy local and market demand for food, which in turn leads to emergent water use. City agents satisfy demand via food production and trade. How each city satisfies demand differs based on the heterogeneous socioeconomic and environmental conditions in their hinterland and the socioeconomic and infrastructural networks that link

5 them. The fine-scale interactions among cities and their environment bring about higher-level emergent patterns which provide input conditions for the next simulation step of the IAM and CGE.

Figure 3. City agent attributes

10 **3.1.2 The city and its hinterland**

Each city agent has an associated hinterland. The definition of a hinterland varies in literature but depends upon resource demand in the city and on the ease of transportation between the city and the resource production area, which is determined by geographic, infrastructural and socioeconomic factors (Billen et al., 2009). To capture these elements, we define city hinterlands based on the hierarchical overlay of supra-sub national administrative

15 borders and Thiessen polygon operation among cities based on the gravity equation of trade with mass equal to demand and distance equal to the cost-distance of trade via road, rail and inland water ways (Fig. 4) (Berthelon and Freund, 2008; Chaney, 2013). We base hinterlands on administrative borders so that the framework can capture the impact of heterogeneous policy or socioeconomic conditions at the administrative scale. For many cities, and depending on the food commodity, the effective hinterland will extend beyond these contiguous

20 administrative regions (Billen et al., 2009; Güneralp et al., 2013). However, policy is applied at the scale of these administrative boundaries and cities operate within these policy constraints. If policies stimulate free trade between administrative regions, then the effective hinterland of a city can expand (Knox and McCarthy, 2012). Therefore, the framework allows for the exploration of the impact of policy at different scales on food and water use and virtual water flows. By also basing the size of hinterlands on the cost-distance of trade via road, rail and

25 shipping, we capture the key role that infrastructural networks play in linking demand in cities with environmental resources.

Hinterlands vary in terms of size and composition. The hinterland of a city in Western Australia will be large, with a high proportion of natural landcover and low population density, whilst a hinterland in Eastern China will be smaller with a high proportion of agricultural and urban landcover and high population density. From a

30 socioeconomic perspective, per capita demand will differ among hinterlands based on diet, affluence etc. derived from the IAM. Equally, the agricultural intensification potential of a hinterland in the Netherlands will be greater compared with a sub-Saharan African region owing to factors such as mechanisation of agriculture, access to fertilizers etc. (Stehfest et al., 2014).

35 **Figure 4. The city and its hinterland**

3.2 Food production and water use

Within our framework, city agent food production decisions are constrained by ecohydrological conditions within their hinterlands. To capture ecohydrological conditions, we recommend tight coupling between a dynamic vegetation model (DGVM) such as Lund-Potsdam-Jena managed Land (LPJ-ML) model and a complex

40 hydrological model such as PC Raster Global Water Balance (PCR-GLOBWB) model (Bierkens and van Beek.,

2009; Bondeau et al., 2007) (Fig. 3). In this way, the model would capture the two way water fluxes between vegetation and water in the soil layer and infiltration to the groundwater reservoir, which is key for computing groundwater recharge rates (Hanasaki et al., 2008b). This is a considerable modelling challenge. Vegetative water demand and rooting depths from the DGVM would need to be sent to the hydrological model. Using the detailed

5   soil water profile from the hydrological model, an improved estimate of water availability could be estimated. If water supply is lower than demand from the DGVM, then vegetation growth will be limited due to soil water stress. If water supply is higher than demand from the DGVM, then water infiltrates into the groundwater reservoir in the hydrological model. Each city hinterland has a potential yield and associated water resource usage based on these ecohydrological constraints.

10   Socioeconomic constraints on food production are taken from the IAM based on factors such as the mechanisation of agriculture, access to fertilizers etc. The demand for each food commodity in a city and its hinterland is equal to (per capita demand taken from IAM * population), with population based on spatially explicit grid-scale population estimates (Brinkhoff, 2016; Klein Goldewijk et al., 2011; Stehfest, 2014; UN Population Division, 2015). Cities and their hinterland are either in surplus or deficit for a crop type based on

15   (local production – local demand) (Dermody et al., 2014). Cities with predominantly urbanised hinterlands will have a net demand for food resources whilst others, with large areas of agriculture within their hinterlands, will have a net surplus in food resources. Demand is also based on trade demand calculated in the trade component of the framework (Section 3.3).

Cities adapt to changes in food demand through agricultural expansion/contraction, (de)intensification

20   or trade. Agricultural expansion and intensification potential are estimated using land use algorithms. The algorithms used to calculate agricultural expansion and intensification potential in IAMs such as IMAGE may be extended to include detailed infrastructural data as well as more complex hydrology in determining agricultural suitability (Barber et al., 2014; Wada et al., 2012; Walker et al., 2013). In our framework, cities with increasing demand, low (high) agricultural intensity potential and high (low) expansion potential are likely to expand

25   (intensify) agriculture (Fig. 5). Cities that are constrained from expanding or intensifying agriculture will increase imports to sustain growth. The agent decision process generates land-use maps that are prescribed to the ecohydrological model (Biemans et al., 2013; Wada et al., 2012).

The method for capturing food production outlined, blends macroscale interdependencies between the agricultural and energy sector with small-scale ecohydrological and demographic conditions to estimate land use

30   change, similar to the approach by Hasegawa et al. (2017) and Verstegen et al. (2016). Importantly, our approach also captures how market demand is transmitted heterogeneously within a region or country via infrastructural networks (see section 3.3 for more details). This is a critical step in understanding the critical role infrastructural networks play in determining water resource extraction and virtual water trade patterns (Konar et al., 2016a; Lambin and Meyfroidt, 2011).

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Figure 5. Food production decisions.

3.3 Virtual Water Trade

The trade network that links city agents is hierarchical. The network comprises a lower-level physical

40   infrastructural network and an upper-level network with link weights reflecting bilateral socioeconomic trade

links (Fig. 6). The lower level of the trade network is defined by physical trade infrastructure of roads, rail and shipping lanes (Berthelon and Freund, 2008; Karpiarz et al., 2014; Limão and Venables, 2001). The data required to build this network, such as open street maps and database of cargo ship movements, is openly available (Brinkhoff, 2016; Haklay and Weber, 2008; Kaluza et al., 2010). In a realised version of the framework, each edge of the lower-level network has a different transport cost. For example, the cost of bulk trade is approximately 7-times less by ship than by road (Limão and Venables, 2001). In addition, intermodal transport costs are applied for transferring goods between transport modes (Janic, 2007). Infrastructure development can be projected using infrastructure growth algorithms or manually added to explore the impacts of prospective plans such as the new trans-Eurasian Silk Road Economic Belt on virtual water trade and water use (Ahmed et al., 2013; Arima et al., 2008; Brugier, 2014; Walker et al., 2013). Because the infrastructural network constrains where resources can be extracted from the environment and redistributed to meet demand, all resource flows travel via the lower level physical infrastructural network in a realised version of the model framework (Barber et al., 2014; Khanna, 2016). The upper level network consists of bilateral trade links among countries. Edge weights among countries are calculated using a CGE model. CGEs are constrained with historical data on bilateral trade balances, competitiveness (relative price developments) and trade policies to estimate trade patterns (Hertel et al., 2007; Hertel and Hertel, 1997; Woltjer et al., 2014). If the CGE simulates high trade volumes between two countries, then the edge weight between those countries in our framework will reflect a high probability of bilateral trade.

Figure 6. Virtual Water Trade Network.

In a realised version of the framework, the food produced in the hinterland of cities is either consumed locally or exported to meet market demand. Cities with a demand, import from cities with a surplus based on the cost-distance among cities (Berthelon and Freund, 2008). Thus, the probability of trade among cities decays with increasing cost-distance (Karpiarz et al., 2014; Limão and Venables, 2001). City agents within the same country trade with one another based solely on supply and demand for each food commodity and the cost-distance of trade among cities. Cities in different countries are also constrained by bilateral trade probabilities of the upper-level network (Fig. 6). For example, the probability of trade between Japan and American cities will be determined by the upper level network based on CGE output. However, it is more likely that the demand will be met from hinterlands on the West Coast of the United States owing to the lower cost-distance of trade. The emergent trade patterns are aggregated at the country and region scale of the CGE and fed back into it for the next simulation year. Because city agent trade decisions are stochastic, it allows for alternate emergent trade patterns within the constraints of the same network. Thus, for given constraints there will be a range of possible solutions. The stronger (weaker) the constraints the narrower (wider) the solution space. In this way, the solution space for given environmental, socioeconomic and infrastructural constraints can be explored (An, 2012). Equally, if conditions change at the small scale, this will result in alternative emergent patterns at the large scale (Fig. 7b). In this way, agency, cross-scale processes, socioeconomic, environmental and infrastructural constraints are married with conventional general equilibrium modelling approaches. This is a novel and potentially important step in capturing non-equilibrium dynamics within pre-existing equilibrium modelling approaches (Farmer and Geanakoplos, 2009). It also allows us to begin to uncover the important role of cross-scale feedbacks in linking local water resource change to the dynamics of regional or global markets (Konar et al., 2016a).

Figure 7. Modelling Framework Workflow.

4. Applications of the framework

The framework is designed to be used with IAMs and CGEs, which are influential decision tools but are unable to capture non-linear, emergent change typical of socioenvironmental systems (Rockström et al., 2017; van Vuuren et al., 2016; Verburg et al. 2016). Our approach does not require IAMs or CGEs to be re-engineered, but rather simulates complex socioenvironmental processes within the constraints exogenously applied those models. The emergent patterns may be aggregated at the scale of IAMs and CGEs and used as input conditions for the next simulation step of those models. In this way, the framework blends bottom-up processes captured by the multi-agent network of cities with the top-down approach captured by pre-existing IAMs and CGEs. Thus, a realised version of the framework has the potential to illuminate how the higher-level patterns demonstrated in IAMs and CGEs emerge. In terms of informing policy, this is an important step as it allows policy makers to explore the impacts of policy changes at the different spatial and temporal scales at which policy is applied. In doing so, models based on the framework can help illuminate roadmaps, considering complex dynamics, to reach regional and long-term goals outlined in IAMs (Rockström et al., 2017). For example, it allows the exploration of how scenarios, such as the recently published Shared Socioeconomic Pathway (SSP), which outlines future environmental change according to different socioeconomic development storylines (O'Neill et al., 2015), can be implemented at finer scales and taking account of sectoral and regional interdependencies and cross-scale feedbacks. This can be a potentially important step in extending the usefulness of IAMs and CGEs whilst avoiding adding unwanted complexity to those models (van Vuuren et al., 2016).

The multi-agent network of cities at the core of the framework enables the exploration of the emergent solution space for realizing food and water security requirements based on socioeconomic and environmental constraints. The emergent solution space illuminates how constrained regions or sectors are based on socioeconomic, environmental and infrastructural factors to transition to sustainable and secure water use pathways (Brown et al., 2005; Garud et al., 2010). Those regions or sectors that are locked into unsustainable or vulnerable water use pathways should be prioritised for intervention (Fig. 8) (Liebowitz and Margolis, 1995; Romero-Lankao et al., 2017; Sophocleous, 2012). Within the solution space, sustainable and secure development pathways can be explored. A common approach for exploring multi-dimensional solution space is to use optimality algorithms (Dermody et al., 2011; Konak et al., 2006; Vrugt et al., 2003). Multi-objective optimality algorithms can be used to explore synergistically sustainable solutions across regions, sectors and scales. Such synergistic approaches are key to addressing the challenges set out in the UN Sustainable Development Goals (Costanza et al., 2016; Lu et al., 2015). Thus, the model can be used to inform policies that are sustainable in the administrative region, the economic sector and the scale at which those policies are applied as well as interdependent regions, sectors and scales.

Figure 8. The solution space illustrates how constrained regions or sectors are along their current water use pathway.

Given the importance of cross-scale feedbacks for understanding local water use, it is essential that smaller scale studies on food and water security can be linked with regional-global scale models (Pande and Sivapalan, 2016; Sivapalan and Blöschl, 2015; Verburg and Overmars, 2009). The model framework presented can be used to understand how detailed changes within a city or catchment link to large-scale market or hydrological changes. Thus, models built according to our framework can contribute to, and benefit from, the rapid growth of within-city studies such as studies of urban metabolism studies or sociohydrological studies which focus on the catchment scale (Broto et al., 2012; Liu et al., 2014; van Emmerik et al., 2014; Zhang, 2013). In the case of urban metabolism studies, detailed analysis is done of resources flows into and out of a city. Models based on our framework can illustrate how urban resource flows are teleconnected with environmental change in other parts of the globe. Equally, urban resource budgets can be used to test model performance. In the case of sociohydrological studies, the framework outlined can help illustrate how small-scale changes across multiple catchments can lead to emergent market changes, which in turn feedback on water use within a single catchment.

5. Summary and recommendations

The complex and interdependent nature of food and water security within our globalised and urbanised world requires new models and approaches to inform policy makers. Models built using the framework outlined are ideally suited to informing policy on so-called "wicked problems" associated with water resource use such as regional and sectoral interdependencies and cross-scale feedbacks (Dentoni et al., 2012; Duit and Galaz, 2008; Lach et al., 2005). It is our conviction that models built according to the framework outlined will represent a new wave of decision tools that can help policy makers navigate the complexity of socioenvironmental interactions within our globalised world.

IAMs and hydrological models provide the groundwork for the proposed framework. However, extra efforts are required to achieve an operational model based on the framework presented. The main step required is the construction of a multi-agent network of city nodes and infrastructural links. A multi-agent network of city nodes and infrastructural links will provide a platform for a wide range of research questions on environmental change. The resources required to build this network are openly available but need to be translated to a scalable and flexible network architecture. A summary description of a generalised framework for a multi-agent network of cities and infrastructural links is presented in Table 1.

Table 1. Description of generalised framework of a multi-agent network of city nodes and infrastructural links.

The structure of this network should be designed in collaboration with scientists from different disciplines to ensure the relevant elements are incorporated to meet a range of research questions. To facilitate collaboration in building such a multi-agent network, there is a need for interdisciplinary dialogue and collaboration. Indeed, this is essential for achieving the Sustainable Development Goals which present interdependent challenges across disciplines (Costanza et al., 2016; Lu et al., 2015). In our experience, the theories and methods associated with complex systems science provide an ideal approach for tackling interdisciplinary sustainability challenges (Liu et al., 2015). Complexity is not just a suite of theories and methods, it delivers an

intuitive way of understanding interdependent systems and provides a platform for deep interdisciplinarity collaboration that is required to meet today's sustainability challenges.

Competing interests. The authors declare that they have no conflict of interest.

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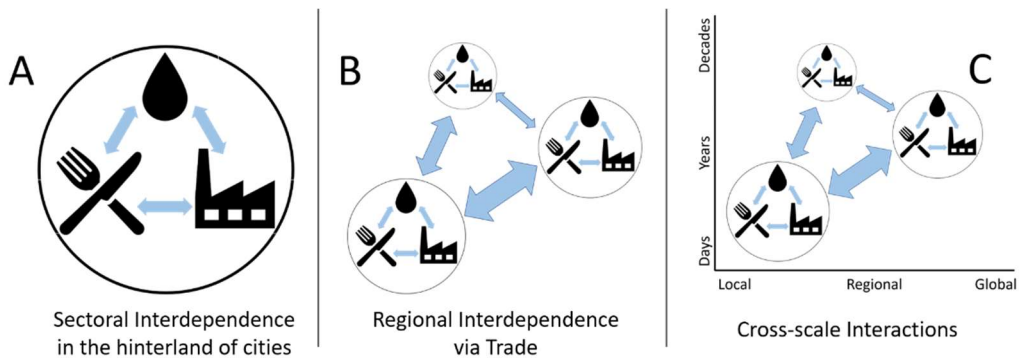
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Figure 1. Complex dynamics within the global food system that lead to emergent water use patterns. (A) Sectoral interdependence in water resources within the food-water-energy nexus **(B)** Regional interdependence in water resources owing to the importance of trade for food security **(C)** Cross-scale feedbacks whereby fine-scale interactions bring about emergent higher-level change. Higher-level, emergent changes may feed back at the fine scale (Sivapalan and Bloschl, 2016).

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Figure 2. Water footprint studies. Water footprint studies exploit hydrological models to estimate blue and green water use in agriculture. This data is combined with data on food trade to estimate the fluxes of virtual water embedded in food trade. **A)** The unsustainable water footprint of agriculture is shown in red, where groundwater abstraction exceeds aquifer recharge (*taken from* Wada and Bierkens, 2014). **B)** Virtual water flows within the United States. States are ranked according to the total trade volume and plotted clockwise in descending order. The size of the outer bar indicates the total virtual water trade volume of each State as a percentage of total U.S. trade. Destination volume is indicated with links emanating from the outer bar of the same colour. Origin volume is indicated with a white area separating the outer bar from links of a different colour (*taken from* Dang et al., 2015).
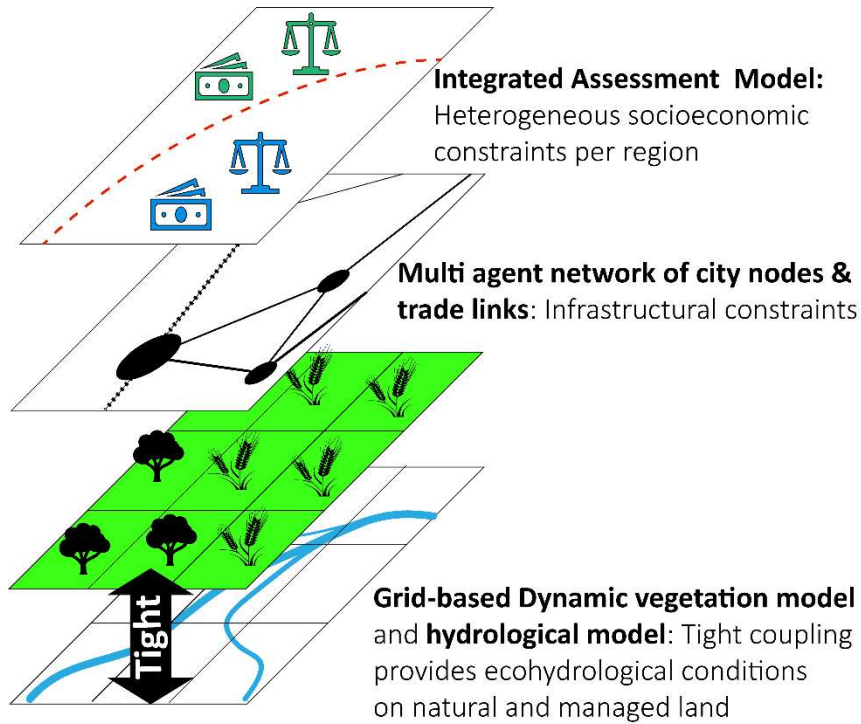
Figure 3. City agent attributes. In our framework, city agents receive ecohydrological conditions from a tight coupling between a dynamic vegetation model and hydrological model. They receive socioeconomic constraint information from an Integrated Assessment Model. Ecohydrological conditions on natural and managed land determine food production potential and associated water use. The IAM captures heterogeneous socioeconomic conditions that constrain the ability of cities to exploit ecohydrological conditions for food production. At the time of writing, to our knowledge, a tight coupling between a dynamic vegetation model and a complex hydrological model has yet to be implemented.
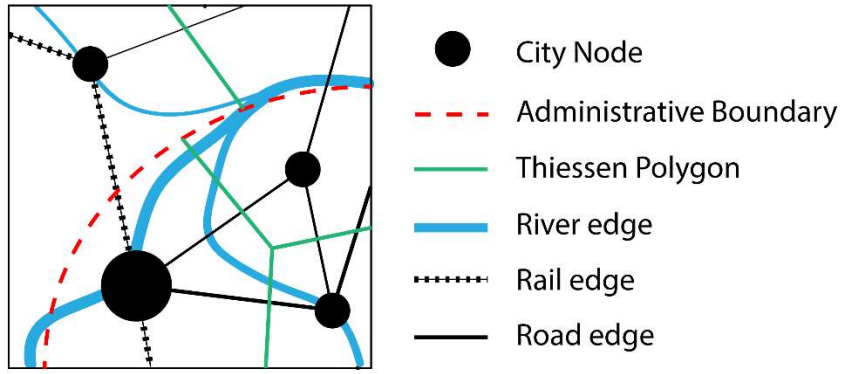
Figure 4. The city and its hinterland. City agent hinterlands are defined by a hierarchical overlay of supra-sub-national administrative boundaries and Thiessen interpolation among city nodes based on the gravity equation of trade. Cities are linked by physical infrastructural network where edges represent the cost-distance of trade via roads, rail and shipping routes.
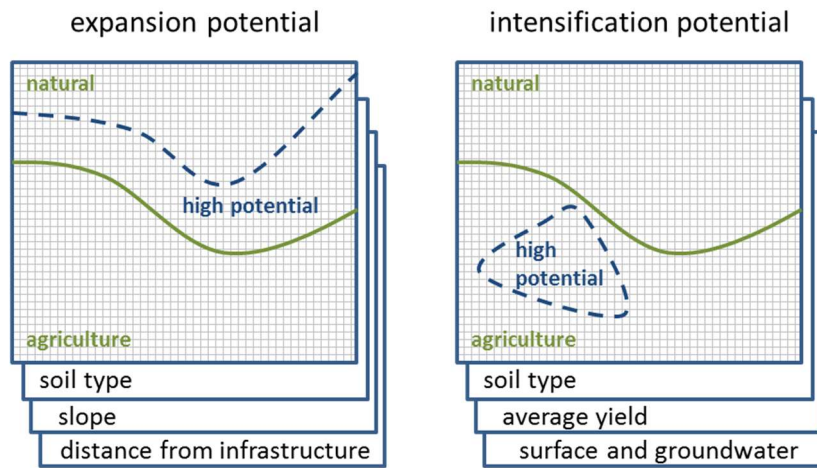
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Figure 5. Food production decisions. City agents decide on agricultural expansion (left side) or intensification (right side) based on demand and spatially explicit crop production potential in their hinterlands.
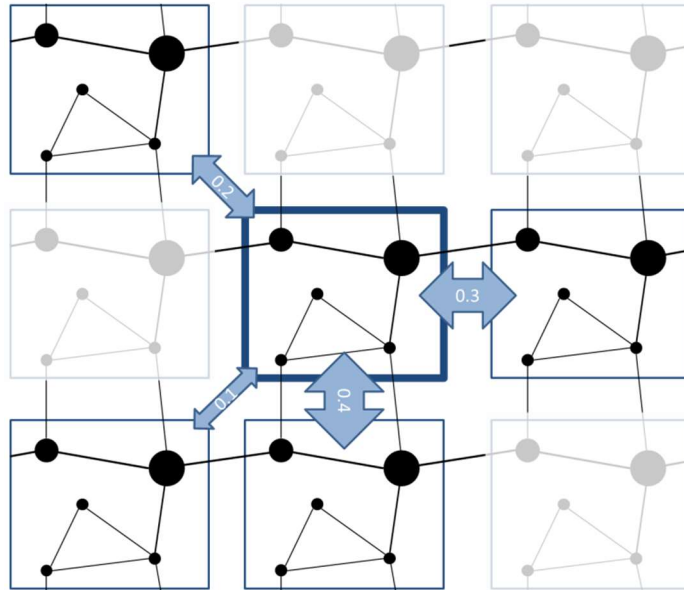
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Figure 6. Virtual Water Trade Network. The trade network is hierarchical, containing an upper-level network with edge weights capturing the probability of trade among countries. The link weights of the upper level network are calculated using a CGE model based on factors such as historical trade patterns, trade agreements etc. The lower level network comprises an infrastructural network of roads, raid and shipping routes. Edge weights capture the cost distance of trade via roads, rail and shipping. Because the infrastructural network constrains where resources can be extracted from the environment and redistributed to meet demand, all resource flows travel via the lower level physical infrastructural network in a realised version of the model framework
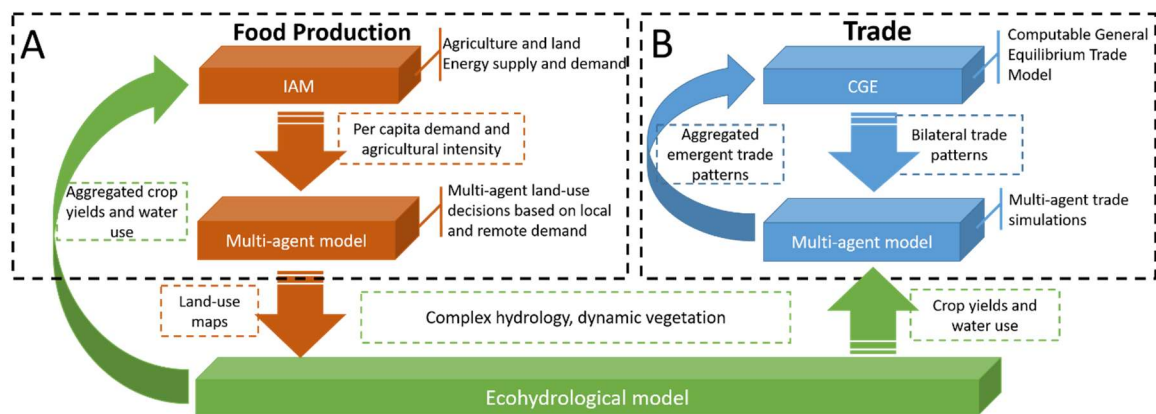
Figure 7. Modelling Framework Workflow. The multi-agent network sits at the interface between the IAM and an ecohydrological model **(A)** The IAM, calculates per capita food demand at a regional scale, which is converted into spatially explicit demand using population maps. The IAM also calculates agricultural intensity constraints. Based on these constraints and demand, agents make food production decisions which change ecohydrological conditions in their catchment. The emergent crop production and water use patterns are aggregated and feedback to the IAM **(B)** A CGE trade model coupled to the IAM provides edge weights for the upper level trade network. Virtual Water Trade among cities is calculated based on supply and demand and cost-distance of trade via the infrastructural trade network. The emergent aggregated trade patterns feedback to the CGE as input for the next simulation year.
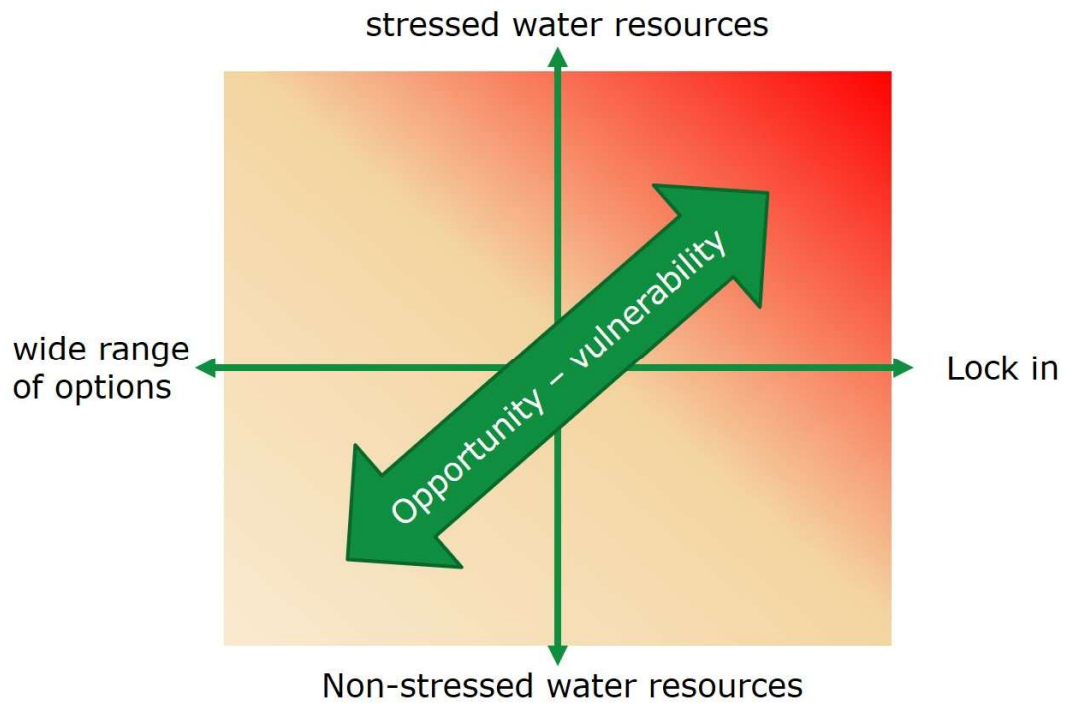
Figure 8. The solution space illustrates how constrained regions or sectors are along their current water use pathway. The solution space emerges from the multi-agent simulations and illuminates how locked-in regions or sectors are along their current water use pathway. The solution space can be explored using optimality algorithms to find pathways towards sustainable water futures, whilst taking account of regional and sectoral interdependencies and cross-scale feedbacks.

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Table 1. Description of generalised framework for a multi-agent network of city nodes and infrastructural links. The description follows the ODD +D Protocol (Müller et al., 2013) for describing agent-based models.

Overview	**1.1 Purpose** A multi-agent network of cities and infrastructural links will provide a platform for a wide range of research questions related to global environmental change. The framework is designed to be coupled with IAMs, CGEs and grid-based environmental models. The framework enables the simulation of regional and sectoral interdependencies and cross-scale feedbacks within the constraints provided by these models.
	1.2 State variables and Scales The multi-agent network consists of 1 type of agent, the city. City agents interact with the environment within their own hinterland and with other city agents by trading resources via the infrastructure network. Each agent has a geographic node location which is linked to a hinterland polygon from which agent attributes are derived. The distance among agents is based on the cost distance of trade via the infrastructural network. The network is scalable depending on the detail of analysis. The scaling is based on infrastructure hierarchies and population. For example, at a global scale, only freeway roads are captured and cities below a certain population threshold are aggregated into larger city nodes.
	1.3 Process Overview and Scheduling Each year, cities receive socioeconomic constraint information from an IAM. Cities have a certain resource demand based on their internal demand and demand from other cities in the network. Cities make resource use decisions based on demand, socioeconomic constraints and environmental conditions in their hinterland. The output of the multi-agent model may be aggregated at the scale of IAMs or CGEs and used as input for the next iteration of those models.
Design Concepts	**2.1 Theoretical and empirical background** The model is built to test the hypothesis that socioenvironmental interactions across regions, sectors and scales are mediated by cities and physical trade infrastructure that link environmental resources with socioeconomic demand.
	2.2 Individual Decision making The decision model is based on the generalisable theory that cities competitively interact for environmental resources to sustain growth. City agent decisions are individual but socioeconomic constraints on decision-making may be applied at a higher level, e.g. state level.
	2.3 Learning Optimisation algorithms may be applied to explore solution space within exogenously applied socioeconomic and environmental constraints.
	2.4 Individual Sensing City agents sense exogenous socioeconomic constraint information from an IAM. City agents sense exogenous environmental conditions from an environmental model. Cities sense endogenous resource demand from other agents.
	2.5 Individual Prediction Agents perceive temporal changes in resource demand.
	2.6 Interaction Interactions among agents are determined by each agent's surplus or deficit for a resource and the cost distance among agents in the network.
	2.7 Collectives Agents do not belong to collectives.
	2.8 Heterogeneity Agent attributes are heterogeneous and based upon socioeconomic constraint information, environmental conditions and population within their hinterland. The local topology of the infrastructure trade network is also heterogeneous among agents.
	2.9 Stochasticity Socioeconomic constraint information is applied as probability distributions, meaning agent decisions are stochastic and based on these probability distributions. Agent-Agent trade decisions are stochastic and based on supply and demand and the cost distance between agents in the infrastructure network. The probability of trade decreases with increasing cost distance, assuming uniform supply and demand.
	2.10 Observation

	Emergent agent decisions are sent to an environmental model as land-use change maps. The environmental model calculates environmental processes based on these land-use changes. The observable output is environmental change in forest cover, water resources, crop yields etc. The second observable output is resource consumption. Emergent resource consumption of agents is aggregated at a scale relevant for IAMs, e.g. the regional scale. The third observable output are trade patterns. Emergent trade patterns are aggregated at a scale relevant for CGEs, e.g. countries and regions.
Details	**3.1 Implementation** The framework is not yet implemented, and a software platform has not yet been chosen.
	3.2 Initialisation It is envisaged that a model based on the framework presented can be initialised for past conditions and run until present to test the model's performance. The model can also be run for scenarios that are implemented within the IAM framework. Because the model is stochastic, an ensemble of simulations can be run for the same socioeconomic constraint information and used to explore different pathways for given constraints.
	3.3 Input Data The input data to define city agents are the global city database and population density maps. Administrative boundaries combined with Thiessen polygon analysis are used to define hinterlands of cities. The infrastructural trade network consists of road and rail networks and shipping lanes and ports. Other infrastructure relevant for resource extraction such as energy redistribution infrastructure could also be captured with the framework.