Environmental Modelling and Software 115 (2019) 19–37

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

A coupled simulation architecture for agent-based/geohydrological modelling with NetLogo and MODFLOW

Marc Jaxa-Rozen[a], Jan H. Kwakkel[a,*], Martin Bloemendal[b,c]

[a] Faculty of Technology, Policy and Management, Delft University of Technology, Jaffalaan 5, Delft, 2628, BX, the Netherlands
[b] Faculty of Civil Engineering and Geosciences, Delft University of Technology, Stevinweg 1, 2628, CN, Delft, the Netherlands
[c] KWR Watercycle Research Institute, Groningenhaven 7, Nieuwegein, 3433, PE, the Netherlands

ARTICLE INFO

Keywords:
Agent-based modelling
Social-ecological systems
Groundwater modelling
NetLogo
MODFLOW

ABSTRACT

The modelling of social-ecological systems can provide useful insights into the interaction of social and environmental processes. However, quantitative social-ecological models should acknowledge the complexity and uncertainty of both underlying subsystems. For example, the agent-based models which are increasingly popular for groundwater studies can be made more realistic by incorporating geohydrological processes. Conversely, groundwater models can benefit from an agent-based depiction of the decision-making and feedbacks which drive groundwater exploitation. From this perspective, this work introduces a Python-based software architecture which couples the NetLogo agent-based platform with the MODFLOW/SEAWAT geohydrological modelling environment. This approach enables users to design agent-based models in NetLogo's user-friendly platform, while benefiting from the full capabilities of MODFLOW/SEAWAT. This workflow is illustrated for a simplified application of Aquifer Thermal Energy Storage (ATES).

1. Introduction

Agent-based models (ABMs) are an increasingly popular complement to conventional analytical approaches for the study of environmental problems, by allowing for the simulation of systemic outcomes which emerge from the behavior of individual entities. The bottom-up perspective offered by ABMs is especially relevant in the context of social-ecological systems (SESs), which are complex adaptive systems driven by interacting but relatively distinct social and biophysical subsystems (Ostrom, 2009). These interactions typically include time-dependent feedbacks between environmental and social variables; these feedbacks may lead to a regime shift, i.e. a persistent, significant change in the state of the coupled system (Scheffer et al., 2001), which may otherwise not arise from changes in a single subsystem. However, these interactions and their contribution to transient system behaviour may be overly simplified or left out of scope by conventional modelling approaches, such as computable equilibrium models (Filatova et al., 2016).

ABMs provide an intuitive framework for the study of SESs (Hare and Deadman, 2004). By accounting for interactions across heterogeneous decision-makers as well as interactions across system levels, they can yield insights regarding the impact of cross-system feedbacks on coupled system behaviors (Schlter et al., 2012). ABMs can similarly be combined with other paradigms: Vincenot et al. (2011) discuss the complementarities of agent-based models and System Dynamics models, in the case of systems which combine divisible and whole components - which is typical of coupled socio-environmental systems. However, regardless of the modelling paradigm used, quantitative SES models generally face a range of conceptual and technical challenges due to the complexity of the underlying systems, and the different disciplinary perspectives involved (e.g. Filatova et al., 2013; Voinov and Shugart, 2013). SES models may thus need to combine methods from social and natural sciences to properly represent the coupled dynamics of social and ecological subsystems. As described by Tavoni and Levin (2014), this interdisciplinary approach may be required to fully acknowledge the complexity of environmental and socio-economic systems, and increase the policy relevance of academic models.

To this end, different studies have focused on coupling physical models of environmental systems together with agent-based simulations of socio-economic processes (e.g. Bithell and Brasington, 2009; Kelly et al., 2013; Reeves and Zellner, 2010). Groundwater resources are a particularly relevant case for coupled agent-based/physical simulation: these resources are widely exploited and often scarcely available, and their management can involve complex interactions between heterogeneous users, making ABMs an appropriate modelling option. Furthermore, groundwater resources are often difficult to track

* Corresponding author.
E-mail addresses: m.jaxa-rozen@tudelft.nl (M. Jaxa-Rozen), j.h.kwakkel@tudelft.nl (J.H. Kwakkel), j.m.bloemendal@tudelft.nl (M. Bloemendal).

https://doi.org/10.1016/j.envsoft.2019.01.020
Received 25 January 2019; Accepted 25 January 2019
Available online 01 February 2019

Software Availability

Name of Software Netlogo-modflow
Description The software offers a way of coupling ABM developed in NetLogo with Modflow. For this, Python is used as a glue language. The presented code depends on Flowpy, and PyNetLogo and their respective dependencies.
Developer M. Jaxa-Rozen, with contributions from Jan Kwakkel, Martin Bloemendal and the Flowpy developers
Source language Python
Supported systems windows (other os require updating the reference to the executable of Modflow)
License BSD 3 clause

and monitor in the subsurface. Numerical modelling can therefore provide useful insights for their management.

However, coupled agent-based/groundwater models may present particular challenges due to the long time scales and model runtimes which are typically involved. Castilla-Rho et al. (2015) describe four issues with conventional approaches for the coupled modelling of such groundwater systems: the limitations of simplified lumped models, the technical complexity introduced by the use of linked software packages and data-exchange libraries, a lack of flexibility in developing scenarios, and the impracticality of performing sensitivity analysis on separate models. To address these limitations, they introduce an interactive environment which directly implements groundwater flow equations in the popular NetLogo agent-based platform. Given an ongoing trend towards increasingly complicated agent-based models of human-environmental systems (Sun et al., 2016), which correspondingly become more difficult to design, this has the advantage of providing a user-friendly environment for the design and use of agent-based groundwater management models.

Nonetheless, this NetLogo-based approach still has drawbacks for those groundwater management problems where geohydrological models are already available and could be directly reused, or where detailed geohydrological modelling is required. This includes problems related to aquifer pollution, in which the transport of contaminants plays a role, or studies in which groundwater conditions are subject to significant changes in salinity or temperature - for example due to coastal saltwater intrusion or energy storage, which are complex coupled processes of flow in porous media, chemical reactions, transport and/or heat transfer.

To address this gap, this paper introduces a simple coupled simulation architecture which can be used to connect the NetLogo platform with the MODFLOW/SEAWAT geohydrological simulation packages, using the Python object-oriented language. This approach retains NetLogo's simplicity while allowing users to account for complex hydrological processes, or to directly interface the agent-based model with existing MODFLOW/SEAWAT models. Furthermore, the issues raised by Castilla-Rho et al. in relation to scenario design and sensitivity analysis are addressed by relying on existing Python libraries, to establish an easily repeatable workflow for the analysis of coupled agent-based/geohydrological models.

Section 2 follows this introduction by describing Aquifer Thermal Energy Storage (ATES) as an example of a social-ecological system which requires detailed geohydrological modelling, motivating the development of an appropriate simulation architecture. This is then placed in the context of recent work related to the coupled agent-based simulation of social-ecological systems. Section 3 introduces the different software platforms used in this work; section 4 then describes the object-oriented architecture which is used to couple NetLogo and MODFLOW/SEAWAT. This architecture is applied in section 5 for a simplified case study of Aquifer Thermal Energy Storage. Section 6 summarizes the paper, along with recommendations for further work.

2. Background

2.1. Aquifer Thermal Energy Storage as a social-ecological system

ATES systems are used to seasonally store thermal energy in aquifers, which - in combination with a heat pump - can significantly reduce the energy demand of buildings for heating and cooling in temperate climates. These systems involve at least one pair of coupled wells, which inject and extract groundwater at different locations or depths of the aquifer; in winter conditions, relatively warmer water is thus extracted from one well and passed through a heat exchanger for heating, then re-injected into a cold well at a lower temperature (typically 5–10C). Conversely, in summer conditions, the flow across the wells is reversed - so that the cooler water injected in winter is used for cooling, then reinjected into the warm well at a temperature of 15–25C. This process is illustrated on the left of Fig. 1. This eventually creates thermal zones around each well, which can have a radius of a few dozen meters (shown in plan view for a typical urban layout on the right of Fig. 1).

The properties of these thermal zones are crucial for the performance and management of ATES systems. They are affected by local geohydrological conditions, such as the porosity of the aquifer or the

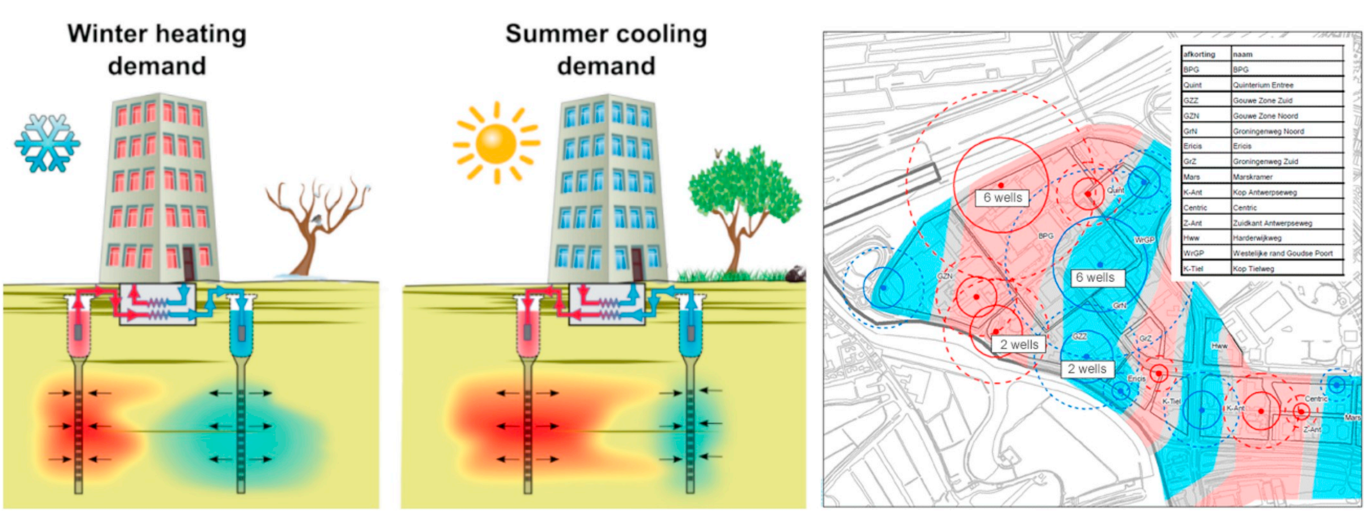

Fig. 1. Basic ATES operation (left); ATES thermal zones (right) (Bonte, 2013).

presence of a regional groundwater flow; thermal interferences between neighbouring systems can also reduce thermal recovery if cold and warm wells are located too closely, while wells of similar temperatures can have beneficial interactions by reducing dissipation from the stored thermal volumes to the ambient medium. These geohydrological and operational factors cause significant uncertainties regarding subsurface conditions and the resulting performance of ATES systems. Furthermore, at the building level, the demand for heating or cooling is difficult to forecast due to variations in building occupancy, weather conditions, or long-term changes in climate. The actual operation of ATES systems (and their associated use of subsurface space) can therefore differ significantly from the expected conditions which are used for permitting and design. For example, although the cold and warm wells would ideally be used symmetrically over the seasons for cooling and heating, ATES systems often have a significant level of thermal imbalance in practice.

Given that local temperature disturbances can persist in the subsurface over a period of decades, these geohydrological and operational variations can cause unforeseen long-term changes in aquifer temperature distributions - which, in turn, can affect the performance of ATES systems, and eventually their continued adoption by building owners. The use of the subsurface for thermal storage can essentially be perceived as a common-pool resource (CPR) problem, due to the subtractable yield of subsurface storage and to the relatively difficult exclusion of potential users (in the absence of appropriate institutional arrangements). As such, some of the problems facing ATES development and planning - e.g. the layout of systems in dense urban areas, or thermal imbalances and interferences - can be related to generic CPR issues such as crowding effects and resource overuse (Kunneke and Finger, 2009). This makes ATES particularly relevant as a case for coupled agent-based/geohydrological simulation: technology adoption dynamics and CPR management are classic applications for agent-based modelling, while the complexity of the underlying subsurface processes requires a full-featured geohydrological simulation approach.

2.2. Coupled agent-based models for social-ecological simulation

As a complement to analytical methods and empirical studies, the ability of agent-based models to link individual decision processes with aggregate system outcomes has made them increasingly relevant for the study of SESs (Janssen, 2006). These systems are complex and uncertain, and involve extensive feedbacks between social and environmental changes - factors which may not be fully recognized by traditional methods used in policy analysis (Schlter et al., 2012). By representing different hypotheses related to social and economic decision processes within environmental models, agent-based simulation can be used to explore SES dynamics and contribute to the design of appropriate policies. This may for instance foster a more participative approach to policymaking by providing clear assumptions about user behavior (Matthews et al., 2007). An (2012) extensively reviews decision models for agent-based models of social-ecological systems, covering microeconomic, psychosocial, institutional, participatory and heuristic approaches. Existing frameworks for the study of SESs, such as the IAD and SES frameworks, can also be applied to the conceptualization of agent-based models (Ghorbani, 2013).

CPR problems have been a core application of agent-based models of SESs. The institutional arrangements which are used for the management or self-governance of CPRs involve relationships between multiple system levels, at different temporal and spatial scales - which makes agent-based models a useful tool for their study (Janssen and Ostrom, 2006). As such, Deadman et al. (2000) and Jager et al. (2000) considered the influence of individual decision-making heuristics on collective outcomes in CPR experiments. Other authors have focused on specific case studies, notably in the field of agricultural water management (Becu et al., 2003; Berger, 2001; Schlter and Pahl-Wostl, 2007).

The agent-based modelling of social-ecological systems can benefit from an accurate representation of environmental dynamics using specialized physical models, but this integration entails additional challenges for modellers. Matthews et al. (2005) review different approaches and challenges for the development of such coupled agent-based models; from a technical perspective, a potential drawback is the complexity of the resulting architecture, making the models more difficult to test and interpret. Similarly, the design of appropriate interfaces and data exchange processes can lead to an overly complex and impractical software architecture.

More fundamentally, addressing different temporal and spatial scales in the social and environmental components is likely to be a key challenge for coupled models. The choice of spatial scale can on its own significantly affect the behavior of a SES model: larger scales may for instance reduce the relative importance of local interactions and heterogeneity across agents (Gotts and Polhill, 2010). Furthermore, while reconciling spatial and temporal scales across models may be a relatively simple technical issue, it may be more difficult to meaningfully exchange information across models designed for different purposes and scales (Voinov and Shugart, 2013). This can for instance involve aggregating lower-level results (in space or time), at the risk of ignoring important feedbacks. A starting point towards addressing this challenge may be to design models with enough flexibility to test the implications of different choices of scale on the coupled system's behavior.

From this perspective, Bithell and Brasington (2009) recommend a stepwise approach for the development of coupled SES models, with additional detail being added as necessary to describe critical processes. Examples of this approach include Bithell and Brasington (2009)'s coupling of an agent-based decision model, an individual-based forestry model, and a spatially explicit hydrological model, to study spatial dynamics in subsistence farming. Similarly, Reeves and Zellner (2010) coupled a groundwater model with an agent-based layer for the study of land-use changes in Michigan, although this approach only included unidirectional communication between the model components.

While these coupled modelling methods can help capture the complex behaviors of social-ecological systems, the use and interpretation of the models should acknowledge the uncertainties which are present at different levels of the system. On a technical level, model runtimes, large parameter spaces and interactions between components can make it difficult to perform sensitivity analysis on coupled models. This may affect the practical usefulness of the models for decision support or policy analysis, and ultimately their credibility (Saltelli and Annoni, 2010).

Modellers should also acknowledge the fundamentally unpredictable nature of complex adaptive systems. For instance, a typical groundwater management problem will include conventional probabilistic uncertainties such as aquifer heterogeneity, which can be modelled using geostatistical methods, then assessed with a sensitivity analysis. However, the behavior of the coupled system will also be driven by deep uncertainties (i.e. uncertainties for which probability distributions or structural relationships are unknown; Lempert et al., 2003), which are not amenable to a probabilistic treatment. These include exogenous drivers such as long-term climate conditions, or structural assumptions about decision-making in the social subsystem - which can ultimately produce significantly different emergent outcomes from equally justifiable assumptions. These uncertainties imply that the models would be invalid for predictive purposes, so that their use for decision-making requires a different approach.

Under such conditions, exploratory modelling (e.g. Bankes et al., 2013) can help understand the behavior of the coupled system by using the models for computational experiments, for instance by generating a wide ensemble of plausible models to assess the effect of different uncertainties and modelling assumptions. By representing a broad set of hypotheses about parameters or relationships, exploratory modelling can help identify counterintuitive outcomes, as well as key sensitivities which may usefully guide the collection of empirical data. Furthermore, techniques for scenario discovery can be used as a complement to sensitivity analysis to explore the conditions under which a system may present a specific behavior - for instance, to identify assumptions which would lead to the failure of a simulated policy (Bryant and Lempert, 2010). This approach can contribute to the design of policies which are more robust, i.e. which perform acceptably over a broad range of uncertain futures (Lempert et al., 2006; Rosenhead et al., 1972), rather than attempting to maximize performance under an a priori best-estimate set of uncertain conditions.

3. Software description and availability

3.1. NetLogo

NetLogo (Wilensky, 1999) is an open-source environment for the design, implementation and analysis of agent-based models, which has become a leading platform for this purpose due to its user-friendliness and active user community. This tool is primarily implemented in Java and Scala, and includes a range of functions and methods to support the rapid development of spatially-explicit agent-based models. Different extension modules are also available, for instance to allow an interface with GIS datasets, or to link NetLogo with the R package (Thiele et al., 2012); for this work, the pyNetLogo connector (Jaxa-Rozen and Kwakkel, 2018) will be used as a link to the Python programming language. This connector is compatible with NetLogo 5.x and 6.0. As such, NetLogo offers a suitable starting point for the purposes of this work, by facilitating the design of agent-based models and enabling users to focus on the properties of the system under study, rather than on the technical details of software implementation.

3.2. MODFLOW/SEAWAT

MODFLOW (Harbaugh, 2005) is a standard code for the simulation of steady and transient groundwater flow in the subsurface, using a finite-difference approach to solve the three-dimensional flow equations for a rectangular grid. It allows for the simulation of representative subsurface conditions (e.g. heterogeneous hydraulic conductivities and transmissivities), as well as external stresses such as precipitation and flows through wells and drains. Additionally, the SEAWAT version (Langevin et al., 2008) couples MODFLOW with the MT3DMS code (Zheng and Wang, 1999); the latter provides a multi-species transport model for the simulation of advection, dispersion, and sorption. This coupling enables the simulation of groundwater flow with variable density and viscosity, and can be applied to study the transport of solutes and heat. This makes the SEAWAT version especially relevant for problems related to aquifer contamination (Zhang et al., 2013), or for the study of open or closed geothermal systems (e.g. Bakr et al., 2013; Hecht-Mndez et al., 2010). The simulation architecture described in this paper is currently compatible with MODFLOW-2005 and SEAWAT 4.

3.3. Python

Python is a general-purpose, object-oriented programming language which is increasingly popular for scientific and engineering applications. An extensive set of libraries is available for general data manipulation and analysis, such as Numpy (Walt et al., 2011) and pandas (McKinney, 2010), as well as interfaces with specific software packages and other environments. As such, the pyNetLogo connector is used to interactively communicate with the NetLogo API from Python. In addition, the FloPy library (Bakker et al., 2016) is used for pre/post-processing MODFLOW/SEAWAT input and output files, by reading and writing these files from storage and interfacing them with standard Python data structures. The coupled simulation architecture is executed using the EMA Workbench Python package (Kwakkel, 2017). This package can be used to design experiments (e.g. for sensitivity analysis) and provides different features for exploratory modeling and analysis, such as parallel simulation of multiple experiments and built-in visualization.

The Python modules used in this work will be made available under the following repository: https://github.com/quaquel/ems_coupledmodel. These modules have been tested with a standard distribution for scientific Python (Continuum Anaconda 3.6); using this distribution, the modules require the additional installation of the pyNetLogo and FloPy Python packages, which are available with the standard pip package manager.

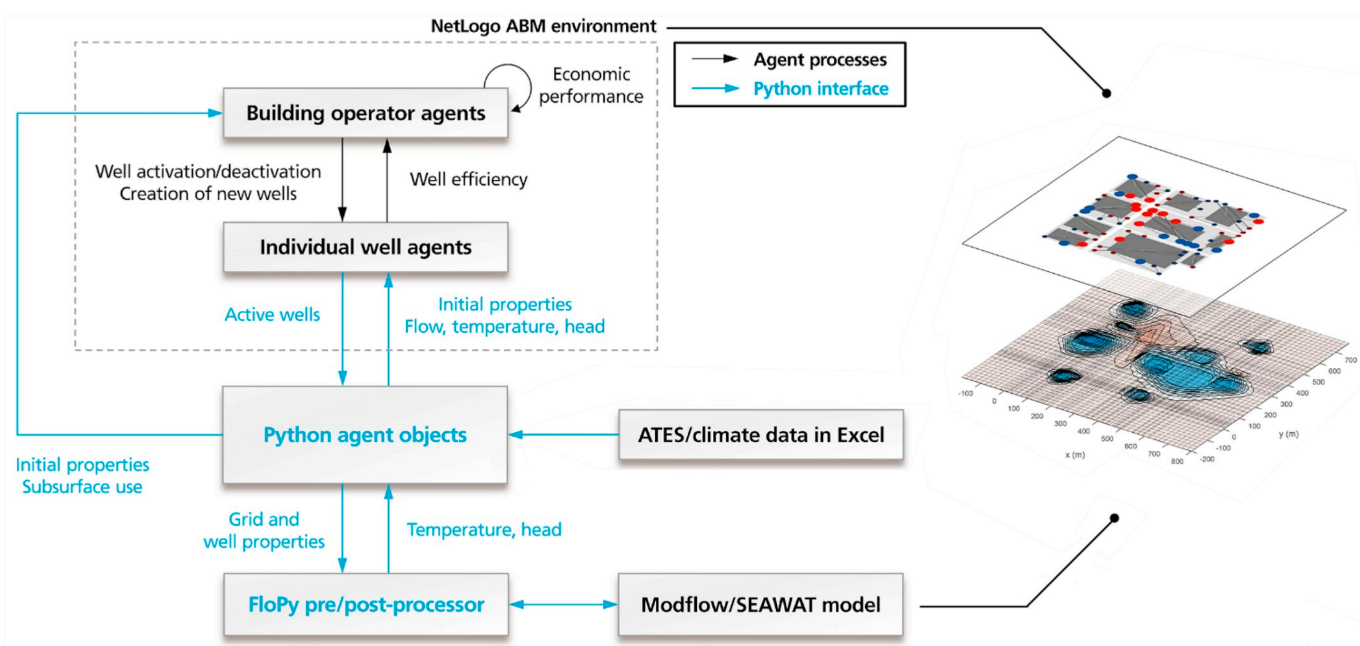

Fig. 2. General overview of the coupled simulation architecture.

4. An object-oriented architecture for coupling NetLogo and MODFLOW

The basic functionality of the pyNetLogo connector can be combined with Python's object-oriented environment to create a link with MODFLOW/SEAWAT models, with Python objects being used as a common interface between the two model components. In the context of groundwater management, interactions are likely to involve stresses such as well flows; using the agent_functions module described in this section, these interactions can be mediated through Python objects representing wells, which are "mapped" to corresponding NetLogo agents using the pyNetLogo functions. Parameters such as well flows or injection temperatures can thus be determined in the agent-based model, then passed to the geohydrological model. Fig. 2 below presents an overview of the overall coupled architecture.

As such, after each step of the NetLogo model, the Python well objects are updated based on the actions taken by NetLogo agents, and generate input files for the geohydrological model using the FloPy library (Bakker et al., 2016). The geohydrological model is in turn executed for one period, after which the Python objects process the resulting binary output files using FloPy's utility functions to obtain arrays for hydraulic head and temperature, or any other simulated concentration (e.g. salinity). By default, the execution periods for each model respectively correspond to one NetLogo "tick" and one MODFLOW stress period. A specified subset of the results (such as the effective head and temperature at the grid location of each well) is then passed to NetLogo, so that the geohydrological output can be used as an input for the decision-making routines of agents. Using Antle et al. (2014)'s terminology, the Python objects and NetLogo agents are thus "closely" coupled at runtime, while the Python objects are "loosely" coupled through data exchanges with the MODFLOW/SEAWAT geohydrological model.

The core classes and methods of the agent_functions module are described in Table 1 below. In addition to the PyAgent generic agent class, the PyGrid class is used to track the properties of the MODFLOW/SEAWAT simulation grid, including spatial and temporal discretization parameters, and output arrays for cell conditions (e.g. hydraulic head, salinity or temperature).

As discussed by Voinov and Shugart (2013), the choice of temporal and spatial resolution is a core question for the development of coupled models of social-ecological systems. By default, the architecture assumes that the models share the same resolution. However, to allow processes to be represented at different resolutions in each model, the time resolution can be modified by setting the tmult attribute of the PyGrid object to a desired multiplier for the NetLogo temporal resolution, relative to MODFLOW/SEAWAT. For instance, a value of 2 implies that NetLogo will be run for two time steps in each MODFLOW/SEAWAT time step; conversely, a value of 0.5 will execute MODFLOW/SEAWAT twice for each NetLogo step. Similarly, the smult attribute sets a conversion factor for spatial resolution between MODFLOW grid cells and NetLogo environment patches, with values larger than 1 implying a coarser NetLogo resolution.

The UML diagrams in Fig. 3 summarizes the class structure and action sequence for this example.

5. Case study

5.1. Case description: a simplified study of ATES

This section uses a simple model which depicts an urban application of Aquifer Thermal Energy Storage (ATES) systems. A more detailed ATES case study is described in Bloemendal et al. (2018); for the purposes of this work, the model was simplified to minimize runtimes while illustrating typical interactions between the model components, and the plausible impacts on coupled system behavior which these feedbacks may cause. Appendix A presents a detailed description of the case following the standard ODD + D protocol (Mller et al., 2013).

For the present case, a set of 10 NetLogo agents represents simulated building owners which are able to create warm and cold ATES storage wells (also defined in NetLogo as agents of a different type) over a 120-month period. These building and well agents are randomly located in a 1000 m × 1000 m environment, with a 20 m nominal NetLogo patch resolution. The wells follow a predefined pumping pattern over time which corresponds to typical seasonal storage cycles, presented in Fig. 4. These well flows are computed in NetLogo at a monthly time resolution, then passed to a single-layer confined aquifer model in MODFLOW/SEAWAT. As discussed by Lo Russo et al. (2014), a monthly discretization should offer reasonable accuracy when simulating typical ATES flow patterns. For this idealized case, this resolution is chosen as a practical compromise between the seasonal discretization used in

Table 1
Basic agent_functions classes and methods.

Class/method name	Description	Arguments	Returns
PyAgent	Generic agent class		
create_NetLogo_agent()	Create a NetLogo agent corresponding to the Python object	Object attributes to be passed to the NetLogo agent (list of strings)	
update_NetLogo_agent()	Update an existing NetLogo agent	Object attributes to be passed to the NetLogo agent (list of strings)	–
update_Python_object()	Update the Python object with properties from the corresponding NetLogo agent	NetLogo attributes to be passed to the Python object (list of strings)	–
PyWell	ATES well class		
calc_LRC()	Locate the well in a PyGrid object to set layer (L)/row (R)/column (C) grid coordinates for MODFLOW/SEAWAT	PyGrid instance	–
PyGrid	Aquifer grid class		
make_grid()	Generate grid properties for MODFLOW/SEAWAT - can be used with existing model input files, or with a list of well objects to dynamically refine the grid	List of well objects (for dynamic grid refinement); MODFLOW.dis filename (optional)	–
clean_grid()	Dynamically refine the MODFLOW/SEAWAT simulation grid using a list of well objects	List of well objects (for dynamic grid refinement); MODFLOW.dis filename (optional)	–
boundaries()	Generate grid boundary properties for MODFLOW/SEAWAT	MODFLOW.dis filename (optional)	–
update_runtime_objectlist()	Compare active NetLogo agents with the existing Python objects, and create/remove Python objects as needed	List of objects to compare with the NetLogo agents; NetLogo attributes to be passed to newly created Python objects (list of strings)	List of Python objects
create_obj_from_NetLogo()	Create a list of Python objects corresponding to NetLogo agents	Python object class to be instantiated; NetLogo attributes to be passed to Python objects (list of strings)	List of Python objects
write_NetLogo_attriblist()	Update a set of NetLogo agents with a list of attributes from a list of Python objects	List of Python objects for which to update corresponding NetLogo agents	–

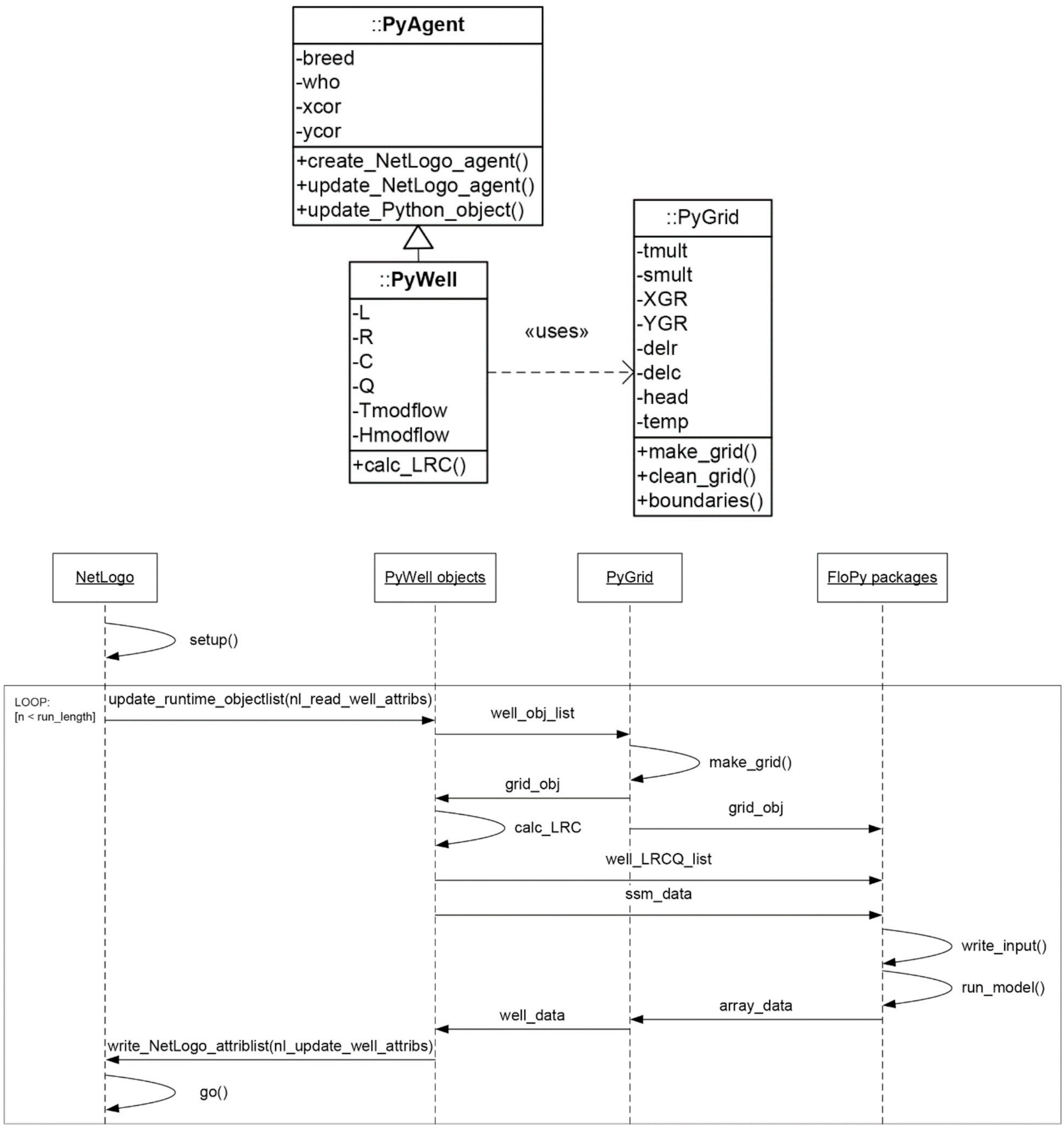

Fig. 3. Simplified class and sequence diagrams.

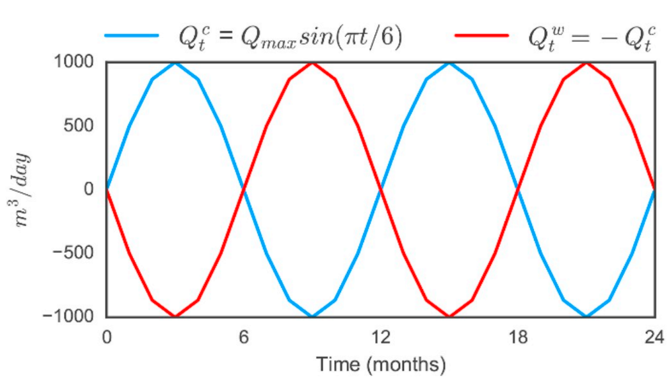

Fig. 4. Seasonal ATES injection/extraction flows.

previous work on ATES (e.g. Bakr et al., 2013), which may lead to inaccurate temperature estimations, and the daily or weekly resolution needed to represent more complex operating patterns (e.g. Bloemendal and Hartog, 2018; Rostampour et al., 2016), which would increase model runtimes.

The geohydrological model extents are set to 1400 m × 1400 m to provide sufficient clearance for temperature distributions to stabilize around the borders of the NetLogo environment, with a 20 m thickness and 4 m nominal spatial resolution. The ambient groundwater flow is set using constant head boundaries, with no ambient flow in nominal conditions. The nominal spatial resolution is chosen to ensure that the expected radius of thermal influence around each well covers at least five grid cells, following recommendations by Sommer et al. (2015) for the numerical study of ATES systems in MODFLOW/SEAWAT; in typical conditions, this resolution allows the estimated thermal efficiency to converge within 1%. After executing the MODFLOW/SEAWAT model over one monthly simulation period, the NetLogo well agents are then updated with the effective hydraulic head and temperature at their location.

Table 2 summarizes the main parameters used for the NetLogo and MODFLOW/SEAWAT components; the ranges indicated for certain parameters will be used in the next subsections for runtime evaluation and sensitivity analysis. Parameters for the geohydrological model are derived from typical operating conditions for ATES systems in the Netherlands (Calje, 2010).

The ATES wells are operated in coupled pairs (or doublets) of cold and warm wells, which inject water at each monthly simulation period t with the Q_t^c and Q_t^w rates given below (with negative values corresponding to an extraction of water from the aquifer). As shown in Fig. 4, the period of the flows is chosen to approximate seasonal storage patterns, with one injection and extraction cycle per 12 months. The total annual pumped volume is representative of a typical commercial building using ATES in the Netherlands. Due to the physical coupling between wells, these flow patterns do not cause any net extraction from the aquifer over a full annual storage cycle.

These flows can be converted to an equivalent amount of injected or retrieved thermal energy per doublet of wells:

$$E_t^{out} = \begin{cases} Q_t^c C_w (T_{out,t}^w - T_{in}^c)\Delta t, & Q_t^c > 0 \\ Q_t^c C_w (T_{out,t}^c - T_{in}^w)\Delta t, & Q_t^c < 0 \end{cases}$$
$$E_t^{in} = Q_t^w C_w (T_{in}^w - T_{in}^c)\Delta t \tag{1}$$

The injection temperatures T_{in}^c, T_{in}^w for cold and warm wells are constant and provided in Table 2. The extraction temperatures $T_{out,t}^c$, $T_{out,t}^w$ are updated at each simulation period from the MODFLOW/SEAWAT simulation grid, and are assumed to correspond directly to the temperature $T_{k,t}$ of the grid cell k in which each well is located. The NetLogo agents then compute the thermal efficiency of each doublet η_t they own, using the ratio of the cumulative retrieved and injected thermal energy:

$$\eta_t = \frac{\sum_1^t E_t^{out}}{\sum_1^t E_t^{in}} \tag{2}$$

The temperatures of the grid cells k are also used to calculate an indicator ε_t, for the fraction of the simulated subsurface volume which presents a significant temperature change relative to the average aquifer temperature T_{amb}. Given that the MODFLOW/SEAWAT cell volumes are uniform, and taking a threshold of 0.1 K:

$$\varepsilon_t = \frac{|\{k \mid |T_{k,t} - T_{amb}| > 0.1\}|}{|\{k\}|} \tag{3}$$

This indicator thus tracks the intensity at which the aquifer is being used for thermal storage over time.

The building agents use simple decision heuristics to build additional wells or deactivate existing wells, based on the thermal efficiency computed from the SEAWAT results using eq. (2) (after an initialization period of 36 months to let temperature distributions stabilize). If the average thermal efficiency of the wells owned by a building is above a certain threshold η_a, the building agent has a given adoption probability α of adding a pair of coupled warm and cold wells at each time step, until a given maximum number n of ATES wells is reached in the simulation. These new wells are located randomly within the simulated area, at a given minimal distance d from existing wells. If the average thermal efficiency is under another threshold η_d (for instance due to excessive thermal interferences), the agents are assumed to deactivate the wells.

5.2. Computational runtime evaluation

Although NetLogo's accessibility has made it popular as a prototyping environment for the development of simple agent-based models, it has also successfully been used for more complex models; these can offer comparable performance to base programming languages such as Java when efficiently implemented (Railsback et al., 2017). To support these capabilities, the coupled simulation architecture therefore needs to be usable with more sophisticated agent-based models without overly increasing runtimes in relation to the individual models. This subsection thus tests a variant of the ATES case study under different parameterizations for the spatial resolution of the agent-based and geohydrological models, as well as different fixed numbers of ATES well agents (i.e. ignoring the decision heuristics otherwise used to create or deactivate well agents).

The NetLogo model is tested with three different environment resolutions from 4 m to 20 m (corresponding to 2500, 22,500 and 62,500 patches), while the MODFLOW/SEAWAT aquifer grid is tested on five different resolutions in the same resolution interval (ranging from 4900 to 122,500 cells). In addition, the NetLogo model is tested with five numbers of ATES well agents, from 20 to 300. To account for cases in which the MODFLOW/SEAWAT grid would be recomputed over time

Table 2
Model parameters for ATES case study.

Parameter	Component	Value or range	Unit	Symbol
Adoption rate	NetLogo	0.02–0.1	period-1	α
Distance policy (min. distance between wells)	NetLogo	50–200	m	d
Efficiency threshold for adoption	NetLogo	0.8	–	η_a
Efficiency threshold for deactivation	NetLogo	0.7	–	η_d
Grid cell (patch) resolution	NetLogo	4–20	m	Δp
Length of each simulation period	NetLogo/SEAWAT	30	day	Δt
Maximum ATES well flow	NetLogo	1000	m^3/day	Q_{max}
Maximum number of ATES wells	NetLogo	20–300	agents	n
Random seed	NetLogo	–	–	θ
Ambient aquifer temperature	SEAWAT	10	°C	T_{amb}
Ambient groundwater flow	SEAWAT	0–20	m/year	v
Aquifer depth	SEAWAT	20	m	Δz
Aquifer porosity	SEAWAT	0.1–0.5	–	p
ATES injection temperature (cold wells)	SEAWAT	5	°C	T_{in}^c
ATES injection temperature (warm wells)	SEAWAT	15	°C	T_{in}^w
Bulk density of aquifer medium	SEAWAT	1760	kg/m^3	ρ_b
Grid cell resolution	SEAWAT	4–20	m	Δg
Horizontal hydraulic conductivity	SEAWAT	10–60	m/day	K
Volumetric heat capacity of water	SEAWAT	$4.18 * 10^6$	J/m^3	C_w

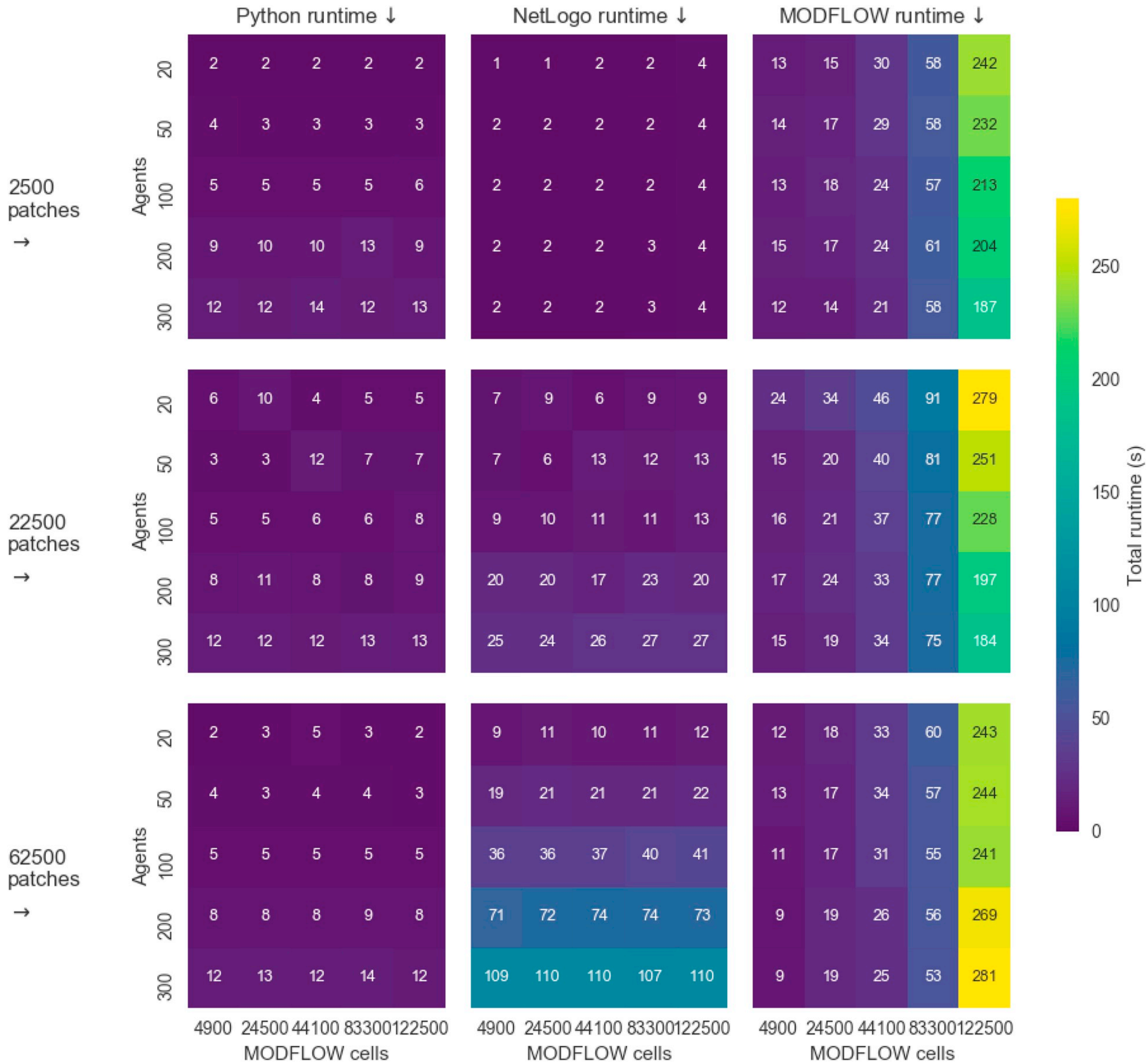

Fig. 5. Runtime for each model component (left column: Python architecture; middle column: NetLogo model; right column: MODFLOW/SEAWAT model). Each row of subplots corresponds to a different resolution of the NetLogo environment. The rows and columns of each subplots correspond to different NetLogo agent counts and MODFLOW/SEAWAT grid resolutions.

due to changes in agent locations, the aquifer model grid is recomputed at each time step. At finer resolutions, the MODFLOW grid is representative of a typical complex groundwater case (such as the large-scale ATES case study presented by Bakr et al. (2013), which used 650,000 grid cells).

Fig. 5 presents the total runtime (in seconds) which is attributed to each model component under these parameterizations, using 30 monthly time periods in each case. For clarity, the figure presents each resolution level as the corresponding total number of NetLogo patches and MODFLOW/SEAWAT grid cells, given that runtimes are more likely to be proportional to these values rather than resolution. Fig. 6 presents these results expressed as a fraction of total runtime across the three simulation components.

It can be observed from Fig. 5 that the runtime attributed to the Python architecture scales proportionally to the number of agents, and is mostly independent of the resolutions used in NetLogo and MODFLOW/SEAWAT. In parallel, NetLogo runtime scales roughly proportionally to the number of environment patches, while MODFLOW runtime increases more than proportionally to the number of grid cells. As such, although the fraction of total runtime attributed to the simulation architecture is significant in Fig. 6 when combined with a large number of agents and coarse model resolutions, it becomes largely negligible at finer resolutions (e.g. 1–3% of total runtime using a 4 m resolution in NetLogo and MODFLOW/SEAWAT).

Fig. 7 further breaks down the runtime performance of the Python architecture in a given parameterization, using 200 agents with 2500 NetLogo patches and 122,500 MODFLOW grid cells. The Python runtime is mostly attributed to interactions between NetLogo and Python through the update_runtime_objectlist() and write_NetLogo_attriblist() functions, with the grid and agent processes (i.e. methods of the PyGrid and PyAgent classes) being relatively negligible.

Based on these results, the coupled simulation architecture is therefore unlikely to significantly increase computational costs, compared to the runtimes which would be associated with each individual model component - in particular given that the cost of data exchanges scales proportionally to the number of agents, whereas the runtime of more complex agent-based models may scale much more quickly due to interactions or links between agents (Railsback et al., 2017).

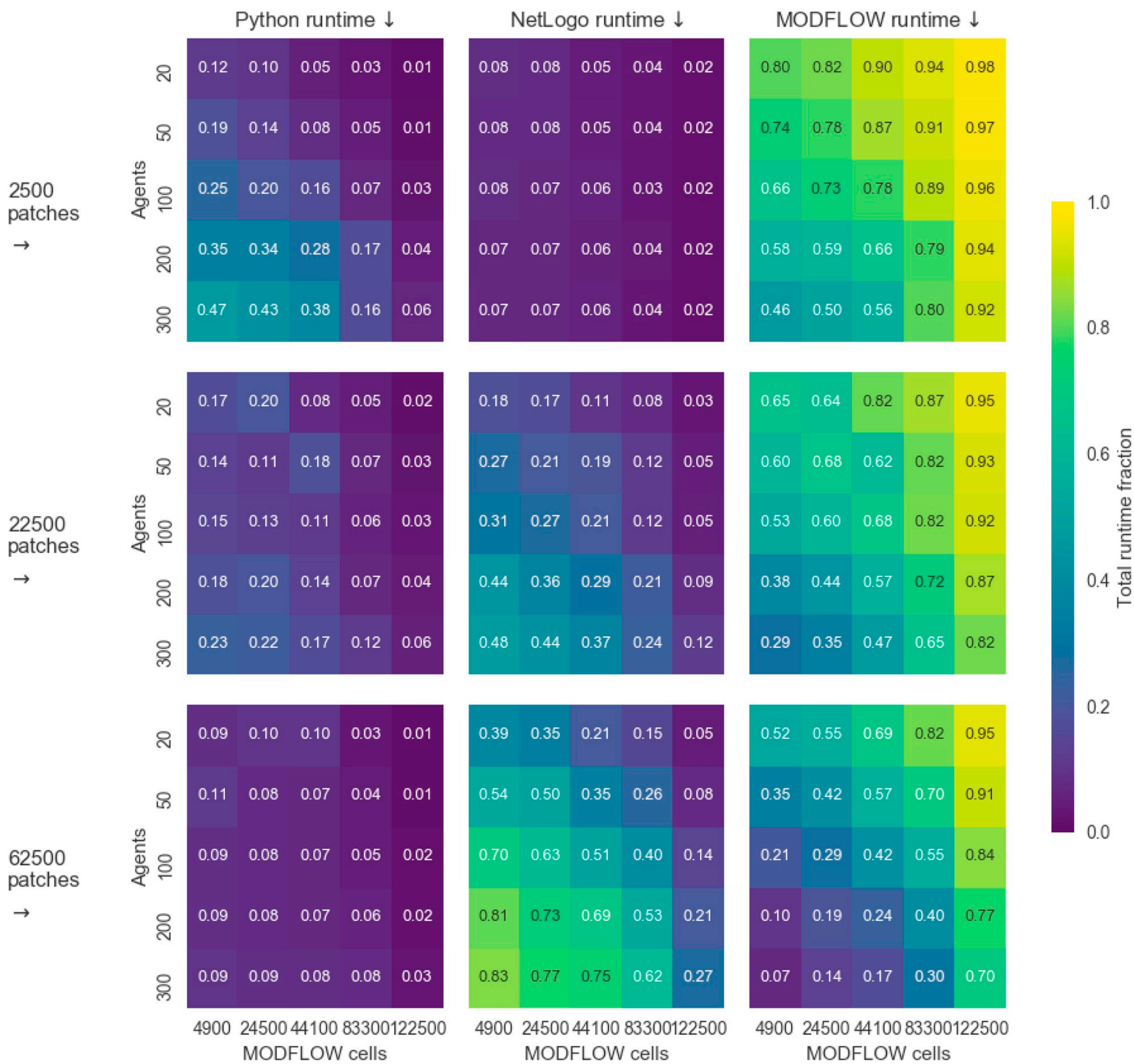

Fig. 6. Fraction of total runtime for each model component (left column: Python architecture; middle column: NetLogo model; right column: MODFLOW/SEAWAT model). Each row of subplots corresponds to a different resolution of the NetLogo environment. The rows and columns of each subplot correspond to different NetLogo agent counts and MODFLOW/SEAWAT grid resolutions.

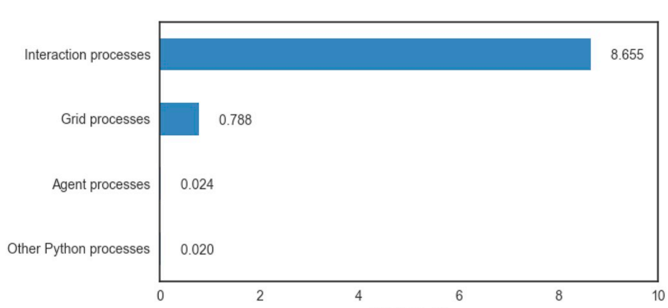

Fig. 7. Distribution of runtime across Python processes (for 200 agents with 2500 NetLogo patches and 122,500 MODFLOW grid cells).

5.3. Analysis under uncertainty

The use of models for decision support under uncertainty can be facilitated by an integrated environment for experimental design and analysis (e.g. Hadka et al., 2015). To highlight the relevance of such an approach for the coupled agent-based/geohydrological models, this subsection uses the EMA Workbench Python package (Kwakkel, 2017) to test the ATES case under parametric uncertainty. The EMA Workbench provides features for experimental design (for instance using Monte Carlo or Latin Hypercube sampling), the parallel execution of simulation runs, and exploratory analysis with techniques for sensitivity analysis or scenario discovery. In the context of this work, it enables a consolidated approach for the analysis of the coupled models,

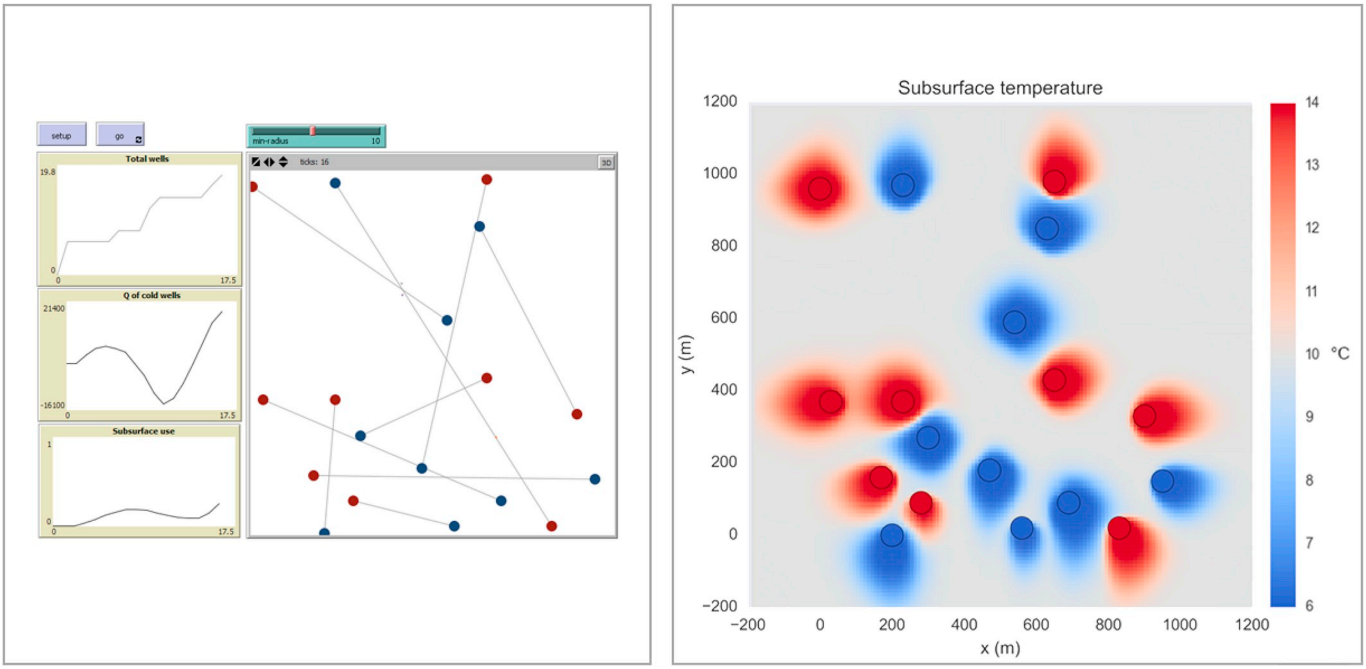

Fig. 8. Example of coupled model output: NetLogo model (left); SEAWAT temperature distribution (right).

for instance by assigning parameters to both model components through a common model interface, and by collecting results from both components within a single data structure.

The Jupyter Notebook provided with this paper documents this analysis, including the integration of the coupled models within the EMA Workbench, the sampling of uncertain parameters in the NetLogo and geohydrological components, and the post-processing of the results.

5.3.1. Basic exploration

Fig. 8 shows an example of output from the coupled models, showing randomly located ATES well agents in the NetLogo environment, and the corresponding temperature distribution in the PyGrid object.

Using a Latin Hypercube sample of 512 experiments to adequately sample the parametric uncertainty ranges listed in Table 2, the coupled simulation yields a broad range of behaviors, illustrated in Fig. 9. The figure presents three key outcomes: the number of active ATES wells over time (left graph), the mean thermal efficiency of the ATES systems (middle graph), and the fraction of the simulated subsurface volume which shows a significant temperature change (right graph). The number of active ATES wells and the subsurface usage respectively summarize the states of the agent-based and aquifer model, with

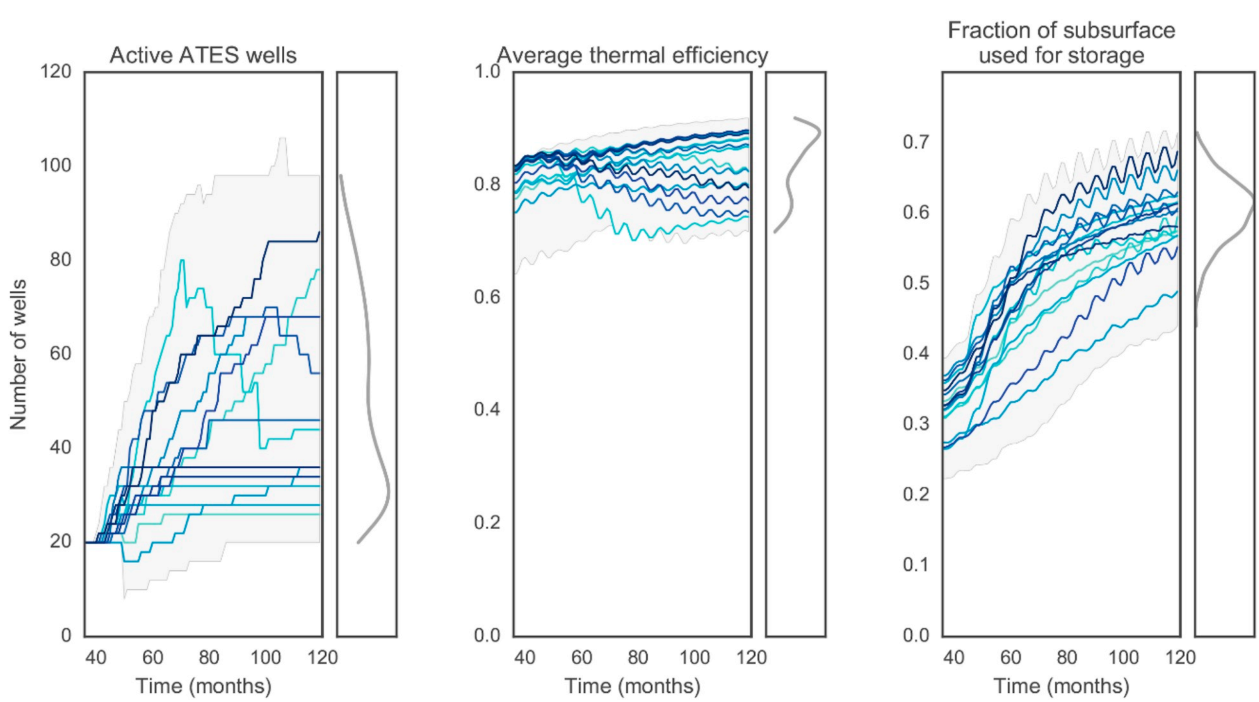

Fig. 9. Coupled model outcomes over time, for a random subset of 16 out of 512 experiments, after an initialization period of 36 months.

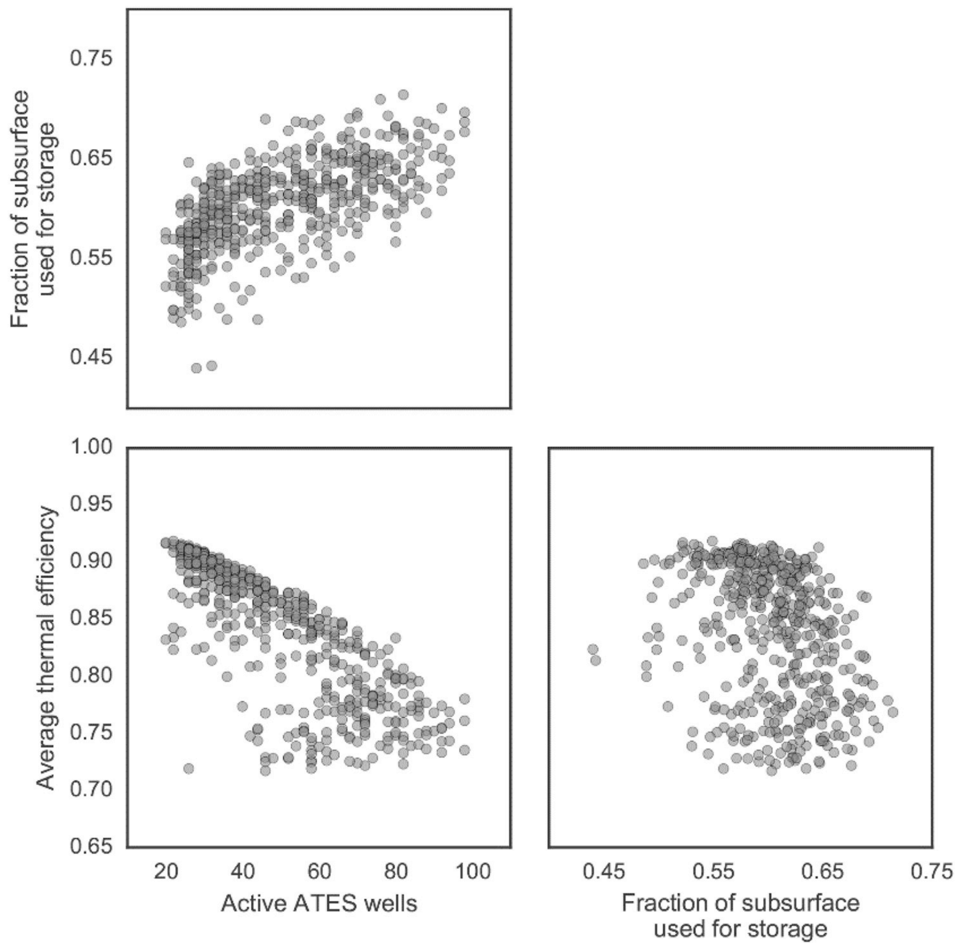

Fig. 10. Scatter plots for outcomes at the end of the simulation.

thermal efficiency as a key link between the models due to its feedback effect on agent decision-making. The graphs show time series for a random subset of 16 experiments (colored in shades of blue) after an initialization period of 36 months, chosen to stabilize thermal distributions after three annual storage cycles. The shaded envelopes show the minimum and maximum values for each outcome over time, and a kernel density estimator (in the panels to the right of the graphs) illustrates the distribution of experiments within this envelope at the end of the simulation.

The graphs point to different modes of behavior for the coupled models, which are affected by interactions across the NetLogo and MODFLOW/SEAWAT components: for instance, under some conditions, a rapid increase in the number of active wells can reduce their average thermal efficiency, due to interactions across neighboring wells - which then leads building agents to deactivate some of the systems. The scatter plots in Fig. 10 indicate basic relationships between the three indicators for all 512 experiments, with the number of active wells in NetLogo being associated positively with the used MODFLOW/SEAWAT subsurface volume and negatively with mean thermal efficiency, while the latter has a weaker relationship with the used subsurface volume.

5.3.2. *Global sensitivity analysis*

To better understand the impact of uncertain parameters on the model outcomes and illustrate a typical analysis workflow, this subsection applies a simple global sensitivity analysis to the coupled models using the SALib library (Herman and Usher, 2017). This library can be directly called from the EMA Workbench to generate appropriate sampling designs for common sensitivity analysis techniques (such as Morris elementary effects, Fourier amplitude sensitivity testing, or Sobol indices) and to analyze the model outcomes.

For this example, SALib was used to sample a set of experiments with the Morris technique, using five uncertain parameters across both models with an additional value for the random seed of the NetLogo model (which corresponds to stochastic uncertainty, and here drives the choice of a random location for newly created wells). Fig. 11 summarizes the sensitivity analysis results using $u*$ indices (Campolongo et al., 2007) obtained from 160 replications, for a total of 160*(N +1) = 1120 samples. The magnitude of the $u*$ values estimates the relative influence of each parameter on model outcomes; the sum of the $u*$ values can thus be normalized to 1 at each time step for each indicator, so that the area graphs below show the relative importance of each variable over time.

This approach enables the comparison of sensitivities over time and across model components, on a common basis. For instance, the number of active wells over time is mostly driven by the NetLogo parameters for adoption rate and distance policy, with the former being predominant earlier in the simulation, while the latter is most influential on values at the end of the simulation (given that it largely determines how many wells can be built in the simulated area). Similarly, the MODFLOW/SEAWAT parameter for aquifer porosity is most influential on the fraction of subsurface volume used for storage early in the simulation (when the number of active wells is still similar across the experiments), but is then overtaken by the parameters which cause different pathways for ATES adoption in the NetLogo model. Although the geohydrological uncertainties remain significant, this implies that the assumptions made

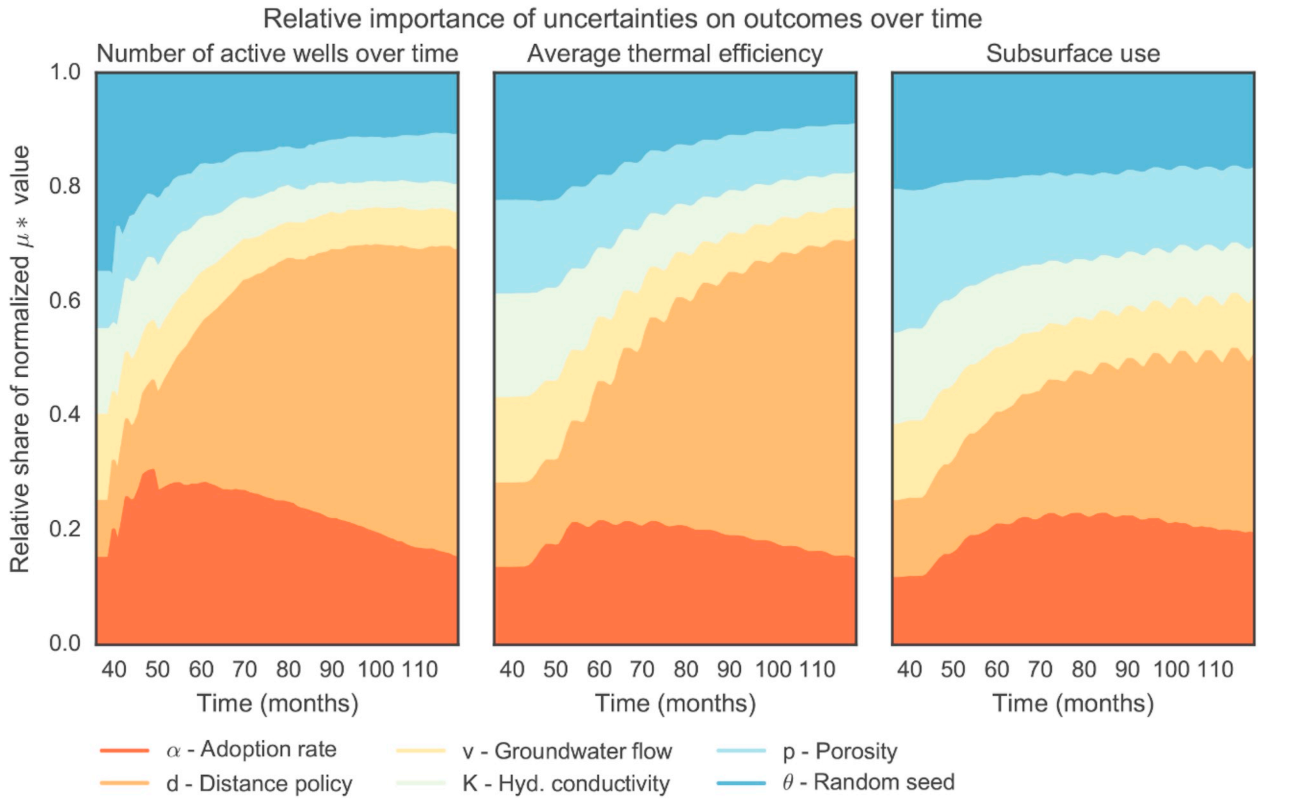

Fig. 11. Normalized Morris sensitivity results over time.

in the NetLogo model are more influential for the overall behavior of the coupled models. It should be noted that this is at least partly driven by the choice of uncertainty ranges: for instance, while the simulated groundwater flow values were typical of average conditions in the Netherlands, approximately 20% of systems in the country are subject to a higher ambient groundwater flow relative to their storage capacity than was simulated in this idealized case (Bloemendal and Hartog, 2018). These systems may encounter significant losses in thermal efficiency, which could lead to different conclusions regarding the relative importance of agent-related or geohydrological uncertainties.

Nonetheless, this finding is broadly consistent with observations made in relation to more realistic models of social-ecological systems (e.g. Schlter et al., 2014): although environmental processes may themselves be significantly affected by deep uncertainties, the design choices made in the conceptualization and formalization of agent decision-making almost inevitably have a substantial impact on the outcomes of SES models. Without resolving these uncertainties, an exploratory modelling approach can at least help clarify the implications of these design choices for the behavior of the system.

5.3.3. Scenario discovery

Scenario discovery (Bryant and Lempert, 2010; Kwakkel and Jaxa-Rozen, 2016) aims to identify the combinations of input uncertainties which tend to be associated with given regions of the model output space, using statistical techniques such as the Patient Rule Induction Method (PRIM) (Friedman and Fisher, 1999) or classification and regression trees (CART). This approach is similar to the "factor mapping" setting discussed in the sensitivity analysis literature (Saltelli et al., 2008), and complements the study of variable importances by focusing on specific outcomes or behaviors of interest.

To complete this example, this subsection therefore applies PRIM on the Latin Hypercube sample of 512 experiments previously used for basic exploration, with a given scenario of interest. This scenario is assumed to correspond to a high usage of the aquifer for thermal

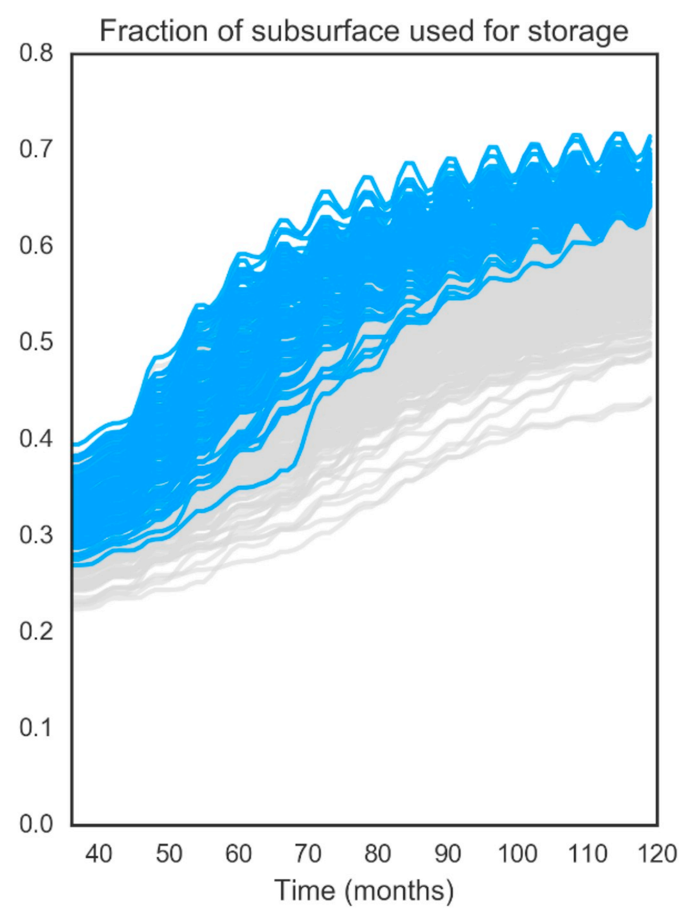

Fig. 12. Cases of interest for scenario discovery.

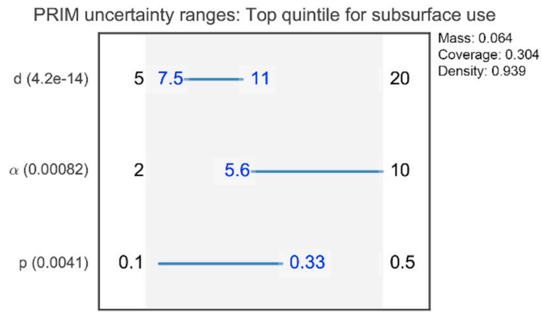

Fig. 13. PRIM uncertainty ranges identified for cases of interest.

storage, defined as cases in which the fraction of used subsurface volume is in the top quintile at the end of the simulation; these cases of interest are highlighted in the full ensemble of results in Fig. 12 below.

Fig. 13 shows an example of a box - or combination of uncertainty ranges - identified by the PRIM algorithm for this scenario. The values next to each variable name indicate the estimated p-value of each parameter, following a binomial test for its significance in this combination. The mass, coverage and density values respectively give the fraction of the total experiments which are within this box, the fraction of all cases of interest for the scenario which are described by the box, and the fraction of experiments within the box which are of interest.

The scenario for a high usage of subsurface volume thus tends to be associated with a low range of the d distance parameter (i.e. between 7.5 and 11 NetLogo patches), a high range for the adoption rate α, and a fairly low range of aquifer porosity p in the SEAWAT model. Based on the density metric, 93.9% of the experiments which combine these input ranges would be in the top quintile of subsurface use. By identifying influential combinations of uncertainties across the coupled models, scenario discovery thus provides useful additional information to complement conventional sensitivity analysis techniques. This is particularly relevant for models which present broad ranges of plausible outcomes or different modes of behavior, and for the study of systems which may need to meet explicit performance thresholds.

6. Conclusions

This paper introduced a coupled simulation architecture which interfaces NetLogo and the MODFLOW/SEAWAT geohydrological simulation codes, using Python's object-oriented features. This architecture was applied for a simplified case study of Aquifer Thermal Energy Storage; the operation and deployment of this technology relies on dynamic agent behavior as well as relatively complex subsurface processes (such as heat transport and sorption), which justified the development of a full-featured simulation architecture which can account for feedbacks between human and groundwater components. As a simple example of the possibilities of this approach, the case study included basic decision heuristics under which simulated ATES owners endogenously adjust the use of the systems based on realized performance. These feedbacks can for instance support more realistic case studies for the long-term adoption of ATES in urban areas, in which adoption patterns are affected by expected technical and economic performance. In parallel, NetLogo's spatial modelling features allow for an intuitive representation of ATES spatial planning, which was here depicted by a minimal distance policy for neighboring storage wells.

As described by Castilla-Rho et al. (2015), the typical drawbacks of coupled agent-based/groundwater modelling include technical complexity, a lack of flexibility in scenario design, and the difficulty of performing coupled sensitivity analysis. The first two of these challenges were here addressed by relying on a simple object-oriented design, which extends the NetLogo model component in an intuitive fashion. Although the coupling requires the external pyNetLogo and FloPy libraries, these libraries are actively supported and at a relatively stable stage of development, which should reduce future compatibility issues. Furthermore, we expect that the possibility of reusing existing MODFLOW/SEAWAT models, while benefiting from the user-friendliness of the NetLogo platform, helps manage the complexity of the overall model development process. An evaluation of the computational costs associated with the different simulation components, under different parameterizations which should be representative of the typical scope of a groundwater management study, also showed that the coupled simulation architecture is unlikely to significantly increase total runtimes relative to the individual models.

The use of the Python language also addresses issues with the coupled analysis of the models, by enabling the straightforward integration of the simulation architecture with different open-source packages available in Python. This approach was demonstrated by using the coupled models with the EMA Workbench; this package can be used to design experiments and analyze the behavior of the coupled models through a common model interface. A typical simulation workflow was illustrated with a global sensitivity analysis of the coupled models, along with a scenario discovery analysis.

As such, while we acknowledge the benefits of a fully integrated platform such as the FlowLogo environment (Castilla-Rho et al., 2015) in terms of technical complexity, we believe that the capabilities of a comprehensive geohydrological modelling environment justify a coupled simulation approach in the case of more complex groundwater management problems. This approach would indeed be required for studies of aquifer pollution or contamination, or the management of coastal aquifers in which saltwater intrusion is significant (which represents an increasingly pressing issue in the context of climate change adaptation, e.g. Rawlani and Sovacool, 2011). To facilitate future work using these features, we have therefore ensured that the architecture modules are available through an online repository, along with interactive notebooks which replicate the analyses presented in the paper.

From a broader view, the results of these analyses highlighted the importance of an integrated view for the treatment of model uncertainties, which can be supported by an approach like exploratory modelling: while this case only involved simple behavioral assumptions in the agent-based component, the behavior of the coupled models was sensitive to different parametric values and combinations across the agent-based and geohydrological components. A separate treatment of these uncertainties would have made it more difficult to identify important relationships between the models. Such a consolidated process for the analysis of coupled models can ultimately help analysts better understand the interactions and feedbacks between socio-technical and environmental variables, and contribute to the design of more robust policies for the management of social-ecological systems.

Acknowledgement

This research was funded by the Dutch National Science foundation, through the Uncertainty Reduction in Smart Energy Systems program.

Appendix A

ODD+D Description

Outline		Guiding questions	Description
I) Overview	I.i Purpose	I.i.a What is the purpose of the study?	The study provides a simple test case for an object-oriented simulation architecture for coupled agent-based/geohydrological modelling. The case uses an idealized application of Aquifer Thermal Energy Storage (ATES) to illustrate data exchanges between the two model components, and plausible system behaviors which may emerge from these feedbacks. ATES is an emerging building technology which provides a suitable case for this purpose: ATES performance depends on thermal subsurface dynamics, which in turn affect the operation of ATES by building owners. This coupled modelling approach can usefully be extended to other management problems which require detailed geohydrological modelling, such as the study of aquifer pollution or coastal saltwater intrusion.
		I.ii.b For whom is the model designed?	Researchers interested in the coupled modelling of human/groundwater systems
	I.ii Entities, state variables, and scales	I.ii.a What kinds of entities are in the model?	Agent-based model (ABM): o ATES system operator agents (e.g. building owners) o ATES well agents (i.e. individual storage wells) o Land parcels Geohydrological model: o Aquifer model grid
		I.ii.b By what attributes (i.e. state variables and parameters) are these entities characterized?	ATES system operator agents (ABM): o Geographic coordinates (fixed) o Set of ATES wells owned by the operator (variable over time) o Mean thermal performance of ATES wells (ratio of cumulative energy recovered over time to injected energy) ATES well agents (ABM): o Physical properties: geographic coordinates (fixed), injection temperature (fixed), flow (predefined as a function of time) o "Owner" system agent o Thermal energy injected and recovered (variable over time) o Aquifer properties at own location (variable over time): temperature, hydraulic head Land parcels (ABM): o Geographic coordinates (fixed) o Availability for creation of new ATES well agents Aquifer model grid (geohydrological model): o Geohydrological properties: horizontal and vertical conductivities, porosity (fixed) o Temperature and head distributions (variable over time)
		I.ii.c What are the exogenous factors / drivers of the model?	o ATES well flow profile over time o Maximum number of ATES well agents o ATES adoption rate o Thermal efficiency thresholds for ATES adoption and deactivation o Distance policy for minimum distance between ATES wells o Aquifer porosity and conductivity
		I.ii.d If applicable, how is space included in the model?	ATES system operators and ATES wells are spatially located within the agent-based model. The wells are mapped to corresponding locations within the aquifer model.
		I.ii.e What are the temporal and spatial resolutions and extents of the model?	The coupled simulation is executed for 120 periods of 30 days. Each spatial layer is modelled with the following nominal values. Additional discretization parameters are tested in the study to evaluate the effect of spatial resolution on model runtime (from 4m x 4m to 20m x 20m in each model component). ABM: • Rectangular grid area of 1000m x 1000m, discretized in land parcels of 20m x 20m. Geohydrological model: • Rectangular grid area of 1400m x 1400m, discretized in cells of 4m x 4m.

Fig. 14. ODD + D documentation of the ATES test case.

	I.iii Process overview and scheduling	I.iii.a What entity does what, and in what order?	For each monthly period: 1) ABM (asynchronous updating with random execution order): o ATES wells calculate their flow based on exogenous flow profile and current time period o ATES wells calculate their thermal efficiency based on geohydrological model results from previous period o ATES system operators calculate the overall thermal efficiency of their ATES wells o ATES system operators build new wells if current system performance exceeds a given efficiency threshold o ATES system operators deactivate their wells if current system performance is below a given efficiency threshold. 2) Geohydrological model: o Based on the new well properties, temperature and head distributions are computed for each grid cell in the aquifer model. Temperature and head values for each grid cell which contains an ATES well are passed back to the corresponding agent in the ABM.
II) Design concepts	II.i Theoretical and Empirical Background	II.i.a Which general concepts, theories or hypotheses are underlying the model's design at the system level or at the level(s) of the submodel(s) (apart from the decision model)? What is the link to complexity and the purpose of the model?	The dynamic hypothesis for the system's behavior under certain parameterizations (e.g. the possible emergence of a "tragedy of the commons") follows the literature on common-pool resource governance (e.g. Hardin, 1968; Ostrom, 2009). This behavior may emerge from delayed feedbacks between the adoption of ATES systems based on expected performance, and the dynamics of stored thermal energy in the subsurface (i.e. feedbacks between the human and natural systems represented by each model component).
		II.i.b On what assumptions is/are the agents' decision model(s) based?	The decision model assumes that ATES system operators are boundedly rational; the adoption of new ATES wells is based on "satisficing" thresholds and past performance without explicit foresight, and with limited knowledge of subsurface conditions (i.e. the temperature at the location of each owned well)
		II.i.c Why is a/are certain decision model(s) chosen?	There is currently a lack of specific data on ATES adoption processes. However, current experience (e.g. Agterberg, 2016) suggests that the use of ATES by building owners is largely driven by expected technical and economic performance. Given that the study focuses on the role of feedbacks between the human and natural systems, rather than a detailed study of ATES operation, this assumption is represented in a simplified manner by using fixed performance thresholds to show how expected performance may affect the behavior of the coupled system.
		II.i.d If the model / a submodel (e.g. the decision model) is based on empirical data, where does the data come from?	Agent-based model (ABM): o ATES well flow profile over time: representative of seasonal pumping patterns for a typical small building using ATES in the Netherlands (50,000 m^3/year) o Thermal efficiency thresholds: representative of expected thermal performance (65-90%) in typical urban conditions (Calje, 2010) Geohydrological model: o Horizontal and vertical conductivities, groundwater flow, and aquifer porosity: typical of aquifer conditions for ATES use in the Netherlands (Calje, 2010)
		II.i.e At which level of aggregation were the data available?	N/A
	II.ii Individual Decision Making	II.ii.a What are the subjects and objects of decision-making? On which level of aggregation is decision-making modeled? Are multiple levels of decision making included?	Decision-making is modelled at the level of ATES systems, who are assumed to correspond to individual building operators. When deciding to deactivate wells, the operators uniformly change the status of all wells under their control.

		II.ii.b What is the basic rationality behind agents' decision-making in the model? Do agents pursue an explicit objective or have other success criteria?	ATES system operators behave in a "satisficing" approach, building new wells as long as thermal performance meets a given threshold.
		II.ii.c How do agents make their decisions?	At each time step, ATES system operators create new wells if the thermal efficiency of their wells (cumulative over time) is above a given threshold, or deactivate existing wells if it is below another threshold.
		II.ii.d Do the agents adapt their behavior to changing endogenous and exogenous state variables? And if yes, how?	ATES system operators decide whether to deactivate existing wells or build new wells based on current thermal performance, which is driven by endogenous aquifer conditions in the geohydrological model.
		II.ii.e Do social norms or cultural values play a role in the decision-making process?	N/A
		II.ii.f Do spatial aspects play a role in the decision process?	New ATES wells may only be built on available land parcels. The subset of available parcels is restricted by planning policies which require a minimum distance between wells.
		II.ii.g Do temporal aspects play a role in the decision process?	Calculated thermal performance is based on the cumulative recovered and injected thermal energy over time. Delayed feedbacks are present in the aquifer model (due to the evolution of temperature distributions over time), but are not explicitly accounted for in the decision process of agents.
		II.ii.h To which extent and how is uncertainty included in the agents' decision rules?	Uncertainty is not explicitly considered in the decision rules.
	II.iii Learning	II.iii.a Is individual learning included in the decision process? How do individuals change their decision rules over time as consequence of their experience?	N/A
		II.iii.b Is collective learning implemented in the model?	N/A
	II.iv Individual Sensing	II.iv.a What endogenous and exogenous state variables are individuals assumed to sense and consider in their decisions? Is the sensing process erroneous?	ATES system operators perceive aquifer conditions (temperature and head) at the location of the wells under their control. Sensing errors are not explicitly modelled; however, as operators only perceive aquifer conditions at each well, they only have limited information about subsurface conditions.
		II.iv.b What state variables of which other individuals can an individual perceive?	N/A
		II.iv.c What is the spatial scale of sensing?	Local (geohydrological grid cell)
		II.iv.d Are the mechanisms by which agents obtain information modeled explicitly, or are individuals simply assumed to know these variables?	Information sharing mechanisms are not explicitly modelled for this case study.
		II.iv.e Are costs for cognition and costs for gathering information included in the model?	N/A
	II.v Individual Prediction	II.v.a Which data uses the agent to predict future conditions?	ATES operators use past system performance as an indicator for adoption. Foresight is not explicitly modelled.
		II.v.b What internal models are agents assumed to use to estimate future conditions or consequences of their decisions?	N/A

		II.v.c Might agents be erroneous in the prediction process, and how is it implemented?	Effective system performance will differ from past performance due the construction of new wells over time in the agent-based model, and to thermal processes in the geohydrological model.
	II.vi Interaction	II.vi.a Are interactions among agents and entities assumed as direct or indirect?	ATES operators interact indirectly through the geohydrological model, due to positive or negative thermal interactions between wells.
		II.vi.b On what do the interactions depend?	Thermal interactions depend on the location and flow properties of ATES wells, and on the geohydrological properties of the aquifer.
		II.vi.c If the interactions involve communication, how are such communications represented?	N/A
		II.vi.d If a coordination network exists, how does it affect the agent behaviour? Is the structure of the network imposed or emergent?	N/A
	II.vii Collectives	II.vii.a Do the individuals form or belong to aggregations that affect, and are affected by, the individuals? Are these aggregations imposed by the modeller or do they emerge during the simulation?	ATES well agents are grouped into sets belonging to a given ATES operator agent.
		II.vii.b How are collectives represented?	N/A
	II.viii Heterogeneity	II.viii.a Are the agents heterogeneous? If yes, which state variables and/or processes differ between the agents?	ATES well agents share the same flow profile, and ATES system agents share performance thresholds used in decision-making. Other physical properties (current temperature/head) are heterogeneous based on aquifer conditions.
		II.viii.b Are the agents heterogeneous in their decision-making?	All ATES system agents use the same decision model.
	II.ix Stochasticity	II.ix.a What processes (including initialization) are modeled by assuming they are random or partly random?	ATES system operator agents and new ATES well agents are initialized at random locations (within policies for minimal distances between wells).
	II.x Observation	II.x.a What data are collected from the ABM for testing, understanding, and analyzing it, and how and when are they collected?	ATES system operators o Number of active wells o Realized system performance ATES wells o Thermal performance: energy injected/recovered Aquifer o Fraction of total aquifer volume used for thermal storage o Temperature and head distributions The data are collected at each time step in each model layer.
		II.x.b What key results, outputs or characteristics of the model are emerging from the individuals? (Emergence)	ATES adoption dynamics are affected by the minimal required distance between wells. Insufficient distances may result in rapid adoption followed by a collapse in performance, as interference between wells eventually reduces thermal efficiency. Larger distances will increase the individual efficiency of systems but limit the total number of wells which can be built.

III) Details	III.i Implementation Details	III.i.a How has the model been implemented?	Agent-based model: NetLogo 6.0 Geohydrological model: MODFLOW-2005/SEAWAT 4 The model components are linked through an object-oriented architecture developed using Python 3.6, with NetLogo agents mapped to corresponding Python objects. The FloPy library (Mark Bakker et al., 2013) provides a pre-/post-processing interface between Python and the geohydrological model. The coupled architecture is executed using the EMA Workbench Python package for experiment design and exploratory modelling and analysis (Kwakkel, 2017).
		III.i.b Is the model accessible and if so where?	N/A
	III.ii Initialization	III.ii.a What is the initial state of the model world, i.e. at time t=0 of a simulation run?	The model is initialized with 10 randomly located ATES operator agents, each of which initially owns 2 randomly located ATES well agents.
		III.ii.b Is initialization always the same, or is it allowed to vary among simulations?	The random agent locations vary across replications.
		III.ii.c Are the initial values chosen arbitrarily or based on data?	Locations are chosen randomly within policies on the minimum distance between ATES wells.
	III.iii Input Data	III.iii.a Does the model use input from external sources such as data files or other models to represent processes that change over time?	N/A
	III.iv Submodels	III.iv.a What, in detail, are the submodels that represent the processes listed in 'Process overview and scheduling'?	N/A
		III.iv.b What are the model parameters, their dimensions and reference values?	N/A
		III.iv.c How were submodels designed or chosen?	N/A

References

An, L., 2012. Modeling human decisions in coupled human and natural systems: review of agent-based models. Ecol. Model. 229, 25–36.

Antle, J.M., Capalbo, S.M., Elliott, E.T., Hunt, H.W., Mooney, S., Paustian, K.H., 2014. Research needs for understanding and predicting the behavior of managed ecosystems: lessons from the study of agroecosystems. Ecosystems 4, 723–735.

Bakker, M., Post, V., Langevin, C.D., Hughes, J.D., White, J.T., Starn, J.J., Fienen, M.N., 2016. Scripting MODFLOW Model Development Using Python and FloPy, Groundwater. (n/a–n/a).

Bakr, M., van Oostrom, N., Sommer, W., 2013. Efficiency of and interference among multiple Aquifer Thermal Energy Storage systems; A Dutch case study. Renew. Energy 60, 53–62.

Bankes, S., Walker, W.E., Kwakkel, J.H., 2013. Exploratory modeling and analysis. In: Gass, S.I., Fu, M.C. (Eds.), Encyclopedia of Operations Research and Management Science. Springer US, pp. 532–537.

Becu, N., Perez, P., Walker, A., Barreteau, O., Page, C.L., 2003. Agent based simulation of a small catchment water management in northern Thailand: description of the CATCHSCAPE model. Ecol. Model. 170, 319–331.

Berger, T., 2001. Agent-based spatial models applied to agriculture: a simulation tool for technology diffusion, resource use changes and policy analysis. Agric. Econ. 25, 245–260.

Bithell, M., Brasington, J., 2009. Coupling agent-based models of subsistence farming with individual-based forest models and dynamic models of water distribution. Environ. Model. Softw 24, 173–190.

Bloemendal, M., Hartog, N., 2018. Analysis of the impact of storage conditions on the thermal recovery efficiency of low-temperature ATES systems. Geothermics 71, 306–319.

Bloemendal, M., Jaxa-Rozen, M., Olsthoorn, T., 2018. Methods for planning of ATES systems. Appl. Energy 216, 534–557.

Bonte, M., 2013. Impacts of Shallow Geothermal Energy on Groundwater Quality, PhD Thesis. Vrije Universiteit Amsterdam, Amsterdam.

Bryant, B.P., Lempert, R.J., 2010. Thinking inside the box: a participatory, computer-assisted approach to scenario discovery. Technol. Forecast. Soc. Change 77, 34–49.

Calje, R., 2010. Future Use of Aquifer Thermal Energy Storage below the Historic Centre of Amsterdam, Master's Thesis. Delft University of Technology.

Campolongo, F., Cariboni, J., Saltelli, A., 2007. An effective screening design for sensitivity analysis of large models. Environ. Model. Softw 22, 1509–1518.

Castilla-Rho, J.C., Mariethoz, G., Rojas, R., Andersen, M.S., Kelly, B.F.J., 2015. An agent-based platform for simulating complex humanaquifer interactions in managed groundwater systems. Environ. Model. Softw 73, 305–323.

Deadman, P., Schlager, E., Gimblett, R., 2000. Simulating common pool resource management experiments with adaptive agents employing alternate communication routines. J. Artif. Soc. Soc. Simulat. 3.

Filatova, T., Verburg, P.H., Parker, D.C., Stannard, C.A., 2013. Spatial agent-based models for socio-ecological systems: challenges and prospects. Environ. Model. Softw 45, 1–7.

Filatova, T., Polhill, J.G., van Ewijk, S., 2016. Regime shifts in coupled socio-environmental systems: review of modelling challenges and approaches. Environ. Model. Softw 75, 333–347.

Friedman, J.H., Fisher, N.I., 1999. Bump hunting in high-dimensional data. Stat. Comput. 9, 123–143.

Ghorbani, A., 2013. Structuring Socio-Technical Complexity: Modelling Agent Systems Using Institutional Analysis, PhD Thesis. Delft University of Technology.

Gotts, N.M., Polhill, J.G., 2010. Size matters: large-scale replications of experiments with fearlus. Adv. Complex Syst. 13, 453–467.

Hadka, D., Herman, J., Reed, P., Keller, K., 2015. An open source framework for many-objective robust decision making. Environ. Model. Softw 74, 114–129.

Harbaugh, A.W., 2005. MODFLOW-2005, the US Geological Survey Modular Ground-Water Model: the Ground-Water Flow Process. U.S. Geological Survey.

Hare, M., Deadman, P., 2004. Further towards a taxonomy of agent-based simulation models in environmental management. Math. Comput. Simulat. 64, 25–40.

Hecht-Mndez, J., Molina-Giraldo, N., Blum, P., Bayer, P., 2010. Evaluating MT3dms for heat transport simulation of closed geothermal systems. Gr. Water 48, 741–756.

Herman, J., Usher, W., 2017. SALib: an open-source Python library for Sensitivity Analysis. The Journal of Open Source Software 2.

Jager, W., Janssen, M.A., De Vries, H.J.M., De Greef, J., Vlek, C.A.J., 2000. Behaviour in commons dilemmas: Homo economicus and Homo psychologicus in an ecological-economic model. Ecol. Econ. 35, 357–379.

Janssen, M., 2006. Chapter 30 governing social-ecological systems. In: In: Judd, L.T.a.K.L. (Ed.), Handbook of Computational Economics Vol. 2. Elsevier, pp. 1511–1548.

Janssen, M., Ostrom, E., 2006. Empirically based, agent-based models. Ecol. Soc. 11, 37.

Jaxa-Rozen, M., Kwakkel, J., 2018. PyNetLogo: linking NetLogo with Python. J. Artif. Soc. Soc. Simulat. 21, 4.

Kelly, R.A., Jakeman, A.J., Barreteau, O., Borsuk, M.E., ElSawah, S., Hamilton, S.H., Henriksen, H.J., Kuikka, S., Maier, H.R., Rizzoli, A.E., van Delden, H., Voinov, A.A., 2013. Selecting among five common modelling approaches for integrated environmental assessment and management. Environ. Model. Softw 47, 159–181.

Kunneke, R., Finger, M., 2009. The Governance of Infrastructures as Common Pool

Resources, Fourth Workshop on the Workshop. WOW4, Bloomington, IN.
Kwakkel, J.H., 2017. The Exploratory Modeling Workbench: an open source toolkit for exploratory modeling, scenario discovery, and (multi-objective) robust decision making. Environ. Model. Softw 96, 239–250.
Kwakkel, J.H., Jaxa-Rozen, M., 2016. Improving scenario discovery for handling heterogeneous uncertainties and multinomial classified outcomes. Environ. Model. Softw 79, 311–321.
Langevin, C.D., Thorne Jr., D.T., Dausman, A.M., Sukop, M.C., Guo, W., 2008. SEAWAT Version 4: a Computer Program for Simulation of Multi-Species Solute and Heat Transport, Technical Report. U.S. Geological Survey.
Lempert, R., Popper, S., Bankes, S., 2003. Shaping the Next One Hundred Years: New Methods for Quantitative, Long-Term Policy Analysis, Technical Report MR-1626. RAND Corporation, Santa Monica, CA.
Lempert, R.J., Groves, D.G., Popper, S.W., Bankes, S.C., 2006. A general, analytic method for generating robust strategies and narrative scenarios. Manag. Sci. 52, 514–528.
Lo Russo, S., Gnavi, L., Roccia, E., Taddia, G., Verda, V., 2014. Groundwater Heat Pump (GWHP) system modeling and Thermal Affected Zone (TAZ) prediction reliability: influence of temporal variations in flow discharge and injection temperature. Geothermics 51, 103–112.
Matthews, R., Polhill, J., Gilbert, N., Roach, A., 2005. Integrating agent-based social models and biophysical models. In: MODSIM05-International Congress on Modelling and Simulation: Advances and Applications for Management and Decision Making, Proceedings, pp. 1617–1623.
Matthews, R., Gilbert, N., Roach, A., Polhill, J., Gotts, N., 2007. Agent-based land-use models: a review of applications. Landsc. Ecol. 22, 1447–1459.
McKinney, W., 2010. Data structures for statistical computing in Python. In: Walt, S. v. d., Millman, J. (Eds.), Proceedings of the 9th Python in Science Conference, pp. 51–56.
Mller, B., Bohn, F., Dreler, G., Groeneveld, J., Klassert, C., Martin, R., Schlter, M., Schulze, J., Weise, H., Schwarz, N., 2013. Describing human decisions in agent-based models ODD + D, an extension of the ODD protocol. Environ. Model. Softw 48, 37–48.
Ostrom, E., 2009. A general framework for analyzing sustainability of social-ecological systems. Science 325, 419–422.
Railsback, S., Aylln, D., Berger, U., Grimm, V., Lytinen, S., Sheppard, C., Thiele, J., 2017. Improving execution speed of models implemented in NetLogo. J. Artif. Soc. Soc. Simulat. 20, 3.
Rawlani, A.K., Sovacool, B.K., 2011. Building responsiveness to climate change through community based adaptation in Bangladesh. Mitig. Adapt. Strategies Glob. Change 16, 845–863.
Reeves, H.W., Zellner, M.L., 2010. Linking MODFLOW with an agent-based land-use model to support decision making. Gr. Water 48, 649–660.
Rosenhead, J., Elton, M., Gupta, S.K., 1972. Robustness and optimality as criteria for strategic decisions. Oper. Res. Q. (1970-1977) 23, 413–431.
Rostampour, V., Bloemendal, M., Jaxa-Rozen, M., Keviczky, T., 2016. A control-oriented model for combined building climate comfort and aquifer thermal energy storage system. In: European Geothermal Congress, Strasbourg, France.
Saltelli, A., Annoni, P., 2010. How to avoid a perfunctory sensitivity analysis. Environ. Model. Softw 25, 1508–1517.
Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S., 2008. Global Sensitivity Analysis: the Primer. John Wiley & Sons.
Scheffer, M., Carpenter, S., Foley, J.A., Folke, C., Walker, B., 2001. Catastrophic shifts in ecosystems. Nature 413, 591.
Schlter, M., Pahl-Wostl, C., 2007. Mechanisms of resilience in common-pool resource management systems: an agent-based model of water use in a river basin. Ecol. Soc. 12, 4.
Schlter, M., Mcallister, R.R.J., Arlinghaus, R., Bunnefeld, N., Eisenack, K., Hlker, F., Milner-Gulland, E., Mller, B., Nicholson, E., Quaas, M., Stven, M., 2012. New horizons for managing the environment: a review of coupled social-ecological systems modeling. Nat. Resour. Model. 25, 219–272.
Schlter, M., Hinkel, J., Bots, P.W.G., Arlinghaus, R., 2014. Application of the SES framework for model-based analysis of the dynamics of social-ecological systems. Ecol. Soc. 19.
Sommer, W., Valstar, J., Leusbrock, I., Grotenhuis, T., Rijnaarts, H., 2015. Optimization and spatial pattern of large-scale aquifer thermal energy storage. Appl. Energy 137, 322–337.
Sun, Z., Lorscheid, I., Millington, J.D., Lauf, S., Magliocca, N.R., Groeneveld, J., Balbi, S., Nolzen, H., Mller, B., Schulze, J., Buchmann, C.M., 2016. Simple or complicated agent-based models? A complicated issue. Environ. Model. Softw 86, 56–67.
Tavoni, A., Levin, S., 2014. Managing the climate commons at the nexus of ecology, behaviour and economics. Nat. Clim. Change 4, 1057–1063.
Thiele, J.C., Kurth, W., Grimm, V., 2012. RNETLOGO: an R package for running and exploring individual-based models implemented in NETLOGO. Methods in Ecology and Evolution 3, 480–483.
Vincenot, C.E., Giannino, F., Rietkerk, M., Moriya, K., Mazzoleni, S., 2011. Theoretical considerations on the combined use of System Dynamics and individual-based modeling in ecology. Ecol. Model. 222, 210–218.
Voinov, A., Shugart, H.H., 2013. Integronsters, integral and integrated modeling. Environ. Model. Softw 39, 149–158.
Walt, S. v. d., Colbert, S.C., Varoquaux, G., 2011. The NumPy array: a structure for efficient numerical computation. Comput. Sci. Eng. 13, 22–30.
Wilensky, U., 1999. NetLogo.
Zhang, H., Xu, W.L., Hiscock, K.M., 2013. Application of MT3dms and geographic information system to evaluation of groundwater contamination in the sherwood sandstone aquifer, UK. Water, air, & Soil Pollution 224, 1438.
Zheng, C., Wang, P.P., 1999. MT3dms: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and Users Guide.