Hydroinformatics in multi-colours—part green: applications in aquatic ecosystem modelling

Hong Li, Arthur E. Mynett and Qing Hua Ye

ABSTRACT

The present paper focuses on demonstrating the capabilities of modern hydroinformatics tools in the field of environmental systems by integrating biotic and abiotic process modelling. Abiotic processes like hydrodynamic flow and transport phenomena are often formulated based on physical principles like conservation of mass, momentum and energy. These processes are adequately represented mathematically by second order partial differential equations that can be solved numerically in a variety of ways. However, in aquatic ecosystem modelling, biological/ecological processes play an important role and these processes are not always understood at the required level of detail to be captured in terms of conservation principles. In this paper two modelling approaches for biotic processes are explored for representing spatial pattern dynamics of aquatic ecosystems: (i) cellular automata (CA) and (ii) multi-agent systems (MAS) models, in combination with Delft 3D-WAQ for advanced flow and transport modelling. It is shown that CA are quite capable of capturing discrete growth phenomena like outcompeting plant species which are known to depend mainly on local effects. A MAS approach can combine nonlinearity, randomness and complexity of aquatic ecosystems, which can then be used to enhance the capabilities of available physics-based software systems like the DELFT3D software suite.

Key words | aquatic ecosystem modelling, cellular automata, DELFT3D software suite, DELWAQ open process library, environmental hydroinformatics, multi-agent systems

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INTRODUCTION

Hydroinformatics found its origin in the advancement of computational hydraulics in the early 1990s but has expanded considerably, both in scope and in application areas. It is now not only being applied in the fields of hydraulics and hydrology (often indicated by the colour blue), but also in urban applications (red), as well as in knowledge systems and knowledge management (yellow). The present article focuses on 'Hydroinformatics in green', demonstrating the capabilities of hydroinformatics in environmental science and technology. It is part of a sequence of articles, each focusing on a particular field (colour) of hydroinformatics, which together constitute a multi-coloured rainbow of application areas that hydroinformatics has expanded into over the past two decades or so. The combined articles on 'Hydroinformatics in multi-colours' were presented as the opening keynote of the Workshop on Advances in Hydroinformatics held in Niagara Falls, June 2007, as reported by Coulibaly *et al.* (2009). The first article of the sequence focused on 'Hydroinformatics in red' taking urban flood and disaster management as an example (Mynett & Vojinovic 2009). The present paper focuses on 'Hydroinformatics in green' demonstrating the capabilities of hydroinformatics tools and technologies in integrating biotic and abiotic processes in environmental systems modelling.

Hydrodynamic flow and transport processes are conventionally based on physical (conservation) principles of mass, momentum and energy which are well represented by continuous partial differential equations. These often form the basis of many professional software packages like the

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DELFT3D software suite, dealing with abiotic processes (flow velocities, nutrient transport rates, etc.) which have been successfully applied in many practical cases. Due to the elliptic nature of the governing equations, solutions obtained for the entire domain are determined by initial and boundary conditions at the *global* level. However, in case of biotic processes, spatial pattern dynamics for aquatic populations often arise as a result of individual growth properties and *local* interactions amongst the species themselves as well as with local flow conditions and local changes of substances in the water body.

In the field of environmental hydroinformatics (Mynett 2002, 2004), a range of modelling paradigms can be employed in aquatic ecosystem modelling: discrete modelling like cellular automata (CA) for harmful algal bloom prediction (Mynett & Chen 2004; Li *et al.* 2006), individual-based modelling for mussel population dynamics (Morales *et al.* 2006; Mynett & Morales 2006) and agent-based approaches like Multi-Agent Systems (MAS) for out-competing species interaction (Li 2009; Li *et al.* 2010).

Only a limited number of references can be found in the literature on modelling spatial pattern dynamics of macrophytes or other aquatic plants using physically-based models (Van Nes *et al.* 2003; Velez & Mynett 2006). On the other hand, several researchers have developed non-spatially explicit mathematical formulations for aquatic plant (or macrophytes) growth (Scheffer *et al.* 1993; Asaeda & Van Bon 1997; Carr *et al.* 1997; Asaeda *et al.* 2000; Madsen *et al.* 2001; Scheffer 2009). Such formulations can then be coupled with spatially explicit methods like hydrodynamic flow modelling and have been successfully applied in practice. Velez & Mynett (2006) added a non-spatial plant growth function into the Delft3D-WAQ open process library (OPL) that enabled spatial pattern dynamics simulation for emerging aquatic plants (water hyacinths) in Sonso Lagoon, Colombia. Li (2009) modelled the spatial pattern dynamics of water lily growth using CA combined with high resolution photographs. Some literature on modelling macrophytes growth consider spatial patterns as a stochastic process (Chiarello & Barrat-Segretain 1997). Li *et al.* (2010) applied a MAS approach for revealing the spatial pattern dynamics of two interacting macrophytes.

One of the difficulties in modelling aquatic plant dynamics is that the large variety of species with very different characteristics cannot be represented only in terms of biomass. In the literature, many references describing the growth of a particular species use detailed physiological data relevant to the species of interest (Van Nes *et al.* 2003), which seems a more reasonable approach than using some generic formulation. Still, growth simulation models often do not consider the spatial extension of aquatic plant growth. This requires a different approach from mathematical formulae, such as empirical rules or a knowledge-based approach, or a spatially explicit modelling concept.

One such spatially explicit modelling approach, namely CA, has attracted many researchers in various fields of science since the concept was introduced (Von Neumann 1949). CA models deal with spatial variation and local interactions. They provide simple discrete deterministic mathematical models for physical, biological and computational systems in which many simple components act together to produce complicated patterns of behaviour (Packard & Wolfram 1985; Wolfram 2002).

MAS have grown from artificial life and are widely accepted in many fields (Lesser 1999), especially in social sciences (Joshua & Robert 1996; Ferber 1999). MAS allow aquatic spatial pattern dynamics to emerge from the behaviour of individuals or groups of individuals and their interactions, which gives insights into their growth, interaction and spreading mechanisms.

Since environmental hydroinformatics is concerned both with abiotic and biotic processes, one of the major research efforts in this field is to combine different mathematical approaches into one coherent modelling framework. Clearly, this is not an easy task since it involves the coupling of different processes with different spatio-temporal scales; the integration of different types of information and data sources, as well as the linking of different modelling concepts. Regarding appropriate scales, it may be noted that hydrodynamic and advection-diffusion processes can have a dynamic time scale of seconds, while water quality (WAQ) conditions may range from hours to days, whereas aquatic plants generally change at a much slower pace with characteristic time scales on the order of weeks or months. Although the concept of *integration* in aquatic ecosystem modelling is not novel (Jorgensen & Bendoricchio 2001), a synthesis of multi-agent based discrete modelling with physically-based continuous modelling for simulating aquatic population dynamics has only recently emerged in the literature (Li 2009; Li *et al.* 2010).

This paper aims to demonstrate some available alternative modelling approaches in environmental hydroinformatics using practical examples. First, a case study is presented using CA to emulate macrophytes growth in a confined pond, comparing the simulated spatial growth patterns with observations from high resolution photographs (Li 2009). Second, a synthesis of the MAS approach into a physically-based modelling framework was tested extending from Li (2009) for modelling two types of outcompeting underwater macrophytes.

DISCRETE MODELLING USING CELLULAR AUTOMATA

Basic concept

A two-dimensional CA is conventionally defined as a double array of lattices (topologically similar to a rectangular grid) on which a number of different neighbourhood schemes (computational stencils) can be defined. Some classical neighbourhood schemes include: (i) a five-cell (Von Neumann) scheme, (ii) a nine-cell (Moore) scheme, and even (iii) a 13 cell (Extended Moore) scheme (Figure 1). The underlying concept is based on the assumption that the future state of the centre cell depends on the states of the neighbouring cells. Classical neighbourhood schemes consider equal weights for all the neighbouring cells, and the rules are applied homogeneously over the whole domain.

When setting up a CA model, neighbourhood schemes, appropriate space and time steps, initial conditions, boundary conditions and transition rules have to be established.

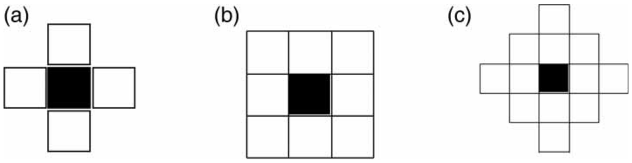

Figure 1 | Neighbourhood schemes: (a) Von Neumann, (b) Moore, and (c) Extended Moore.

The selection of appropriate grid size and time step depends on the particular process to be modelled; in the case of macrophytes growth simulation, this is directly related to the growth properties of the considered plant. The initial and boundary conditions can be obtained from other models or from *in situ* measurements like remote sensing images, aerial photographs, etc. The transition rules define that all cells change their state S at discrete time-steps based on the current state of the cell itself and of its neighbouring cells, through certain transition rules f as expressed by Equation (1):

$$S_i^{n+1} = f(S_i^n, S_{i1}^n, S_{i2}^n, S_{i3}^n, S_{i4}^n \ldots\ldots) \tag{1}$$

where: n is the current time level, $n+1$ is one time step ahead, S_{i1}, S_{i2}, S_{i3}, S_{i4} etc. are the neighbouring cells of S_i, while each cell uses the same rules f. The initial pattern constitutes the '*seeds*' of the system. Each generation is a function of the previous generation and the rules are applied simultaneously to every cell in the whole domain at each discrete moment in time. The rules continue to be applied repeatedly to create a next generation of states, etc.

Boundary conditions need to be defined for the particular domain of interest. If the domain is a closed water body like a pond or a lake, fixed/closed boundary conditions can be applied. However, if the research domain can have mass exchange across some boundaries (like a seaward boundary in the case of coastal zone modelling), open boundary conditions have to be supplied.

Expert (biological/ecological) knowledge is usually required to define the appropriate spatio-temporal dependences. Also, in aquatic population dynamics modelling there are several possibilities for constructing the local rules f in CA modelling: (a) by using simple if-then-else rules based on the data and empirical or experimental knowledge (Li 2009); (b) by using weighted rules which emphasize the importance of distance or other factors that can bias contributions from neighbouring cells, e.g. a particular hydrodynamic flow pattern; (c) fuzzy inference rules obtained from training using the available data and combining with expert knowledge into a set of transition rules (Chen 2004); (d) probabilistic rules which can be used to create a stochastic CA model; (e) rules automatically generated by the available data using machine learning techniques (Li *et al.* 2012), e.g. artificial neural networks, which can be quite suitable provided sufficient data are available.

Photography-based cellular automata in aquatic plant dynamics modelling

Spatial pattern evolution is a crucial aspect of aquatic plant growth that also affects other species in the same ecosystem. Locally, plants interact mainly with their immediate neighbours only, while on a larger scale patterns arise that are characterized by their overall density and shape, commonly referred to as *patchiness*. During the last decade or so, there is an increasing trend in research on spatial pattern dynamics modelling (Mynett & Chen 2004) with special attention being paid to spatial plant evolution (Chen *et al.* 2002; Freckleton & Watkinson 2002; Giusti & Marsili-Libelli 2006; Hogeweg 2007). Among the various modelling approaches, cell-based locally interactive models CA seem to have great potential for representing the spatial patterns evolving predominantly from local interactions.

The CA model developed in this research for mimicking macrophytes growth in a small pond was based on combining time series of high-resolution photos, meteorological data and plant properties (Li 2009). The effects of cell size and neighbourhood scheme for capturing the specific biological characteristics are explored, as briefly summarized below.

Influencing factors for water lily growth

In the food web of an ecosystem, macrophytes are sources of food and shelter for other species like fish and ducks. They contribute to nutrient recycling, flow condition stabilization, and can also change the hydraulic roughness of the bottom of lakes or ponds. One particular type of macrophytes considered here, the water lily (*Nymphaeaceae*), is rooted in the soil in bodies of shallow water (optimal depth less than about 1 m), with leaves and flowers floating on the water surface. The *Nymphaeaceae* family contains round leaves (diameter 6–11 cm) that are able to store sufficient energy for growth. One water lily plant can typically attain 1 m or so in height (from the bottom) and cover a surface space with a diameter ranging between 0.5 and 1.0 m, while its flower can have a diameter of 3–6 cm. Water lilies are well adapted to their habitat. They grow and live on the edge of ponds and lakes, and in the shallow water parts. The climate of their habitat is usually warm and they live in water that is rich in oxygen and receives a great deal of sunlight.

Plant growth in a pond depends on the ecological interactions and is also constrained by abiotic conditions (Brönmark & Hansson 2005). In case of small lakes or ponds, conditions such as light penetration, water temperature and nutrients availability are in general homogenous and therefore contribute mainly to the temporal dynamics rather than to the spatial patchiness of aquatic plants. Local interactions, bathymetric features and even more importantly initial seeding positions, were considered to be the main factors when developing the CA model for water lily growth. In order to set up and calibrate the CA model, weekly high resolution photos were used which show the spatial distribution of macrophytes (water lily) at the water surface in a small pond (about 52 × 26 m).

Model development

The development of the CA model for water lily growth was carried out in the Matlab environment. The photo of week 18 was processed and taken as the initial matrix (Figure 2) for the basic model and for all subsequent scenarios applied in this case study. The general assumptions for this basic CA

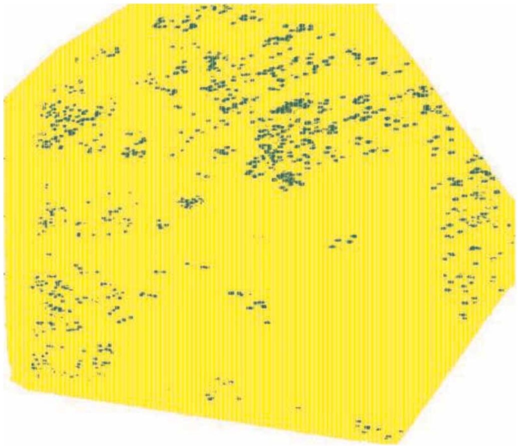

Figure 2 | Initial model condition retrieved from high resolution photo in week 18 (grey background is water, dotted spots are water lilies).

model are: (1) CA model cell states – there are only two states (water lily with value 1 and water with value 0; (2) CA model background – there is no nutrient limitation, there is no influence from hydrodynamics and wind; (3) CA neighbourhood schemes – spatial extension by seeding or by new leaves only happens in the nearest neighbouring cells, namely in the case of the Von Neumann neighbourhood scheme, only in the nearest 4 cells; and (4) CA transition rules – all neighbouring cells have equal rights to contribute to the growth of the central cell and rules are applied homogeneously throughout the entire domain.

The considered factors influencing the water lily spatial pattern dynamics for the basic CA model are: (i) weekly averaged water temperature (and differences); (ii) weekly accumulated sunshine duration; (iii) specific plant properties (e.g. life span, specific age, etc.); (iv) conditions in neighbouring cells. The considered neighbourhood schemes are Von Neumann and Moore neighbourhood schemes, respectively. Model cell size is based on the resolution of the photos; in this case, a cell size of 4 × 4 cm served as the basic model grid. The model time step is taken to be 1 week.

The rules are if-then-else rules based on the above influencing factors in combination with the available data and information: photos of spatial coverage, measured water temperature, as well as specific properties of the macrophytes obtained from expert knowledge. Some examples of simple rules employed in this case study are as follows:

1. Growth rate: the normal growth and the fastest growth are defined. For example, one of the rules for the fastest growth is that when the temperature is higher than 16 °C and the sunshine duration is more than 40 h a week – then, under such conditions and as long as there is at least one neighbouring cell that has a plant, a plant will grow in this cell as well.
2. Life span: a threshold of 18 weeks was considered; after a plant exists for 18 weeks, it will die.
3. Spatial extension of the plants: if there are favourable weather conditions, and at an age less than 18 weeks, and neighbouring cells are relatively empty – then the plant expands to its neighbouring cells either with the form of newly growing plants or by expansion of the leaves of existing plants.
4. Mortality rate: varies with temperature, sunlight duration and temperature differences. For instance, if the temperature is between 15 and 12 °C, and the temperature drop is more than 3 °C compared to the previous week, then those cells which have less than two neighbouring cells with plants will die.

Table 1 | Scenarios for model cell configuration

Scenarios	S1	S2	S3	S4	S5
Cell size (cm^2)	4 × 4	8 × 8	12 × 12	20 × 20	40 × 40

Different scenarios were carried out to explore the effects of model structure including different neighbourhood schemes and cell sizes. The selection of proper scales depends on many factors including the availability of measurement data, the characteristics of the type of plants, and the chosen model structure. The cell size was based on the photo resolution and multiples of 4 × 4 cm basic grid size to form the basic scenario (S1). Scenarios were conducted with a multiplier of the original cell size from the basic model S1:S2 with 2 times (8 × 8 cm), S3 with 3 times (12 × 12 cm), S4 with 5 times (20 × 20 cm) and S5 with 10 times (40 × 40 cm) the original cell size (Table 1). In addition, modelling results are also influenced by the selection of the particular neighbourhood scheme. Therefore, these five scenarios are implemented both for Von Neumann and for Moore neighbourhood schemes.

Analysis of results

The basic model, which has 4 × 4 cm grid size, is considered as the reference to check whether it is possible to depict the patterns exhibited on the photos by using a CA model with simple if-then rules. The spatial pattern of week 30 is shown in Figure 3(a) for the Von Neumann neighbourhood scheme

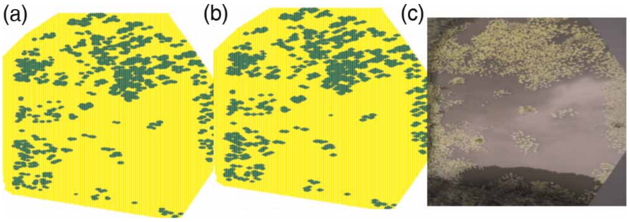

Figure 3 | Spatial patterns predicted by the basic model (a) with Von Neumann, (b) with Moore (c) photo observation for week 30.

and in Figure 3(b) for the Moore neighbourhood scheme. The modelling results are compared with the photo in Figure 3(c) taken at that same week.

Since the pond is quite static and no nutrient limitation seems to be present, the spatial pattern of the modelling results evolving from this basic model are seen to agree quite well both in patchiness and in terms of total plant coverage, compared with the photo observation. However, some of the areas seem to have a lesser density compared with the photo. The resulting water lily coverage in the whole pond, together with the occupation percentages retrieved from the photos, is shown in Figure 4.

Compared to the ratios of plant cells and total cells calculated from the weekly photos (percentage of plant cells), it is seen that the model can capture the growth trend quite well compared with the data retrieved from the photos, although in general the models seem to slightly underestimate the growth. The use of a Moore neighbourhood scheme seems to provide slightly better results than the Von Neumann neighbourhood scheme in the growth process (from modelling time step 1 to 25). Both modelling results using Von Neumann and Moore neighbourhood scheme provide a good match in the decay period. The underestimation of water lily growth indicates that there are also other factors influencing the modelled growth patterns. Therefore, sensitivity analyses for the models were carried out to investigate the effect of CA cell size in aquatic plant dynamics modelling.

For sensitivity analyses, the five scenarios shown in Table 1 were explored for both Von Neumann and Moore neighbourhood schemes. The comparisons between photos and modelled water lily spatial patterns for different cell sizes and percentages of water lily spatial occupation indicate that not only the factors included in the basic model can influence the model results, but the choice of cell size and configuration can also be vital for the simulation of water lily growth dynamics. The Root Mean Squared Errors (RMSEs) in spatial occupation was also calculated. The results shown in Table 2 indicate that the best scenario was S2 with Von Neumann neighbourhood scheme, namely double the original 4 × 4 cm cell size, closely matched by a Moore scheme with original S1 cell size. It should be noted that both Von Neumann S2 and Moore S1 stencils have approximately the same stencil size, corresponding to a typical mature water plant leave.

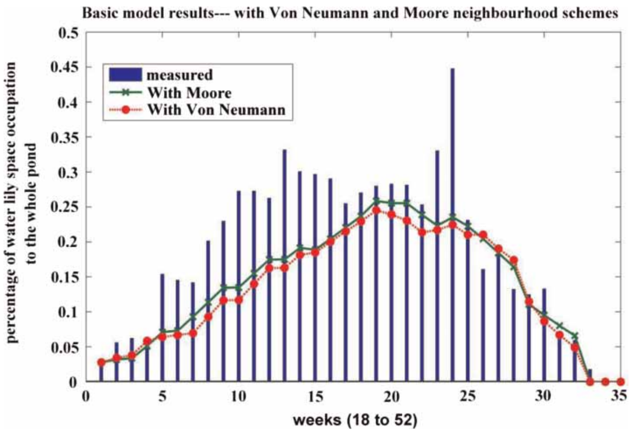

Figure 4 | Comparison of plant occupation percentages: model results using Moore and Von Neumann neighbourhood schemes vs. retrieved from photos.

This leads to the general conclusion from the case study that the model performs best when the selected neighbourhood configuration has the characteristic dimensions of the particular plant species.

The case study explored here was a stagnant pond which has little environmental dynamics and no other interacting species. However, most of the lakes or ponds are much more complicated than the situations in this example. One way of including more complex interactions and influences from other dynamical processes as well, is to use a MAS approach as described hereafter.

SYNTHESIS OF DISCRETE MAS AND CONTINUOUS WAQ MODELS

The main purpose to achieve a synthesis between discrete MAS and continuous process formulations stored in the DELFT3D-WAQ OPL is to achieve online coupling of different dynamical processes involved in aquatic ecosystem modelling, as shown by Li (2009) in the case of macrophytes dynamics. The synthesis model includes the dynamical

Table 2 | RMSEs of resulting water lily spatial occupations compared to the photo of week 30

Scenarios	S1	S2	S3	S4	S5
RMSE with Von Neumann	0.082	**0.073**	0.122	0.201	0.307
RMSE with Moore	**0.075**	0.076	0.123	0.179	0.190

changes in flow patterns and WAQ factors that influence aquatic plant behaviour. Such models can include information and data available as intermediate results to be used as inputs for other processes, which sometimes cannot be obtained from measurements. There are two main parts in the synthesis model: the MAS model for macrophytes dynamics developed in Li *et al.* (2010) and the conventional WAQ and hydrodynamic flow model. The shell used for the synthesis of these two parts is the DELWAQ OPL.

Multi-agent systems

The concept of Individual Based Model (IBM), Agent-Based Model (ABM) and MAS can be traced back to the Von Neumann Computing Machine in the late 1940s. Since then, ABM has been developing and forming its own theory from various elements in artificial intelligence. They are employed in complex systems theory and evolutionary programming in computer science. This field developed significantly when the first widely available computer package designed for ABM (SWARM) was developed by the Santa Fe Institute at the end of the 1980s and during the early 1990s. Nowadays, ABM is a booming field in many applications. One of the commonly accepted concepts for MAS is from Ferber (1999): 'A MAS contains multiple environments, objects and agents (the agents being the only ones to act), relations between all these entities, a set of operations that can be performed by the entities and the changes of the universe in time and due to these actions.'

In the Multi-Agent Based model developed by Li *et al.* (2010), the main actors were: (i) two types of macrophytes as agents, and (ii) their environmental background, such as water temperature, water depth, flow, and WAQ, etc. Each agent has its own processes, e.g. growth, death, interaction, spatial extension and energy gain or loss by motion or feeding under the given environment. There are interactions between agents especially when they are close to each other in space: they may need to compete for food or other energy sources, or one type of agent can be the predator or grazer of another type of agent. There are also interactions between agents and environmental factors, which can be constraints from the environment on agents, and there can be feedbacks from the behaviour of agents to their environment.

Similar to CA, MAS models can be applied to a discrete modelling domain consisting of either structured or unstructured grids that provide the spatial computational background. Contrary to CA, MAS can not only model local interactions (through neighbouring cells) but can also act over longer distances (i.e. extend their influence over distances of multiple cells), represent individual behaviours and include more complicated and flexible interactions among agents and between agents and their environments. Each agent has its own position in the background environment with its own properties and behaviour. There can be interactions amongst different agents themselves, subject to constraints from their surrounding environment. Also, different types of agents can coexist in each and the same background cell and their competition can be both within the cell as well as within the neighbouring regions of the cell, depending on the individual properties assigned to each agent. Because of this, a MAS approach is both flexible and robust, although sometimes computations can become elaborate and time consuming. However, this becomes less and less of a problem because of the continuing advances in computational power.

In the case study of coexisting plant species described in (Li *et al.* 2010), the authors derived the behavioural aspects for each agent (namely here, macrophytes *Pp* and *Cs*) and the interaction and communication between plants and their environment, which led to variations in aquatic plant density, and the equations describing the rate of change of aquatic plant density within each computational cell were summarized.

Also in Li *et al.* (2010), extended Lotka-Volterra (LV) equations were integrated into a MAS modelling approach in order to consider not only competitions due to resources availability, but more importantly to consider the formulation for competition and interaction among species both in space and time. In this way, density variations for each species at each location can be obtained from individual growth properties in combination with other processes such as seed dispersal, seed germination, spatial interaction and extension, interspecies and intraspecies competition, as well as mortality. Furthermore, a small random variation (R) can be considered to represent the stochasticity in aquatic ecosystems. Further details on MAS macrophytes modelling can be found in Li *et al.* (2010).

DELWAQ Open Process Library

A first version of the DELWAQ WAQ module within the DELFT3D software suite was developed in the 1980s by Postma (2007). A flexible process software library was initiated in the early 1990s and the OPL was made available some time later (WL | Delft Hydraulics 2006, 2007). The DELWAQ OPL follows an object-oriented approach where each substance is represented as an object. The interaction between different substances such as WAQ kinetics is also seen as an object. This has very powerful implications. In the OPL, there are several WAQ components: substances (e.g. concentrations or densities of nutrients), processes (e.g. growth of algae), items (e.g. input/output variables of a process) and fluxes (a special class of items consisting of fluxes between substances). The library currently includes more than 200 substances/organisms and fractions of substances which are considered to be universally applicable, as well as more than 400 processes that represent the interactions between substances. Besides, some library functions can be re-used for different substances having the same behaviour, by changing parameter settings or inputs into the function calls. However, not all processes and substances can be specified *a priori* into a process library, especially not processes that depend on evolving spatial pattern dynamics like for macrophytes and other species different from phytoplankton. This would require having an open interface which allows users to add substances and processes, depending on the requirements of each specific process.

The concept of an OPL was developed precisely for this. The DELWAQ process library is an extensible library of WAQ components. The OPL is the developer environment of the Delft Process Library Configuration Tool. Such a developer environment is to facilitate the process of 'creating' new substances, processes, parameters and their settings to become part of the DELWAQ Library Suite. Once the substances, processes, etc. are added, the users can easily decide to switch them on or off without having to bother about the underlying software connections between them. Besides, users can also specify which items they want to be editable through the user interface, or which items they want to add to the output list. Within the OPL, the system takes care of all necessary connections, such as invoking component processes, connecting to outputs and keeping track of fluxes between substances. When the user switches on certain processes, the system identifies all editable items whether they are provided as a constant, as a single time function for the whole area, as a spatially distributed constant or as a spatially distributed time function. The resulting WAQ model configuration contains all choices and is saved for later reference.

Li (2009) explored the use of the DELWAQ OPL to link continuous processes including hydrodynamics (flow) and WAQ (transport) with discrete processes such as spatial pattern evolution of aquatic plants, by developing a synthesis between continuous physically-based models and discrete multi-agent-system models. Since the DELWAQ process library follows an object-oriented approach, it provides an ideal environment for developing such a synthesis model, as illustrated in a case study of two outcompeting species in an inland lake, as discussed next.

State variables and scales

In the case of submerged macrophytes, many different properties need to be represented in the modelling system. Given the large number of macrophytes in a small area (e.g. chara can have 1,000 stems m^{-2}), we consider one of the state variables of vegetation to be the stem density (Np, stem m^{-2}, the number of stems per square metre). The increment of stem density per time step is assumed to be modelled based on an extended logistic function as described in Li *et al.* (2010). In the computational segments, there is a maximum stem density for each species as carrying capacity defined as Np_max (stem m^{-2}). Consequently, the Np/Np_max<=100%.

Each stem has some properties, such as age, lifespan, height (from bed level) and diameter, etc. Due to the high density of macrophytes, populations of macrophytes located within one computational cell are considered as one agent and their values are assigned at the centre of each computational cell. Thus, the model can be seen as a metapopulation model or super-individual model (Grimm & Railsback 2005). Some precaution is needed on the units of each state variable in the programming process. This has to do with how the program couples the different scales of the hydrodynamics model, WAQ model and the macrophytes growth model. Assuming a unified spatial scale for all processes, only the time steps of different processes need to be coupled. For WAQ processes, a typical (default) time step may have the unit of one day. However, for macrophytes growth processes the time scale may be 1 week while hydrodynamic processes may change every few minutes or so.

The synthesis model considers all relevant processes, among them the aquatic plant dynamics module including germination, growth, spatial extension, competition, mortality, seed dispersal. These processes are interacting with the processes of hydrodynamics and WAQ. As indicated in Figure 5, the latter two processes are well developed and modelled by the Delft3D software package, whereas the processes of aquatic plant dynamics are modelled by using a MAS concept (Li *et al.* 2010).

Hydrodynamic conditions can be treated as engines for seeds transportation and for spatial extension, and also can be a limitation for plant germination (higher flow leads to lower germination). Meanwhile, the resulting spatial pattern can also have very important impacts on hydrodynamic patterns although this is not the main focus of this research. In terms of WAQ processes, we see that the most direct link should be that the growth of plants requires nutrients to be available in a local region including the waterbed and the water column, while the photosynthesis of plants provides an input of oxygen into the water body. This can influence the nutrient level and lead to better WAQ conditions (Asaeda *et al.* 2000) by reducing excessive nutrients from the water column.

By using the DELWAQ OPL as the carrier for the synthesis model, the aquatic plant dynamics module is embedded into the WAQ module and is calculated together with other WAQ processes when the model scenarios are set up. The substances group in this case is 'macrophytes' added in the DELWAQ process library and two different types of submerged aquatic plants are considered in this example: *Potamogeton pectinatus* (*Pp*) and *Chara aspera* (*Cs*). The processes included here are based on the detailed description in Li *et al.* (2010) with minor revisions to fulfil the requirements within the Delft3D software package.

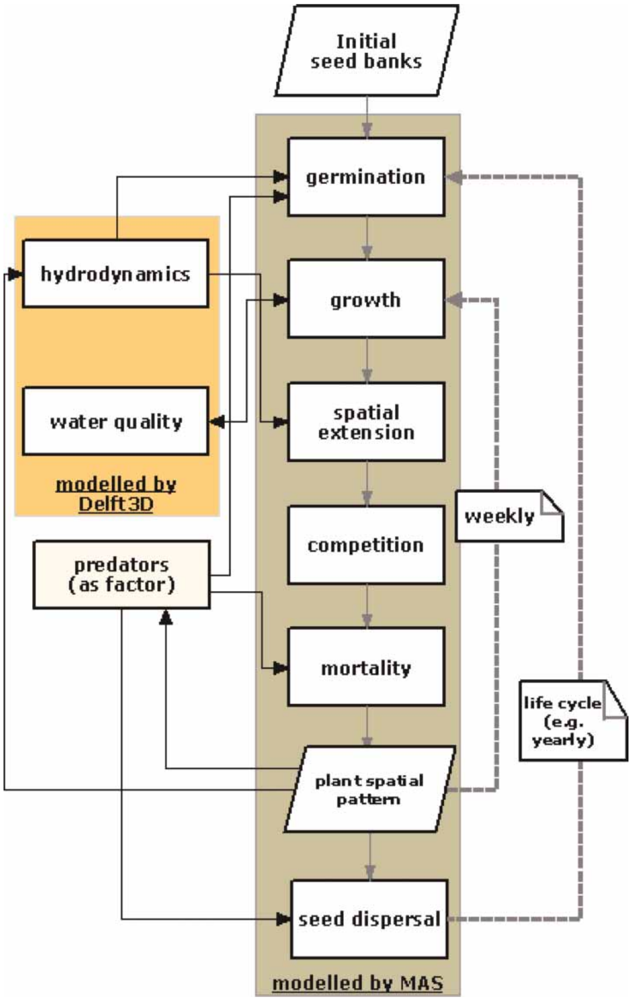

Figure 5 | Processes involved in aquatic plant dynamics modelling (Li 2009).

Application of the synthesis model in Lake Veluwe

Lake Veluwe (*Veluwemeer*) is a shallow (average water depth 1.55 m) and small (about 30 km^2) artificial lake at the centre of the Netherlands (Figure 6). It is currently a macrophyte-dominated system. Since the late 1960s and early 1970s, submerged vegetation has been affected by eutrophication, which led to the first big shift of vegetation in this lake from varieties of macrophytes to only sparse patches of submerged *Potamogeton pectinatus* (*Pp*). In 1979, measures were taken to reduce excessive phosphorus loading (Hosper 1997; Van den Berg *et al.* 2001), which gradually increased the quality of this lake. Between 1987 and 1993, the dominance of *Potamogeton pectinatus* (*Pp*)

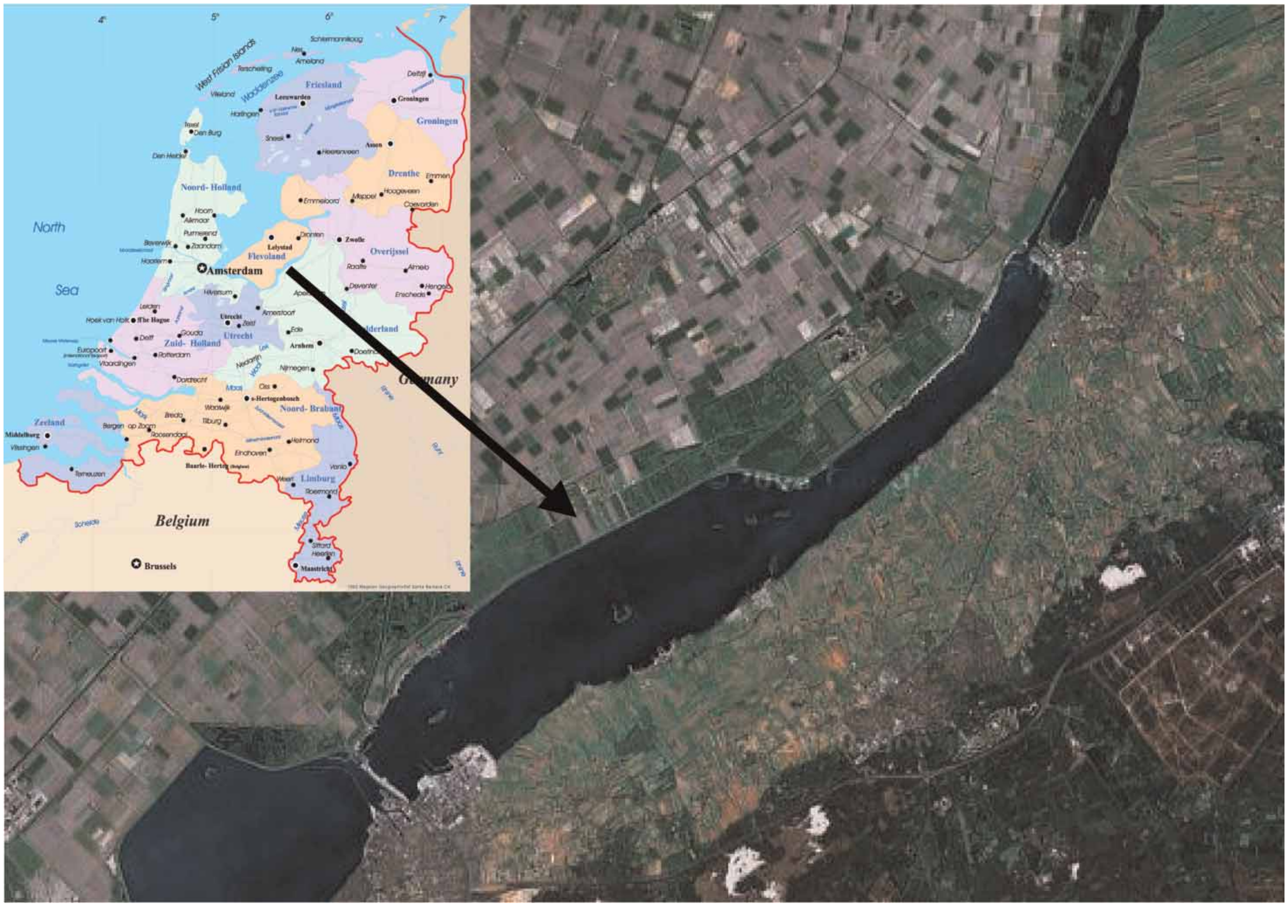

Figure 6 | Location of Lake Veluwe, the Netherlands.

decreased, while Charophyte meadows (e.g. *Chara aspera* (*Cs*)) expanded during the same time interval, which is currently the dominant macrophyte in this lake. Pattern changes of the dominant macrophytes might have resulted from the combination of different processes and effects including hydrodynamics conditions, nutrient conditions, their own biological properties, as well as the interactions among species, etc. Some research has indicated that the pattern change was also due to the change in underwater light climate (Coops & Doef 1996; Van den Berg *et al.* 1998). According to Van den Berg (1999), *Pp* is a better competitor for light and temperature than *Cs* due to the shading effects of its canopies and the capability of nutrient storage at earlier growth stages under lower temperatures. On the other hand, *Cs* has a much shorter life span than *Pp*, and spreads many more seeds (on the order of 1 million per m^2) and germinates much more than *Pp*. Furthermore, based on the experiments of Van den Berg (1999), the growth of *Cs* was associated with dissolved inorganic carbon (DIC) depletion. At lower DIC (high *pH*), *Cs* has a higher photosynthetic rate than *Pp* therefore leading to an even higher *Cs* concentration. Strong decrease of DIC was observed in Lake Veluwe especially in the spring and summer period (Van den Berg 1999). Therefore, in the area dominated by *Cs*, *Pp* can hardly grow.

The data sources available in this case study include point measurements and GIS annual density maps (Figure 7) for the two types of macrophytes *Cs* and *Pp*. Bathymetry data were supplied by the Dutch National Water Board (Figure 8).

A sensitivity analysis was conducted which showed that besides plant growth, the processes of seed dispersal, spatial extension and species interactions are indispensable processes in modelling aquatic plant spatial pattern dynamics,

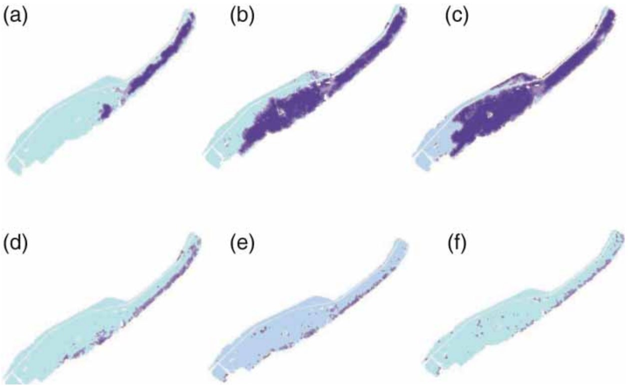

Figure 7 | *Cs* and *Pp* densities and distributions in year 1994, 1997 and 1999 (a) *Cs*: 1994, (b) *Cs*: 1997, (c) *Cs*: 1999, (d) *Pp*: 1994, (e) *Pp*: 1997, (f) *Pp*: 1999 (areas with darker colour: macrophytes; lighter colour: water).

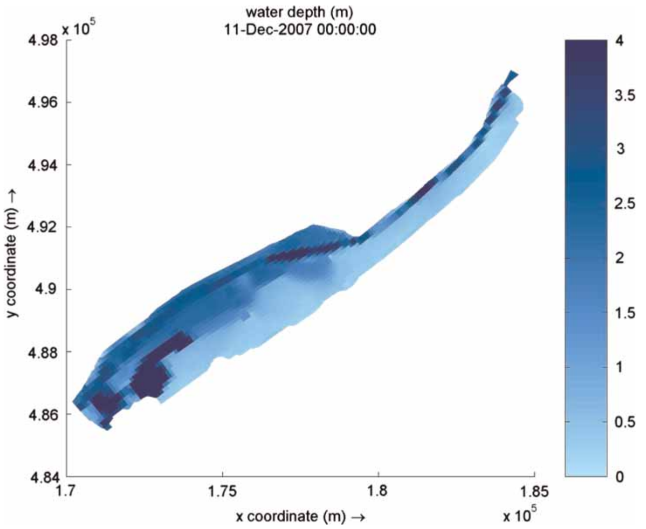

Figure 8 | Averaged water depth of Lake Veluwe.

especially for the extension of patterns representing biological diffusive phenomena (Li 2009). The synthesis of modelling was preliminarily applied to the Lake Veluwe case, in order to compare modelling results with the MAS model described in Li *et al*. (2010).

Initial plant maps obtained from GIS density maps of the year 1994 are shown in (Figures 7a and d). For the application in Lake Veluwe, a simplified flow dynamics model driven by wind was adopted and no nutrient limitation was considered. Due to the aquatic plants' ability of absorbing nutrients from the lake bed, it is assumed that nutrients are sufficiently available even without additional input from outside the domain. In this application, water depth and velocity contain dynamic changes, especially velocity due to the changes in wind condition.

After running the simulation for a few years, the resulting spatial patterns were simulated to become as indicated in Figure 9. Light areas show open water surface while the dark areas represent the cells covered by *Cs* with darker colours indicating higher density. *Cs* is seen to extend to larger spatial coverage after several years of growth and extension, whereas *Pp* has a decreasing trend, as observed in reality.

Comparing the GIS density map and the resulting *Cs* map obtained from the MAS model for the year 1997 (Figure 10), the resulting density map from the synthesis model appears quite similar in spatial coverage. One of the possible reasons of slightly less coverage compared to the previous example in Li *et al*. (2010) may be that the hydrodynamics is simplified to only a wind-driven flow field. Besides, the random seeding considered in the previous example is not taken into account as a process in the synthesis model. Still, the overall comparison and features of the synthesis model seem to represent the observations quite well.

SUMMARY AND DISCUSSION

The paper has illustrated the use of hydroinformatics techniques in environmental systems modelling with two examples.

The capabilities of CA for discrete modelling of macrophytes (i.e. water lily plant) growth in a confined pond were demonstrated and compared with high resolution photographic images. The case study showed that a fine-scale CA model is quite capable of capturing the individual behaviour of water lily growth, including seasonal variation and the development of patchiness behaviour. It was shown that high resolution photography can be a cheap and practical source of data for verifying plant population dynamics at the water surface (provided a stable platform for taking photos is available). Detailed patchiness and local patterns even at the smaller scales can be obtained when using a detailed CA model having a cell size of the same magnitude as the characteristic dimensions of the particular plant. In general, it was seen to be vital to develop proper geometrical CA rules when modelling real biological systems.

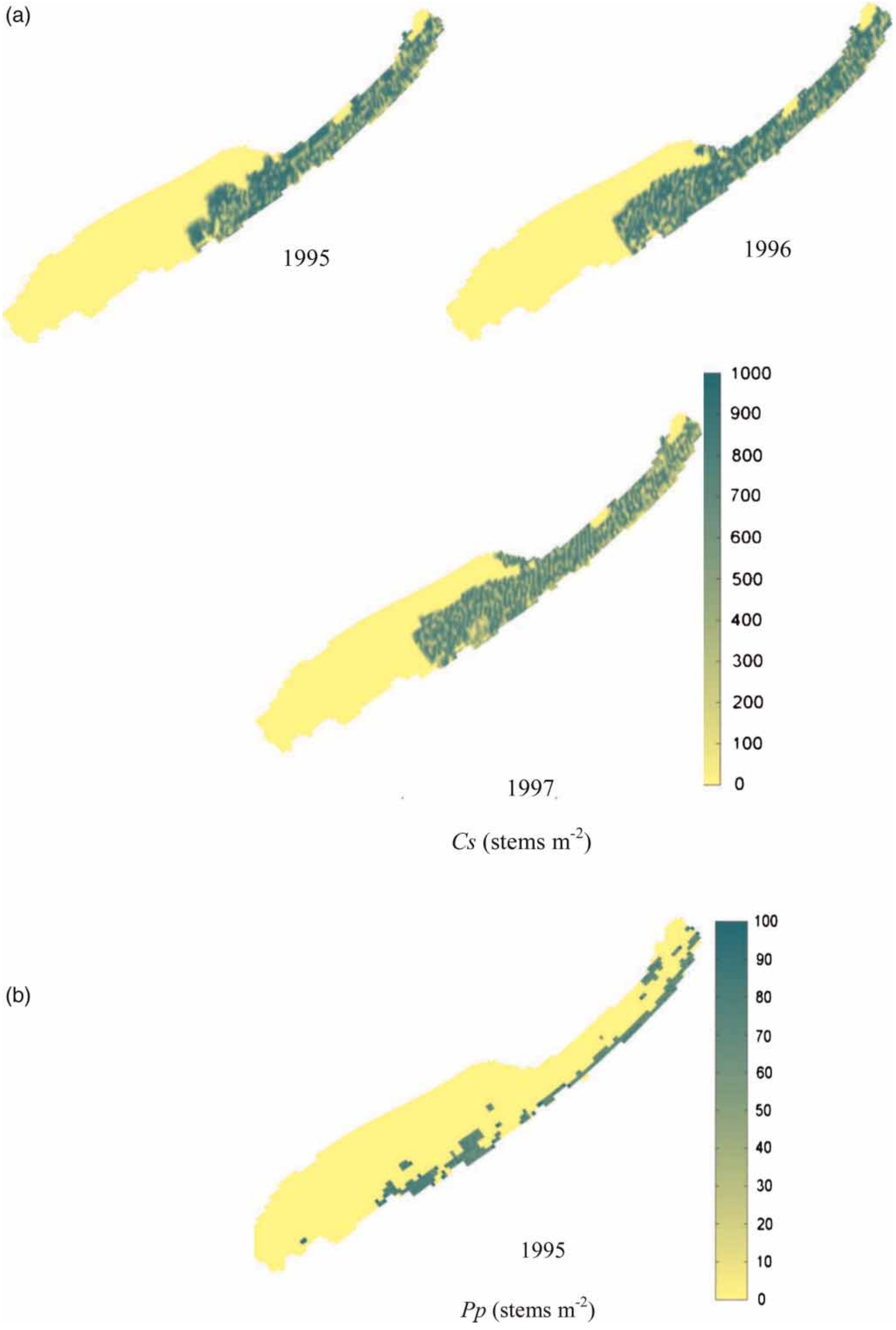

Figure 9 | Resulting density maps (a) *Cs*, (b) *Pp*.

In order to take into account not only the simulation of growth and decay of two different macrophytes, and the interactions among macrophytes, but also the dynamic interactions of their living environment (flow, WAQ, etc.), special emphasis was given in this paper to how to achieve a synthesis model combining a range of processes in non-linear aquatic population dynamics modelling. The concept is based on coupling a continuous physically-based WAQ model (i.e. DELFT3D-FLOW-WAQ) and a discrete multi-agent macrophytes growth model (i.e. MAS). In the case

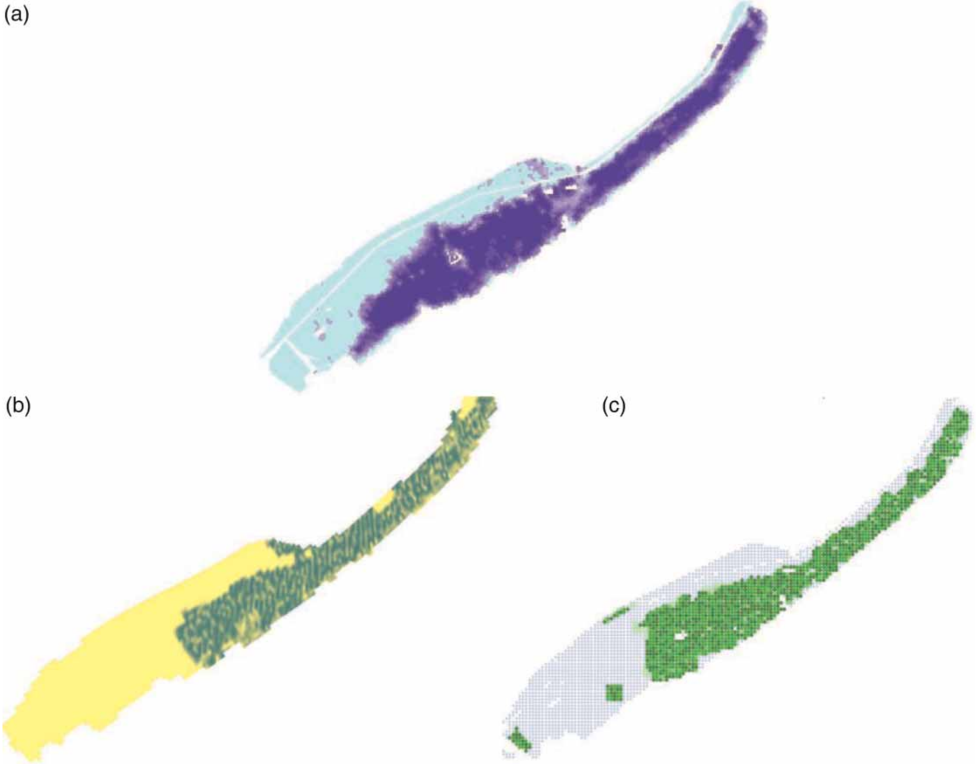

Figure 10 | Resulting density maps (*Cs*, 1997) of (a) GIS density map, (b) synthesis model (from Li 2009), and (c) MAS (from Li *et al*. 2010) (lighter colour: water; darker colour: macrophytes).

study for Lake Veluwe, the synthesis model was able to reproduce the very peculiar behaviour of two outcompeting macrophyte species as observed in the lake over a sequence of years, as analysed by Li *et al*. (2010). The multi-process, non-linear synthesis model showed a useful way of combining a range of hydroinformatics techniques, in this particular case integrating continuous processes with discrete processes in a computer-based environment. Such a synthesis model is able to include biological/ecological growth and spreading processes, accounting for local effects and conditions into a coherent modelling framework, thereby further enhancing conventional (partial) differential-equation based modelling.

In both cases in this study, the local effects and individual properties of specific aquatic plants are indispensible processes and factors in forming global spatial patterns. Different macrophytes with different properties determine their growth and extension patterns under certain environments. In particular, for rooted macrophytes, the seed dispersal/germination has vital effects to the spatial pattern dynamics.

The Lake Veluwe case study shows a challenging field which calls for further research on understanding the underlying mechanisms and mathematical formulations of aquatic environmental systems modelling. This synthesis model has a first step of integrating continuous hydrodynamic and WAQ formulations with discrete multi-agent aquatic vegetation growth models. Further attempts are ongoing to extend and further develop this synthesis model with MAS concept into a Delft3D vegetation dynamics module by including better formulation of biological and ecological processes and combining feedback mechanisms from biotic processes (in this case aquatic plant growth) to the hydrodynamic and advection-dispersion behaviour of the surrounding flows and morphological changes. The research on the influence of vegetation to flow dynamics (biogeomorphological research) has been developing as a separate field of science in itself (Uittenbogaard 2003; Baptist 2005; Paarlberg *et al*. 2005; Temmerman *et al*. 2007).

The use of discrete modelling techniques and agent-based modelling approaches explored in this paper was seen to represent the spatial pattern dynamics quite well both qualitatively and quantitatively, while also achieving a better understanding of some of the fundamental underlying mechanisms. The results of the various combined modelling approaches can further help in quantifying spatial habitat complexity in environmental systems. Along with the fast development in measurement techniques and the wider availability of spatially distributed data from e.g. sensor networks, radar observations, etc., a combination of multi-data sources and different modelling approaches seems to hold great potential for better simulating and predicting spatio-temporal aquatic population dynamics, and can contribute greatly to achieving better water management strategies and improved sustainable development of the aquatic environment. The environmental hydroinformatics techniques and synthesis framework introduced in this paper can be seen as first steps towards a next generation systems in aquatic ecosystem modelling.

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