Modular ecosystem modeling

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Abstract

The Library of Hydro-Ecological Modules (LHEM, http://giee.uvm.edu/LHEM) was designed to create flexible landscape model structures that can be easily modified and extended to suit the requirements of a variety of goals and case studies. The LHEM includes modules that simulate hydrologic processes, nutrient cycling, vegetation growth, decomposition, and other processes, both locally and spatially. Where possible the modules are formulated as STELLA® models, which adds to transparency and helps reuse. Spatial transport processes are presented as C++ code. The modular approach takes advantage of the spatial modeling environment (http://giee.uvm.edu/SME3) that allows integration of various STELLA models and C++ user code, and embeds local simulation models into a spatial context. Using the LHEM/SME the Patuxent landscape model (PLM) was built to simulate fundamental ecological processes in the watershed scale driven by temporal (nutrient loadings, climatic conditions) and spatial (land use patterns) forcings. Local ecosystem dynamics were replicated across a grid of cells that compose the rasterized landscape. Different habitats and land use types translate into different modules and parameter sets. Spatial hydrologic modules link the cells together. These are also part of the LHEM and define horizontal fluxes of material and information. This approach provides additional flexibility in scaling up and down over a range of spatial resolutions. Model results show good agreement with data for several components of the model at several scales. Other applications include several subwatersheds of the Patuxent, the Gwynns Falls watershed in Baltimore, and others.

Keywords: Landscape modeling; Modularity; Scaling; Dynamic spatial modeling; Land use change

Software availability

Program title Library of Hydro-Ecological Modules (LHEM)
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Year first available 2000
Hardware required UNIX workstation or Linux PC, Mac (OS X) or Windows PC
Software required STELLA, SME
Program language C++, STELLA

1. Introduction

The General Ecosystem Model (GEM) (Fitz et al., 1996) has been designed to simulate a variety of ecosystem types using a fixed model structure, in hope that the generic nature of the model will help alleviate the “reinventing-the-wheel” syndrome of model development. A general ecosystem model in theory should eliminate the need for continuous remaking of models for different systems and/or sites and can form the basis of spatially explicit ecosystem process models. Such characteristics logically lead to one of the broader objectives in ecosystem research: with a standard structure for developing a (model) synthesis of a system, comparisons among systems may be facilitated. The model was to be
**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B_t$</td>
<td>biological time counter (°C)</td>
</tr>
<tr>
<td>$BM_a$</td>
<td>above ground biomass (kg/m²)</td>
</tr>
<tr>
<td>$b_r$</td>
<td>biological time threshold for reproductive organs to develop (°C)</td>
</tr>
<tr>
<td>$C_h$</td>
<td>horizontal conductivity (m/day)</td>
</tr>
<tr>
<td>$C_S$</td>
<td>infiltration rate for a given type of soil (m/day)</td>
</tr>
<tr>
<td>$C_{Hab}$</td>
<td>habitat type modifier for infiltration (0 &lt; $C_{Hab}$ &lt; 1)</td>
</tr>
<tr>
<td>$C_{si}$</td>
<td>slope modifier for infiltration (°)</td>
</tr>
<tr>
<td>$C_{ij}$</td>
<td>cell size weighted horizontal conductivity in cell $(i,j)$ (m/day)</td>
</tr>
<tr>
<td>$C_n$</td>
<td>half-saturation coefficient ($n = N$ for nitrogen, or $P$ for phosphorus) (g/m²)</td>
</tr>
<tr>
<td>$C_{tr}$</td>
<td>habitat dependent transpiration rate (1/day)</td>
</tr>
<tr>
<td>$C_{vc}$</td>
<td>soil dependent vertical hydraulic conductivity parameter (m/day)</td>
</tr>
<tr>
<td>$D$</td>
<td>day length (hours)</td>
</tr>
<tr>
<td>$D_{DOM}$</td>
<td>deposited organic material (kg/m²)</td>
</tr>
<tr>
<td>$D_h = UW_d(t) - UW_d(t-1)$</td>
<td>change in unsaturated water depth over one time step (m)</td>
</tr>
<tr>
<td>$D_l$</td>
<td>labile detritus (kg/m²)</td>
</tr>
<tr>
<td>$D_{min}$</td>
<td>total amount of mineralized detritus (kg/m²)</td>
</tr>
<tr>
<td>$D_S$</td>
<td>stable detritus (kg/m²)</td>
</tr>
<tr>
<td>$d_0$</td>
<td>rate of stable detritus transformation (1/day)</td>
</tr>
<tr>
<td>$d_1$</td>
<td>rate of stable to labile detritus flow (1/day)</td>
</tr>
<tr>
<td>$E$</td>
<td>elevation above sea level (m)</td>
</tr>
<tr>
<td>$F_{NPP}$</td>
<td>net primary production (kg/m²/day)</td>
</tr>
<tr>
<td>$f_a$</td>
<td>nutrient uptake ($n = N$ for nitrogen, or $P$ for phosphorus) (1/day)</td>
</tr>
<tr>
<td>$f_{in}$</td>
<td>value of the temperature limitation function at maximal temperature ($L_i(T_{max}) = f_{in}$)</td>
</tr>
<tr>
<td>$f_0$</td>
<td>value of the temperature limitation function at zero temperature ($L_i(0) = f_0$)</td>
</tr>
<tr>
<td>$g$</td>
<td>separation parameter between surface and subsurface storage of detritus</td>
</tr>
<tr>
<td>$H$</td>
<td>humidity (%)</td>
</tr>
<tr>
<td>$H_E$</td>
<td>evaporation from surface water (m)</td>
</tr>
<tr>
<td>$H_I$</td>
<td>amount of water that the vegetation can intercept (m)</td>
</tr>
<tr>
<td>$H_P$</td>
<td>percolation rate (m/day)</td>
</tr>
<tr>
<td>$H_T$</td>
<td>amount of evapotranspiration (m)</td>
</tr>
<tr>
<td>$I$</td>
<td>incoming solar radiation (kcal/m²)</td>
</tr>
<tr>
<td>$I_p$</td>
<td>potential infiltration (m)</td>
</tr>
<tr>
<td>$I_s$</td>
<td>saturation level for irradiation (kcal/m²)</td>
</tr>
<tr>
<td>$k$</td>
<td>tolerance coefficient to high water stage</td>
</tr>
<tr>
<td>$L_i$</td>
<td>light limitation</td>
</tr>
<tr>
<td>$L_N$</td>
<td>nutrient availability limitation factor</td>
</tr>
<tr>
<td>$L_T$</td>
<td>temperature limitation factor</td>
</tr>
<tr>
<td>$L_{sw}$</td>
<td>water availability limitation factor</td>
</tr>
<tr>
<td>$m$</td>
<td>draught tolerance factor</td>
</tr>
<tr>
<td>$NPH$</td>
<td>non-photosynthetic biomass (kg/m²)</td>
</tr>
<tr>
<td>$NPH_a$</td>
<td>above ground non-photosynthetic biomass (kg/m²)</td>
</tr>
<tr>
<td>$NPH_b$</td>
<td>below ground non-photosynthetic biomass (kg/m²)</td>
</tr>
<tr>
<td>$NPP$</td>
<td>net primary production (kg/m²/day)</td>
</tr>
<tr>
<td>$n_{C_s}$</td>
<td>nutrient concentration in the sediment (g/m³)</td>
</tr>
<tr>
<td>$n_{C_{sw}}$</td>
<td>concentration of nutrient on the surface ($n = N$ for nitrogen, or $P$ for phosphorus) (g/m²)</td>
</tr>
<tr>
<td>$n_{D_d}$</td>
<td>separation coefficient for nutrients that are dissolved and further infiltrated into groundwater and the nutrients that are retained in the subsurface layer ($R_s$)</td>
</tr>
<tr>
<td>$n_{U_{sw}}$</td>
<td>parameter for nutrient requirements of photosynthesis ($n = N$ for nitrogen, or $P$ for phosphorus)</td>
</tr>
<tr>
<td>$n$</td>
<td>litterfall intensity</td>
</tr>
<tr>
<td>$P$</td>
<td>porosity</td>
</tr>
<tr>
<td>$p_{min}$</td>
<td>minimal foliage biomass (kg/m²)</td>
</tr>
<tr>
<td>Variable</td>
<td>Description</td>
</tr>
<tr>
<td>----------</td>
<td>-------------</td>
</tr>
<tr>
<td>PH</td>
<td>photosynthetic biomass (kg/m²)</td>
</tr>
<tr>
<td>PHM</td>
<td>maximal photosynthetic biomass (kg/m²)</td>
</tr>
<tr>
<td>PHmax</td>
<td>maximal biomass reached during the season (kg/m²)</td>
</tr>
<tr>
<td>R</td>
<td>amount of rainfall (m)</td>
</tr>
<tr>
<td>R₀</td>
<td>distance to the saturated layer at which the capillary effect starts (m)</td>
</tr>
<tr>
<td>Rd</td>
<td>root zone depth (m)</td>
</tr>
<tr>
<td>Rexp</td>
<td>index of the capillary root suction from the saturated layer</td>
</tr>
<tr>
<td>Rs</td>
<td>depth of the subsurface layer (m)</td>
</tr>
<tr>
<td>S</td>
<td>water in saturated layer, $S_{ij}$ saturated water in cell $(i,j)$ (m)</td>
</tr>
<tr>
<td>Sn</td>
<td>nutrient ambient concentration ($n = N$ for nitrogen, or $P$ for phosphorus)</td>
</tr>
<tr>
<td>Sp</td>
<td>amount of rainfall infiltrated into saturated storage (m)</td>
</tr>
<tr>
<td>Sr</td>
<td>amount of water in the subsurface layer (m)</td>
</tr>
<tr>
<td>S_SW</td>
<td>flow from saturated storage to the surface (m)</td>
</tr>
<tr>
<td>SW_S</td>
<td>flow from surface water into the saturated storage (m)</td>
</tr>
<tr>
<td>S_I</td>
<td>surface water, $SW_{ij}$ surface water in cell $(i,j)$ (m)</td>
</tr>
<tr>
<td>s₁</td>
<td>curvature parameter for temperature limitation function</td>
</tr>
<tr>
<td>T</td>
<td>ambient temperature (°C)</td>
</tr>
<tr>
<td>T_max</td>
<td>maximal temperature after which the growth stops (°C)</td>
</tr>
<tr>
<td>T_opt</td>
<td>optimal temperature (°C)</td>
</tr>
<tr>
<td>TR</td>
<td>total transpiration (m)</td>
</tr>
<tr>
<td>TRp</td>
<td>Penman–Monteith potential transpiration (m)</td>
</tr>
<tr>
<td>TRs</td>
<td>transpiration from the saturated zone (m)</td>
</tr>
<tr>
<td>TRu</td>
<td>transpiration from the unsaturated zone (m)</td>
</tr>
<tr>
<td>U</td>
<td>unsaturated moisture proportion</td>
</tr>
<tr>
<td>U_c</td>
<td>unsaturated capacity (m)</td>
</tr>
<tr>
<td>U_d</td>
<td>drying capacity (0.5 $U_i$)</td>
</tr>
<tr>
<td>U_f</td>
<td>field capacity</td>
</tr>
<tr>
<td>U_w</td>
<td>wilting point (0.1 $U_i$)</td>
</tr>
<tr>
<td>UW</td>
<td>water in unsaturated layer, $UW_{ij}$ unsaturated water in cell $(i,j)$ (m)</td>
</tr>
<tr>
<td>UW_d</td>
<td>depth of the unsaturated layer (m)</td>
</tr>
<tr>
<td>UW_p</td>
<td>amount of rainfall infiltrated into unsaturated storage (m)</td>
</tr>
<tr>
<td>W</td>
<td>wind speed (km/h)</td>
</tr>
<tr>
<td>Wa</td>
<td>available water</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>ratio of photosynthetic biomass to above ground biomass</td>
</tr>
<tr>
<td>$\alpha^*$</td>
<td>maximum ratio of photosynthetic biomass to above ground biomass</td>
</tr>
<tr>
<td>$\alpha_{npp}$</td>
<td>photosynthesis rate (1/day)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>ratio of above ground non-photosynthetic biomass to below ground non-photosynthetic biomass</td>
</tr>
<tr>
<td>$\epsilon_1$</td>
<td>habitat dependent landscape interception parameter</td>
</tr>
<tr>
<td>$\epsilon_2$</td>
<td>vegetation interception parameter</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>litterfall rate (kg/m²)</td>
</tr>
</tbody>
</table>

The GEM approach, generally applied to ecosystems that range from wetlands to upland forests, was intended to provide at least two useful functions in synthesizing our broader understanding of ecosystem properties. It involves using the model as a quantitative template for comparisons of the different controls on each ecosystem, including the process-related parameters to which the systems are most sensitive. Secondly, a simulation model, which is general in process, orientation, and structure, could provide a tool to analyze the influence of scale on actual and perceived ecosystem structure.

While the GEM approach still seems to be extremely important for cross ecosystem and scale comparisons, it turned out to be somewhat insufficient to cover all the possible variety in ecosystem processes and attributes that come into play when going from one ecosystem type to another, and from one scale to another. Modeling is a goal driven process, and different goals in most cases will require different models. There is too much ecological variability to be represented efficiently within the framework of one general model. Either something important gets missed, or the model becomes too redun-
tant to be handled efficiently especially within the framework of larger spatially explicit models. Similarly, when changing scale and resolution different sets of variables and processes come into play. Certain processes that could be considered at equilibrium at a weekly time scale need be disintegrated and considered in dynamic at an hourly time scale. For example, ponding of surface water after a rainfall event is an important process at fine temporal resolution, but may become redundant if the time step is large enough to make all the surface water either removed by overland flows, or infiltrated. Daily net primary productivity fluctuations, that are important in a model of crop growth, may be less important in a forest model that is to be run over decades with only average annual climatic data available. Once again the general approach may result in either insufficiency or redundancy.

The modular approach is a logical extension of the general approach. In this case instead of creating a model general enough to represent all the variety of ecological systems under different environmental conditions, we develop a library of modules simulating various components of ecosystems or entire ecosystems under various assumptions and resolutions. In this case, the challenge is to put the modules together, using consistent and appropriate scales of process complexity, and make them talk to each other within a framework of a full model. The concept of modularity gained strong momentum with the wide spread of the object oriented approach in software development (Silvert, 1993; Sequeira et al., 1997).

Reynolds and Acoc (1997) offer an extensive discussion of modular design criteria and rules in application to plant modeling. The features of decomposability and composability are probably the most important ones. The decomposability criterion requires that a module should be an independent, stand-alone submodel that can be analyzed separately. On the other hand, the composability criterion requires that modules can be put together to represent more complex systems. Decomposability is mostly attained in the conceptual level, when modules are identified among the variety of processes and variables that describe the system. There is a lot of arbitrariness in choosing the modules. The choice may be driven either by purely logical, physical, ecological considerations about how the system operates, or by quantitative analysis of the whole system, when certain variables and processes are identified as rather independent from the other ones.

The composability of modules is usually treated as a software problem. That aspect is usually resolved by use of wrappers that enable modules to publish their functions and services using a common high-level interface specification language (the federation approach) (CORBA, 1996; Villa and Costanza, 2000). The other alternative is the design of model specification formalism that draws on the object-oriented methodology and embeds modules within the context of a specific modeling environment that provides all the software tools essential for simulation development and execution (the specification approach) (Maxwell, 1999). In both cases, as models find themselves in the realm of software developers, the gap between the engineering and the research views on models and their performance starts to grow. From the software engineering viewpoint, the exponential growth of computer performance offers unlimited resources for the development of new modeling systems. With the advent of the Internet, it becomes possible to assemble models from building blocks connected over the Web and distributed over a network of computers (Fishwick et al., 1998). New languages and development tools appear even faster than their user-communities manage to develop.

On the other hand from the research viewpoint, if a model is to be a useful simplification of reality, it should enable a more profound understanding of the system of interest. It is more important as a tool for understanding the processes and systems, than for merely simulating them. In this context, there is a more limited demand for the overwhelming complexity of modeling systems. The existing software may remain on the shelf if it does not really help understand the systems. This is probably especially pertinent to models in biology and ecology, where in contrast to physical science or engineering, the models are much more loose and “black-box” much of the underlying complexity due to the difficulty of parameterizing and simulating all of the mechanisms from a first-principal basis. They may require a good deal of analysis, calibration and modifications, before they may be actually used. In this case, the focus is on model and module transparency and openness. For research purposes, it is much more important to know all the nuts and bolts of a module to use it appropriately. The “plug-and-play” feature that is so much advocated by some software developers becomes of lower priority. In a way it may even be misleading, creating the illusion of simplicity of model construction from prefabricated components, with no real understanding of process, scale and interaction.

Models delivered by means of some of the icon-based systems such as STELLA (HPS, 1995) offer a lot of transparency, especially if they are properly documented. The STELLA software was used to formulate the GEM, which in part contributed to its fairly wide dissemination. STELLA has a number of advantages, but its support of modularity is very limited. There are no formal mechanisms that could put individual STELLA models together and provide their integration. STELLA does allow submodels or sectors within the larger context (such as the sectors in the GEM), allowing each sector to be run independently of the others, or in any combination. However, there is no easy way that a sector
can be replaced or moved from one model into another. One of the important features of the Spatial Modeling Environment (SME) (Maxwell and Costanza, 1995, 1997) is that it can take individual STELLA models and translate them into a format that supports modularity. In addition to STELLA modules, SME can also incorporate user-coded modules that are essential to describe, say, various spatial fluxes in a watershed or a landscape.

Instead of a general model that should represent all the variety of ecosystems, by using SME, we can formulate a general modular framework (Fig. 1), which defines the set of basic variables and connections between the modules. Particular implementations of modules are flexible and assume a wide variety of components that are to be made available through libraries of modules. The modules are formulated as stand-alone STELLA models that can be developed, tested and used independently. However, they can share certain variables that are the same in different modules, using a convention that is defined and supported in the library specification table. When modules are developed and run independently, these variables are specified by user-defined constants, graphics or time series. Within the SME context, these variables get updated in other modules to create a truly dynamic interaction.

For example, spatial dynamics modules can be formulated in C++. They can use some of the SME classes to get access to the spatial data and can then be incorporated into the SME driver and used to update the local variables described within the STELLA modules. In this case, it is hard to offer the same level of transparency as with the STELLA modules. More emphasis should be made on explicit documentation and comments to the code. We also hope that by presenting the various modules of the Library of Hydro-Ecological Modules (LHEM) on the web and offering detailed description of various modules and their functions we can increase their utility for reuse and further improvement.

At this time, the LHEM offers a framework to archive the modules that may be used either as stand-alone models to describe certain processes and ecosystem components, or may be put together into more elaborate structures by using the SME. In this paper, we will describe some of the major modules that are currently included into the LHEM. We will give a brief description of their structure and then refer the reader to the web pages, where the modules can be further explored and downloaded. We will illustrate the concept on the example of the Patuxent landscape model (PLM) that is a fairly complex spatial watershed model and that has been put together entirely from the LHEM modules and then calibrated and used for scenario runs.

2. General conventions

There is a good variety of software currently available that can help build and run models. Between the qualitative conceptual model and the computer code, we may place a number of software tools that can assist us in converting conceptual ideas into a running model. Usually there is a trade off between universality and user-friendliness. On the one extreme, we see computer languages that can be used to translate any concepts and any knowledge into working computer code. On the other extreme, we find realizations of particular models that are good only for the individual systems and conditions that they were designed for. In between there are a variety of more universal tools.

They include modeling languages, which are computer languages designed specifically for model development, and extendible modeling systems, which are modeling packages that allow specific code to be added by the user if the existing methods are not sufficient for their purposes. In contrast, there are also modeling systems, which are completely prepackaged and do not allow any additions to the methods provided. There is a remarkable gap between these packaged and extendible systems in terms of their user-friendliness. The less power the user has to modify the system, the fancier the graphic user interface and the easier the system is to learn. From modeling systems, we go to extendible models, which are actual individual models that can be adjusted for different locations and case studies. In these, the model structure is much less flexible, the user can make choices from a limited list of options, and it is usually just the parameters and some spatial and temporal characteristics that can be changed.

Similarly for modeling environments such as SME there is a certain level of user-friendliness that is usually in reverse proportion to generality. To be able to link both unit and spatial modules together, SME adopts certain conventions on how the modules should be described and what are the formats of data that can be used.

![Fig. 1. Principle modules and their interaction. The local modules are formulated as STELLA models, the spatial modules are C++ code, using SME classes to access spatially explicit variables and parameters.](image-url)
In SME, local modules can be described as sectors in STELLA. Each module is a different STELLA model. The sector name should begin with the $ sign. In what follows we will call state variables, forcing functions and parameters simply variables if they do not need be distinguished. The variables within a sector will be considered as owned by this module. All the external variables that are defined outside of the sector borders can be defined in other modules. Within a module, to make it operable as a stand-alone model, these external variables should be defined as constants or as time series (say, defined as graphs in STELLA) that can change with time or as functions of some other independent variables.

Variables that are shared between modules should have the same name. The SME translator takes the STELLA equations saved as a text file, and translates them into an intermediate formalization, called the Modular Markup Language (MML) (Maxwell and Costanza, 1997). It will find the shared names and link them together. A config file will be produced that contains all the variables from all the modules. This config file can be further edited to change the values used for the variables in the driver. However, these changes will not affect the values that the variables are set to in the STELLA formulations of the modules. Due to STELLA limitations, there is no way back from MML or STELLA equations to the STELLA icon-based diagram and modeling tools. Therefore all the changes that are made to the MML formulation or directly to the driver in C++ will be lost if we export and process a new STELLA equations file.

Whereas most of the local dynamics can be effectively described within STELLA models, it becomes hard if not impossible to represent spatial processes using this formalism. To link individual local models into a spatial network, again, SME can be used, if the appropriate code is provided. The SME allows one to link C++ programs, described as UserCode, with the local ordinary differential (difference) equations (ODE) generated based on STELLA formulations. A number of the SME classes are made available for writing user code in order to provide access to spatial and non-spatial data structures handled by the SME.

Besides, as local dynamics get treated in the SME in a spatial context, it also gets the spatial variability that can be associated with the various parameters being spatially distributed, related to, say, soil or habitat types. In this case, when moving from one spatial locality to another, the same system of ODEs generated from STELLA gets to be solved with a different parameter set, one that is substituted by SME. Currently, SME does not incorporate any extensive database features to serve the needs of describing and archiving the numerous parameters encountered in models and modules. However, there are several well-elaborated input mechanisms that allow one to read the location-dependent data from various file formats. For example, the habitat dependent parameters are accumulated in a file that has various columns representing the different model parameters, and rows describing the various habitats. A parameter described as habitat dependent in the config file is then input from this file based on the information about the particular habitat specified by the Land Use map.

Another alternative that we have explored to integrate individual modules and run them jointly is the MADONNA software (Macey and Oster, 1993), that can take STELLA equations, compile them and run, actually, much faster than STELLA can (which interprets on the fly, not compiling the equations). In MADONNA, it is quite easy to combine equations from several STELLA modules into one Equations file and thus create a new integrated model. The option of viewing the flowchart diagram of this integrated model still will be lost and the joint model will have to be maintained only in the Equations format, thus forfeiting some of the transparency and visualizations that the original modules deliver. There is no functionality to access spatial data, so for running the modular models spatially, SME still remains a better choice.

3. Physical modules

3.1. Variables and major assumptions

There are no state variables in this module. The variables defined here are the forcing functions and parameters that describe the physical environment and include:

- Climatic factors: precipitation, temperature, humidity, wind speed, solar radiation;
- Surface geomorphology: such as elevation, bathymetry, soils;
- Auxiliary variables shared by other modules: such as day length, Julian day, and habitat type.

The module is designed mostly to simplify data preprocessing. It takes care of various conversions when the raw data are input into the model. For particular applications, there is a good chance that some modifications will be required if the data available are presented in some different formats and units. In some cases, additional sub-modules may be formulated. For example, the photoactive solar radiation (PAR) is rarely available in standard climatic data sets. In many cases, this forcing function can be well estimated by empirical formulas based on the latitude of the study area.

3.2. Solar radiation

Currently, there are two modules in LHEM that calculate PAR. The first one is similar to the one used in GEM
(Fitz et al., 1996). It is based on an algorithm derived from Nikolov and Zeller (1992), that begins with a calculation of daily solar radiation at the top of the atmosphere based on Julian date, latitude, solar declination, and other factors. Mean monthly cloud cover is calculated using a regressed relationship based on daily precipitation, humidity, and temperature. This monthly cloud cover value is used to attenuate the daily radiation reaching the surface. Daily radiation (PAR in cal·cm⁻²·day⁻¹) received at the earth surface at a particular elevation, latitude, or time of year in the Northern hemisphere is calculated using the Beer’s law relationship to account for attenuation through the atmosphere.

The second algorithm is a simplification of the Nikolov and Zeller model that matches their results in mid-latitudes (20 < Lat < 64) almost exactly (r² = 0.96). The solar radiation at the earth surface is calculated using an empirical formula:

\[
\text{PAR} = (A + B \cos(T_{\text{rad}}) + C \sin^2(T_{\text{rad}}))(1 - 0.05D),
\]

where \( A = 720.52 - 6.68 \cdot \text{Lat} \); \( B = 105.94 \cdot (\text{Lat} - 17.48)^{0.27} \); \( C = 175 - 3.6 \cdot \text{Lat} \), \( D \) is the cloudiness, and \( T_{\text{rad}} = 2/365 \cdot \text{PI} \cdot (\text{DayJul} - 173) \) is the conversion from days to radian (also see Nomenclature for a list of all variables and parameters).

4. Hydrologic modules

4.1. Variables and major assumptions

The traditional scheme of vertical water movement (Novotny and Olem, 1994), also implemented in GEM (Fitz et al., 1996), assumes that water is fluxed along the following pathway: rainfall → surface water → water in the unsaturated layer → water in the saturated zone. Snow is yet another storage that is important to mimic the delayed response caused by certain climatic conditions. In each of the stages, some portions of water are diverted due to physical (evaporation, runoff) and biological (transpiration) processes, but in the vertical dimension, the flow is controlled by the exchange between these four major phases:

- Surface water (SW),
- Snow/ice (SI),
- Water in unsaturated storage (UW),
- Water in saturated storage (S).

We build our hydrologic module around these four state variables. These variables as well as the associated fluxes are computed within this module and made available for input into other modules. On the input side for the hydrologic module, we use:

- Precipitation,
- Air temperature,
- Humidity,
- Wind velocity,
- Habitat type,
- Soil type,
- Slope,
- Root depth,
- Leaf area index,
- Stream sinuosidity.

In addition to the GEM hydrologic module that proved to be well suited for wetland conditions, we have formulated another module that is better adjusted to terrestrial ecosystems and was used in PLM. Taking into account the temporal (1 day) and spatial (200 m, 1 km) resolution and the available input data, we have simplified the GEM module.

At a daily time step, the model cannot attempt to mimic the behavior of short-term events such as the fast dynamics of a wetting front, when rainwater infiltrates into soil and then travels through the unsaturated zone towards the saturated groundwater. During a rapid rainfall event, surface water may accumulate in pools and depressions but in a catchment scale, over the period of a day, most of this water will either infiltrate, evaporate, or be removed by horizontal runoff. Infiltration rates based on soil type within the Patuxent watershed, range from 0.15 to 6.2 m/day (Maryland Department of State Planning, 1973), potentially accommodating all but the most intense rainfall events in vegetated areas. The intensity of rainfall events can strongly influence runoff generation, but climatic data are rarely available for shorter than daily time steps. Also, if the model is to be run over large areas for many years, the diel rainfall data become inappropriate and difficult to project for scenario runs. Therefore a certain amount of detail must be forfeited to facilitate regional model implementation.

With these limitations in mind, we have implemented the following conceptualization:

- We assumed that rainfall infiltrates immediately to the unsaturated layer and only accumulates as surface water if the unsaturated layer becomes saturated or if the daily infiltration rate is exceeded. Ice and snow may still accumulate.
- Surface water in the model is water in rivers, creeks, ponds, and the like. There is no standing surface water on top of unsaturated layer. Surface water is removed by horizontal runoff or evaporation.
- Within the one-day time step, surface water flux also accounts for the shallow subsurface fluxes that rapidly bring the water distributed over the landscape into the micro channels and eventually to the river. Thus, the surface water transport takes into account the shallow subsurface flow that may occur during rainfall,
allowing the model to account for the significantly different nutrient transport capabilities between shallow and deep subsurface flow.

Conceptually this is similar to the slow and quick flow separations (Jakeman and Hornberger, 1993; Post and Jakeman, 1996) assumed in empirical models of runoff. In this case, the surface water variable accounts for the quick runoff, while the saturated storage performs as the slow runoff, defining the base flow rate between rainfall events.

The following processes are analyzed within this module and therefore may be available in the other modules.

### 4.2. Interception

A certain part of rainfall gets attached to vegetation or other structures on the landscape and further evaporates without even reaching the ground. The net interception loss is typically 10–30% of rainfall (Shuttleworth, 1993), and depends both on the canopy storage capacity and the nature and pattern of the rainfall, since up to half of the evaporation of the intercepted water occurs during the storm itself. Therefore we assume that the amount of water that the vegetation can intercept is in proportion to the total biomass:

$$H_i = \max(\varepsilon_i \cdot R, \varepsilon_L \cdot L_R), \text{ (m)}$$

where \(L_L\) is the leaf area index (LAI); \(\varepsilon_i\) is the habitat dependent landscape interception parameter; \(\varepsilon_L\) is the vegetation interception parameter, and \(R\) is the amount of rainfall (m). In this way, a certain amount is intercepted for any precipitation event and only the remaining part is delivered to the ground.

### 4.3. Evaporation and transpiration

As in GEM, pan evaporation from surface water, \(H_E\), (m/d) is calculated according to the Christiansen model (Saxton and McGuinness, 1982). The model uses temperature \(T\), solar radiation \(I\), wind speed \(W\) and humidity \(H\) as the independent variables.

Evapotranspiration is the process that removes water from the ground and releases it into the atmosphere. In addition to the evaporation process that is responsible for the air–water interface, we also account for the delivery process that makes water available for evaporation. If the surface is vegetated then the biological process of transpiration, that is performed by plants using water from the root zone, brings water to the leaves, pushing it out through the leaf stomatal pores and making it available for evaporation. If there are no plants, ponded water or soil moisture is evaporated.

The portion of land that is covered by vegetation can be approximated by the LAI, \(L_L\). The total amount of evapotranspiration is then

$$H_E = L_L \cdot TR + (1 - \min(1, L_L)) \cdot E.$$

Here, \(E = C_e H_E U_f\) is the evaporation from the ground, \(C_e\) is the ground evaporation rate, \(H_E\) is the pan evaporation for open water defined above, and \(U_f\) is the relative moisture proportion \((U_f = U/P\), where \(U\) is the moisture proportion and \(P\) is the porosity). When the LAI is larger than 1, the ground evaporation process shuts down, and TR, total transpiration, becomes predominant. TR is further subdivided into transpiration from the unsaturated \((TR_u)\) and saturated \((TR_s)\) layers:

$$TR = TR_u + TR_s = \theta_s \cdot TR + (1 - \theta_s) \cdot TR,$$

where \(TR\) is the transpiration, and \(\theta_s\) is the proportion of unsaturated layer transpiration.

$$\theta_s = \begin{cases} W_u \cdot U_W / (R_d + R_{exp}), & \text{if } R_d + R_0 > UW_d, \\ 1, & \text{if } R_d + R_0 < UW_d, \\ 0, & \text{if } UW_d = 0 \end{cases}$$

where \(UW_d\) is the depth of the unsaturated layer, \(R_d\) is the root zone depth, \(R_0\) is the distance to the saturated layer at which the capillary effect becomes pronounced, \(R_{exp}\) is the index of the capillary root suction from the saturated layer that effectively makes saturated water available even when the roots are not yet long enough to reach it \((UW_d > R_d)\):

$$R_{exp} = \exp(-10 \cdot (UW_d - R_d)).$$

\(W_u\) is the water availability index:

$$W_u = \min\left(1, R_{exp} + \begin{cases} 0, & \text{if } U < U_w \\ 1, & \text{if } U > U_w \\ (U - U_w) / (U_d - U_w), & \text{otherwise} \end{cases}\right)$$

that makes water fully available when unsaturated moisture proportion \(U\) is larger than drying capacity \(U_d\), which is usually 50–60% of field capacity \(U_i\), it makes water unavailable when \(U\) is less than the wilting point \(U_w\), (may be assumed equal to 10% of field capacity), and it returns an intermediate value otherwise. This is further modified by the capillary action, potentially making water available even when the unsaturated zone is totally dry, but the roots are close to the saturated storage.

For potential transpiration \(TR_p\), we have implemented the Penman–Monteith resistance based model of evapotranspiration, which is currently considered most advanced in hydrologic practice. The equation is fairly complex and is well documented in the literature (Shuttleworth, 1993). It represents the amount of water that is lost into the atmosphere as a function of climatic
conditions (temperature, humidity, solar radiation, wind velocity), and vegetation characteristics, such as the LAI. Transpiration is then calculated from potential transpiration, by taking into account the water availability \( W_e \):

\[
TR = C_u \cdot TR_p \cdot W_e,
\]

where \( C_u \) is the habitat dependent transpiration rate, and \( TR_p \) is the Penman–Monteith transpiration.

Evapotranspiration is probably one of the most complicated processes in the hydrologic cycle; therefore it is also implemented as a separate module in the LHEM.

4.4. Infiltration

Since the model is run on a daily basis and since we assume that rainfall infiltrates immediately into the unsaturated layer, infiltration is defined by the potential infiltration and by the unsaturated storage that is currently available for water intake (unsaturated capacity). Surface features characterize potential infiltration:

\[
I_p = C_{\text{Hab}} \cdot C_S / C_{\text{Si}},
\]

where \( C_S \) (m/day) is the infiltration rate for a given type of soil, \( C_{\text{Hab}} \) is the habitat type modifier (\( 0 < C_{\text{Hab}} < 1 \)), and \( C_{\text{Si}} \) (degrees) is the slope modifier.

The unsaturated capacity is the total volume of pores in the soil that is not yet taken by water:

\[
U_e = \frac{UW_d(P-U)\max(0,D_{fl})}{C_{\text{Si}}},
\]

where \( P \) is the soil porosity. If \( I_p \) is less than the unsaturated capacity then the potential infiltration is realized and the actual infiltration \( H_t = I_p \). If \( I_p > U_e \) then the incoming water will fill up all the pores, effectively eliminating the unsaturated zone and making it saturated. Therefore in this case, we channel all the infiltrated flow to the saturated storage, add the available unsaturated water to it and set \( UW = 0 \). Whatever water is left after infiltration is surface water that is available for horizontal runoff.

4.5. Percolation

By gravitational force, a certain amount of water percolates from the unsaturated storage further down until it hits the saturated layer. Only the water that is in excess of field capacity is available for percolation. When the unsaturated moisture proportion is below field capacity, capillary and adhesive forces retain all the water. Therefore the amount of water available for percolation is:

\[
U_e = U - U_t,
\]

and the percolation rate is defined by the equation:

\[
H_p = 2 \cdot C_{vc} \cdot P \times U_e^{0.4} / ((P-U_t)^{0.4} + U_e^{0.4}),
\]

where \( C_{vc} \) is the soil dependent vertical hydraulic conductivity parameter.

In addition to the percolation process, additional water is transferred from the unsaturated layer to the saturated layer whenever the water table is moving up. In this case, water that is kept in the pores of the unsaturated layer is added to the water coming up from the saturated layer, further rising the saturated layer. This amount is equal to \( H_{p_0} = \max(0,U-D_h) \), where \( D_h = UW_d(t) - UW_d(t-1) \), which is the change in unsaturated water depth over one time step.

Conversely, if the water table is going down, the moisture at field capacity stays in the soil and is added to the unsaturated storage: \( H_{p_1} = \max(0,U_D-D_h) \).

4.6. Spatial implementation

The algorithms involved in the spatial hydrologic modules have been discussed in more detail elsewhere (Voinov et al., 1998, 1999b). There are three major modules currently available to move water and constituents in the horizontal dimension. SWTRANS1 and SWTRANS2 are used for surface water dynamics, GWTRANS takes care of the aggregated saturated water storage.

SWTRANS1 is mostly useful for relatively flat areas, such as wetlands, coastal plains, and estuaries. In this module, backflow is allowed and the water level is calculated by equilibrating the water in a number of adjacent cells (Voinov et al., 1998). The call to the function is:

SWTRANS1 (S_WATER, MAP, ELEVATION, STUFF)

where S_WATER is the map of surface water, also updated by the unit models; MAP defines the study area; ELEVATION is the elevation map; and STUFF is the map of constituent concentrations.

SWTRANS2 assumes that there is a well-pronounced gradient in elevation that makes sure that water moves only in one direction. This is most appropriate for terrestrial ecosystems, which can usually be described by a link map that clearly indicates in which direction the water is running (Voinov et al., 1999b). The function call is similar to the above.

SWTRANS is a combination of SWTRANS1 and SWTRANS2. Here, water can either equilibrate in relatively flat areas or run downhill, where the gradient is dominant. This function is used for areas that have a combination of steep and flat regions. In this case, another variable is added to the function call: SWTRANS (S_WATER, MAP, HABMAP, ELEVATION, STUFF). HABMAP is the additional coverage that is used to decide where the first algorithm is more appropriate and where the second one should be used. In some cases, it can be the habitat map, where cells in the open water category are the ones that need the equilibration algorithm.

GWTRANS calculates the fluxes of groundwater and updates the concentration of constituents in cells. The
function is based on a modified Darcy formalization of the groundwater flow. The call to the function is:

\[
\text{GWTRANS}({\text{SAT\_WATER}}, \text{POROSITY}, \text{H\_CONDUCT}, \text{MAP}, \text{STUFF}, \text{UNSATW})
\]

where SAT\_WATER is the map of saturated water height, also updated by the unit models; POROSITY is the coverage for soil dependent porosities; H\_CONDUCT is the coverage for specific horizontal conductivity coefficients, that may also be soil dependent, MAP defines the study area; STUFF is the map of constituent concentrations, that can be nitrogen or phosphorus in this case; UNSATW is the amount of water in unsaturated storage. H\_CONDUCT is calculated as the cell size weighted horizontal conductivity: 

\[
\text{H\_CONDUCT} = C_h / \sqrt{A}, \text{ where } A \text{ is the cell size and } C_h \text{ is the conductivity.}
\]

Firstly, the function calculates for each cell, the average conductivity-weighted water storage for the nine cells that are the immediate vicinity of a cell and the cell itself:

\[
H_o = \frac{\sum_{j \in W} S_j C_j / \sqrt{A}}{\sum_{j \in W} P_j C_j}
\]

\(\Omega\) is the vicinity of cell \((i,j)\), that consists of cells \((i-1,j-1), (i-1,j), (i-1,j+1), (i,j-1), (i,j), (i,j+1), (i+1,j-1), (i+1,j), (i+1,j+1)\); \(S_j\) is the SAT\_WATER; \(C_j\) is H\_CONDUCT; \(P_j\) is POROSITY.

Next, it is assumed that the stage in the cell \((i,j)\) will tend towards this equilibrium and for each of the pairwise interactions with the neighboring cells \(k\) the flow \(F_k\) is calculated:

\[
F_k = (H_o P_j - S_j)(C_j + C_k) / 2, \text{ where } k \in \Omega \setminus (i,j).
\]

The new stage is then \(S_j = S_j + \Sigma_k F_k\). Note that when \(F_k > 0\) water is leaving the cell \((i,j)\) and flows into the neighboring cell \(k\). It flows in the opposite direction when \(F_k < 0\). The flow of water also carries the constituents (such as nutrients and sediments), whose concentration in cell \((i,j)\) is updated with each of the pairwise flows calculated:

\[
N_j = N_j - N_j F_k / S_j, \text{ if } F_k > 0; \text{ and }
\]

\[
N_j = N_j + N_k F_k / S_k, \text{ if } F_k < 0. \text{ Here, } N_j \text{ is the amount of the constituent in cell } (i,j), \text{ and } N_k \text{ is the amount of constituent in the neighboring cells } (k \in \Omega(i,j)).
\]

5. Nutrient modules

5.1. State variables

As in GEM, the nutrients considered in the LHEM are nitrogen and phosphorus. Various nitrogen forms, NO\(_2\), NO\(_3\) and NH\(_4\) are aggregated into one variable representing all forms of nitrogen that are directly available for plant uptake. Available inorganic phosphorus is simulated as orthophosphate. There are two nutrient modules currently available. The distinction appears in the conceptualization of nutrients in the vertical dimension. In terrestrial ecosystems, nutrients on the surface are no longer necessarily associated with surface water, and therefore need not be in the dissolved form as in GEM. Since most of the time most of the cells have no surface water, \(n\_SW\) (\(n = N \text{ or } P\)) represents the dry deposition of nitrogen or phosphorus on the surface. Over dry periods \(n\_SW\) continues to accumulate with incoming fluxes from air deposition or mineralization of organic material. When rainfall occurs, a certain proportion of the accumulated \(n\_SW\) becomes dissolved and therefore is made available for horizontal fluxing and infiltration.

The first nutrient module closely follows the hydrologic fluxes and considers nutrients on the surface (\(n\_SW\)), in the unsaturated storage (\(n\_UW\)) and in the saturated layer \((n\_S)\), \(n = N \text{ or } P\).

The second nutrient module is designed to accommodate for the aggregation of surface and shallow subsurface flows in the hydrologic sector. A proportion of nitrogen and phosphorus stored in the upper soil layer is made available for fast horizontal fluxing along with nutrients on the land surface. The depth of this layer is a soil dependent parameter. In most cases, we have assumed this layer to be 10 cm thick, following a similar formalization in the CNS model (Haith et al., 1984), where this upper soil layer was also assumed to be exposed to direct surface runoff. Therefore the spatial allocation of nutrient variables does not quite match that of the water. This is in attempt to minimize the number of variables, since even in this case, measurements that may be used for calibration are fairly scarce. However, the price that we pay for this aggregated representation is more complexity in the formalization of processes, because we have to compensate for the spatial aggregation assumed.

In this case, only \(n\_SW\) (mineral N or P on the surface), and \(n\_S\) (mineral N or P in the sediment) are considered. The phosphorus cycle in both modules, features another variable \(P\_SS\), which is the phosphorus deposited in the sediment in particulate form, no longer available for plants uptake, and effectively removed from the phosphorus cycle.

The input variables in this module are the hydrologic fluxes defined by the hydrologic modules as well as net primary productivity and root depth calculated in the plant dynamics modules.

5.2. Loading

There are five major sources of nutrients in the system: atmospheric deposition, fertilizer application, septic leakage, discharges from sewage treatment plants and natural decomposition of organic material. The atmospheric loading consists of dry and wet deposition. In
most cases, only the wet deposition is reported. To account for dry deposition, we may assume that it is in proportion to wet deposition with a coefficient $D_d$ that may be different for different localities.

The fertilizer loading can be defined by the amount and application time. In most cases, it occurs once or twice during the crop growth season and depends upon the crop, soil type and agricultural practices adopted in the area. One common way to estimate the amount of nitrogen fertilizers applied is to assume the pounds per bushel rule, when the amount of fertilizer applied per area in pounds is equal to the crop yield in bushels expected for the type of soil in the area (Bandel and Heger, 1994). Both atmospheric deposition and fertilizers contribute to the above ground storage of nutrients $n_{SW}$.

The amount of nutrients discharged from sewage treatment operations is usually a point time series that may be fed directly into the model for those cells where the discharge occurs. In most cases, it will contribute to $n_{SW}$, but in some cases, depending upon the engineering of particular discharges may also go to $n_{UW}$ or $n_{S}$. The leakage from septic tanks is a non-point source of pollution that may be estimated based on the amount of nutrients produced per individual per time period. For example, the amount of nitrogen is 4.8 kg/individual/year (EPA report with NCRI). According to other sources, this may vary: 3.5 – 5 kg/individual/year (EPA report with NCRI).

The natural decomposition of dead organic material also contributes to nutrient loading. It occurs both on the surface and in the soil. If $D_{min}$ is the total amount of mineralized detritus, then we assume that $gD_{min}$ is channeled to the surface storage of nutrients, whereas $(1-g)D_{min}$ goes to the subsurface storage. $0 < g < 1$ is the separation parameter, that is hard to measure and usually has to be calibrated.

5.3. Plant uptake

The amount of nutrients used for plant growth is in proportion to the net primary production (NPP). The nutrients in the surface storage are assumed to be available for plant uptake only when there is water to dissolve them. This water is taken to be surface water (SW), plus water contained in the 10 cm subsurface layer ($R_s$ in Fig. 2).

The amount of water in the subsurface layer is

$$S_s = \begin{cases} \frac{UW - R_s}{UW_d}, & \text{if } R_s < UW_d; \\ UW + S(R_s - UW_d)/(E - UW_d), & \text{if } R_s > UW_d; \end{cases}$$

where $UW$ is the water in the unsaturated storage, $S$ is saturated water, $R_s$ is the depth of the subsurface layer ($R_s = 10$ cm), $UW_d$ is the unsaturated layer depth and $E$ is elevation at the given locality. The total amount of water available to dissolve the nutrients is $SW + S$, and the concentration of nutrients is $n_{C_{sw}} = n_{SW}/(SW + S)$. The amount of nutrients available for plant uptake is then equal to the total amount of nutrients on the surface, when surface water is present, or is represented by only a part of $n_{SW}$ that is estimated to be in the subsurface storage:

$$n_{A_{sw}} = \begin{cases} n_{C_{sw}}(SW + S), & \text{if } SW > 0; \\ n_{C_{sw}}(1 - n_{D_d} - S), & \text{if } SW = 0. \end{cases}$$

The coefficient $n_{D_d}$ is used to separate between the amount of nutrients that are dissolved and further infiltrated into groundwater and the nutrients that are retained in the subsurface layer ($R_d$).

Then for the uptake of nutrients from the surface we may assume the rate:

$$n_{SW_{up}} = \min(n_{A_{sw}}, n_{U_{sw} \cdot NPP}),$$

where NPP is the net primary production of plants calculated in the plants module, and $n_{U_{sw}}$ is the parameter for nutrient requirements of photosynthesis.

The description of nutrients uptake from the sediment (both unsaturated plus saturated zone) is more complicated, since we need to parameterize the gradual decrease of nutrient concentration with depth (Fig. 2), also taking into account the depth of the root zone. Assuming that the concentration of nutrients is the same through the unsaturated zone and then decreases to zero at the bottom of the elevation considered, we may write that $n_{S} = \int_{R_s}^{E} N(x)dx$, where $N(x)$ is the vertical distribution of nutrients in the sediment in Fig. 2. Then
the amount of nutrients available for uptake in the root zone $R_d$ is $n_S(y) = \int_{R_d}^{y} n(x)dx$. Therefore the amount of nutrients available for plant uptake in the sediment is:

$$n_A = \begin{cases} 0, & \text{if } R_d < R_s, \\ \frac{n_S(2E-UW_d - R_d R_s)}{(E - R_d R_s - UW_d)}, & \text{if } R_d > R_s < UW_d, \\ \frac{n_S(2R_s - R_d - R_s)}{(E - R_s R_d)}, & \text{if } R_s < R_d < UW_d, \\ \frac{n_S^2}{E + UW_d} \left( \frac{2(UW_d - R_d)}{E - UW_d} \right), & \text{otherwise} \end{cases}$$

Here $R_d$ is the root depth calculated in the plants module. The uptake of nutrients from the sediment is then similar to the one calculated for the surface:

$$n_{SDup} = \min(n_A, n_{Us} \cdot NPP)$$

where $n_{Us}$ is the uptake parameter for the sediment storage of nutrients. In all the above formulas, $n = N$ or $P$ for nitrogen or phosphorus, respectively.

5.4. Vertical transport

Nutrients are dissolved in water and carried with hydrologic flows, both in the vertical and horizontal dimensions. The downflow from $n_{SW}$ to $n_S$ is associated with the infiltration of water from the surface into the sediment:

$$N = n_{Csw} \cdot n_{D_d} (UW_p + S_p + SW_S),$$

where $n_{Csw}$ is the nutrient concentration on the surface, $n_{D_d}$ is the separation coefficient discussed above, $UW_p$ and $S_p$ are the amount of rainfall infiltrated into unsaturated storage and saturated storage, respectively, and $SW_S$ is the flow from surface water into the saturated storage. The reverse process occurs when saturated water hits the surface and flows out:

$$N_{up} = n_{C_s} \cdot S_{SW},$$

where $n_{C_s}$ is the nutrient concentration in the sediment, $n_{C_s} = n_S/(S + SW)$, and $S_{SW}$ is the flow from saturated storage to the surface. Both $S_{SW}$ and $SW_S$ flows are calculated in the hydrologic module.

5.5. Sorption

At higher concentrations, PO$_4$ becomes adsorbed by organic material and metal ions in the soil. The rate of sorption is controlled by the amount of organic material in the soil. At lower concentrations of soluble PO$_4$, in the sediment, P_SS becomes available again and returns back into the nutrient cycle.

5.6. Spatial implementation

The horizontal spatial fluxes of nutrients are closely tied to the hydrologic flows. Therefore they are described together with the hydrologic flows on the surface (SWTRANS1 and SWTRANS2), and in the ground (GWTRANS).

6. Plants

6.1. State variables

In the plant module, we simulate the growth of higher vegetation. It will be the macrophytes in an aquatic environment, trees in forests, crops in agricultural habitats, grasses and shrubs in grasslands. The plant biomass (kg/m$^2$) is assumed to consist of the photosynthetic (PH) and the non-photosynthetic (NPH) components. In addition to that we distinguish between the above ground and the below ground biomasses (Fig. 3).

Another state variable ($B_t$) is employed to track the so-called biological time in the module. Biological time is the sum of effective daily average temperatures over the life span of the plant (growing degree-days). The temperature is called effective if it exceeds a certain value (5 °C in our case). These are the temperatures that are most suitable for the physiological development of the plant. Therefore the total of such temperatures is a good indicator of the plant life stage and may be used to trigger certain processes such as sprouting and appearance of reproductive organs.

The module imports temperature and solar radiation data from the physical module, nutrient availability from the nutrient modules, and water availability from the hydrologic module.

6.2. Temperature limitation

There are a great variety of functions that can be used to represent the temperature ($T$) limitation $L_t$ on growth processes (Jorgensen, 1980). In most cases, a bell-shaped

![Fig. 3. Major plant components considered in the plant module. Plant biomass is assumed to consist of the photosynthetic (PH) and the non-photosynthetic (NPH) biomass. The ratio between above ground non-photosynthetic biomass (NPH$_b$) and below ground non-photosynthetic biomass (NPH$_n$) is assumed to be constant.](image-url)
curve is described, which has a range of optimal temperatures where the limitation is negligible ($L_i = 1$) whereas at other temperatures, the growth slows down or stops completely ($L_i > 0$).

This behavior is provided by a function described by Lassiter and Kearns (1974):

$$L_i = \exp(s_i(T - T_{opt})) \left( \frac{T_{max} - T}{T_{max} - T_{opt}} \right)^{s_i(T_{max} - T_{opt})}.$$  

Here, $T_{opt}$ is the optimal temperature, $T_{max}$ is the maximal temperature after which the growth stops, $s_i$ is the curvature parameter that regulates the form of the curve.

Another function (Voinov and Akhremenkov, 1990) that is more complex, but offers more flexibility in defining the shape of the temperature limitation curve is:

$$L_i = \begin{cases} 
  f_{i0}^{1 - \frac{T}{T_{max}}} & \text{if } T < T_{opt} \\
  f_{i0}^{\frac{T_{max} - T}{T_{max} - T_{opt}}} & \text{otherwise} 
\end{cases}$$

where the additional parameters are $f_{i0}$, the value of the function at zero temperature ($L_i(0) = f_{i0}$); and $s$ is the value of the function at maximal temperature ($L_i(T_{max}) = f_m$).

6.3. Light limitation

Another factor that limits photosynthesis is the availability of light. The light limitation ($L_i$) is defined as:

$$L_i = \frac{I}{I_s} \exp \left( 1 - \frac{I}{I_s} \right),$$

where $I$ is the incoming solar radiation, and $I_s$ is the saturation level for irradiation.

6.4. Water limitation

If there is too much or too little water, the process of plant growth slows down. To account for the deficit of water, the function $W_0$ (Fig. 4) is used.

$$W_0 = \sin(W_s \cdot \pi/2)^m,$$

where $W_s$ is the available water, $m$ is the water deficit tolerance coefficient. When the tolerance is high ($m < 1$), the plant can grow fast enough even under low water availability. When tolerance is low ($m \gg 1$), the plant growth declines whenever water availability becomes below 1.

As with inadequate water availability, excess water may also be detrimental to plant growth. Certain plants require that a proportion of the root zone be above the water table to ensure that there is no limitation. Other plants grow well as long as they are covered by surface water to a certain level, but then if there is more water, their growth becomes inhibited. The function $W_1$ is to take into account both conditions. The coefficient $k$—the tolerance to high water stage—represents the tolerance to surface water stage when it is negative, and represents the requirement of a proportion of the root zone to be above the water table when it is positive:

$$W_1 = \begin{cases} 
  1/(1 + \exp(SW + k)), & \text{if } k < 0 \cup SW > -k; \\
  \min(1, U/W_d/k), & \text{if } k > 0 \cup R_d > 0; \\
  1, & \text{otherwise} 
\end{cases}$$

Here SW is the surface water, UW is the water in the unsaturated storage, and $R_d$ is the root depth. As the surface water stage exceeds the tolerance level, or the unsaturated depth becomes less than $R_d \cdot k$, $W_1$ becomes smaller than 1 and limits the plant growth.

The overall water limitation ($0 < L_w < 1$) is then calculated as $L_w = \min(W_0, W_1)$.

6.5. Nutrient limitation

The standard Michaelis–Menten equation is assumed to calculate the uptake ($f_n$) of each individual nutrient:

$$f_n = S_n/(S_n + C_n),$$

where $S_n$ is the nutrient ambient concentration, $C_n$ is the half-saturation coefficient; $n = N$ for nitrogen or $P$ for phosphorus. The Liebig principle of limiting factors is driving the overall nutrient limitation:
\[ L_a = \min(f_N, f_p). \]

6.6. Net primary production

The four limiting functions for light, temperature, moisture and nutrient availability are assumed to be multiplicative. The NPP is then calculated as

\[ F_{NPP} = \alpha_{NPP} L_i L_w L_o \cdot \text{PH}(1 - \text{PH}/\text{PH}_M), \]

where \( \alpha_{NPP} \) is the photosynthesis rate (1/day), and \( \text{PH}_M \) is the maximal photosynthetic biomass for the given type of plant.

6.7. Planting

Some types of plants, such as agricultural crops, are planted at a certain time, \( i_p \). During planting, a given amount of biomass is introduced into the system and then starts to grow. If seeds are planted, then the biomass introduced is non-photosynthetic. This biomass remains inactive until the biological time \( B_t \) becomes larger than a certain threshold \( B_{a0} \). After that, the translocation process described below starts to channel the biomass from the non-photosynthetic (NPH) to the photosynthetic (PH) storage. As PH appears, photosynthesis begins and the plant starts to grow.

6.8. Translocation

We describe the distribution of new biomass among the model compartments based on the following two proportions: \( \alpha^* = \max(\alpha) = \max(\text{PH}/\text{BM}_a) \), the maximum ratio of photosynthetic biomass to above ground biomass (BM_a); and \( \beta = \text{NPH}_a/\text{NPH}_b \), the ratio of above ground non-photosynthetic biomass (NPH_a) to below ground non-photosynthetic biomass (NPH_b), which is assumed to be constant.

Using these two ratios, we can calculate most of the other model fluxes and compartments. The above ground non-photosynthetic biomass is \( \text{NPH}_a = \beta \text{NPH}/(1 + \beta) \), and the below ground component is \( \text{NPH}_b = \text{NPH}/(1 + \beta) \). When there is more photosynthetic biomass produced than transferred into the non-photosynthetic storage, \( \alpha > \alpha^* \). During periods that are unfavorable for photosynthetic production, \( \alpha \) may become small, \( \alpha < \alpha^* \). However, at all times, the plant is assumed to try and maximize photosynthetic biomass, \( \alpha = \alpha^* \). The two processes that are employed for this purpose are Transup and Transdown. Transup describes the translocation of material from the non-photosynthetic storage (roots, branches) into the photosynthetic parts of the plant (leaves), and dominates at the start of the growth period or during periods unfavorable for growth when stored assimilates are used to maintain plant growth. Reciprocally, the Transdown dominates during periods of effective photosynthesis, when more assimilates are produced than currently needed and a portion can be channeled into storage in the non-photosynthetic parts of the plant. In both cases, the plant tries to maintain the proportion between the photosynthetic and non-photosynthetic parts as close to \( \alpha^* \) as possible.

The above ground biomass \( \text{BM}_a = \text{PH} + \text{NPH}_a = \text{PH} + \beta \text{NPH}/(1 + \beta) \).

Therefore \( \alpha = \text{PH}/[\text{PH} + \beta \text{NPH}/(1 + \beta)] \), and the translocation mechanism should operate is such a way that \( \alpha = \alpha^* \). This condition is altered for certain plants that grow reproductive organs (such as crops). As soon as the reproduction process comes into play, the plant changes the translocation patterns and growth of the reproductive organs becomes a priority. Since we do not have a special variable to account for these organs, we assume that they are part of the non-photosynthetic storage and when biological time exceeds the threshold for reproduction, the translocation is altered in favor of the NPH stock.

The proportion of the newly produced photosynthetic material that is translocated into the non-photosynthetic storage is then described as:

\[ T_\alpha = \begin{cases} \cos((\pi/2)\alpha^*/\alpha), & \text{if } \alpha > \alpha^* \\ 1 - 1/B_t, & \text{if } B_t > b_t \\ 0, & \text{otherwise} \end{cases} \]

where \( b_t \) is the biological time threshold after which reproductive organs start to develop.

The reverse process of translocation from the non-photosynthetic storage to generate photosynthetic biomass, Transup, occurs at the beginning of the vegetation period and is also triggered by the biological time counter \( B_t \).

6.9. Mortality, litterfall and harvest

These three flows occur at different times but they all decrease the plant biomass. Mortality is a natural process of decay of certain plant parts that is assumed to occur at a constant rate as a proportion of the photosynthetic and non-photosynthetic biomasses.

Deciduous plants shed their leaves (PH biomass) in the fall. The process is triggered by changes in day length: once day length becomes smaller than a certain threshold value, the litterfall process starts. The litterfall process starts slow and then accelerates as less photosynthetic biomass is left:

\[ F_L = \begin{cases} 0, & \text{if } D > d_l | D \geq D(t-1) \\ \lambda \cdot (\text{PH}_{\max}/\text{PH})^p, & \text{otherwise} \end{cases} \]

where \( \lambda \) is the litterfall rate, \( \text{PH}_{\max} \) is the maximal photosynthetic biomass, and \( p \) is the litterfall exponent.
Here, the first condition only allows litterfall to occur in fall when the day length $D$ is decreasing and becomes less than the threshold value $d$. The second condition clears the foliage completely after a certain minimal biomass $p_{\text{min}}$ is reached. The third condition is the gradual litterfall that starts when the day length requirement is reached; $\lambda$ is the litterfall rate and $n$ is the intensity ($n=3$); $PH_{\text{max}}$ is the maximal biomass reached during the season. It serves as a reference point from which to decrease the photosynthetic biomass (Fig. 5).

The harvest is another process that removes plant biomass. At harvest time, $t_H$, certain proportions of PH and NPH are taken out of the system. Right after harvest occurs, a certain portion, $\rho$, of the biomass left, is made available for the mortality flows that quickly channel the living biomass into the dead organic pool and make it available for decomposition. For seasonal crops, $\rho=1$, and all the biomass remaining after harvest rapidly dies off. For perennial crops, $\rho \to 0$, and there is no additional mortality caused by the harvest.

6.10. Spatial implementation and crop rotation

The spatial distribution of plants is fixed; plants do not travel horizontally in the landscape. Therefore the only spatial changes that can occur to the vegetation are connected to human activities, such as crop rotation, or other management practices. The spatial module that takes care of crop rotation is called by CROPROT (HAB\_MAP, DAYJUL), where DAYJUL is the Julian day, and HAB\_MAP is the Habitat map of the area. The function scans the whole area and switches land use type from one to another according to the current land use and the Julian day. The sequence of crops is fixed and is determined by the matrix (Fig. 6) where each crop is associated with a certain time interval. For each of the cells $(i,j)$ and each of the crops, we perform the operation:

\[
\text{if}\left(\text{TIME}_{k} = \text{TIME}_{i,j} \& \text{HAB}\_\text{MAP}(i,j) = \text{CROP}_{k-1}\right) \text{HAB}\_\text{MAP}(i,j) = \text{CROP}_{k}
\]

where $\text{TIME}_{k}$ is the planting day for $\text{CROP}_{k}$.

7. Detritus

7.1. State variables

At present, this module serves predominantly to close the nutrient and material cycles in the system, it does not go into all the details of the multi-scale and complex processes of leaching and bacterial decomposition. As biomass dies off, part of it turns into stable detritus, $D_{S}$, whereas the rest becomes labile detritus, $D_{L}$. The proportions between the two are driven by the lignin content, which is relatively low for the PH biomass and is quite high for NPH biomass. Labile detritus is decomposed directly, and stable detritus is decomposed either to labile detritus, or becomes deposited organic material (DOM), $D_{DOM}$.

7.2. Decomposition

Avoiding much of the complexities, we assume the decomposition process as linear. The decay of stable detritus is

\[
F_{DS} = d_{0}DS + d_{1}L_{DT}DS,
\]

where $d_{0}$ is the flow rate of stable detritus transformation into $D_{DOM}$, $d_{1}$ is the flow rate between stable and labile detritus. The latter flow is modified by Vant-Hoff temperature limitation function $L_{DT} = 2^{(T-20)/10}$, where $T$ is the ambient air temperature (°C). The decomposition of labile detritus and DOM are described similarly as linear functions modified by the Vant-Hoff temperature function.

8. Calibration and test runs

We have been mostly using the LHEM for modeling of the Patuxent watershed as well as several of its subwatersheds. Another watershed that was modeled is the Gwynns Falls, a highly urbanized watershed in Baltimore. The details of the PLM and its results have been reported elsewhere (Voinov et al., 1999a; Costanza et al., 2002), and may also be found at http://giee.uvm.edu/PLM. This brief description of the application of the LHEM in a particular project is primarily to illustrate how the modules were assembled and calibrated, and to demonstrate that they can be effectively adjusted to represent a variety of habitats and locations. We are not focusing on particular calibrations, since in any case, recalibration will be required if the LHEM is to be applied in other projects. It is more important to test the parameter ranges in which the modules can still perform and understand how robust they are when applied in various combinations and localities.

The modular approach called for the decomposition of the calibration process into what we termed a multi-
Fig. 6. Diagram of crop rotation most commonly implemented in Maryland. A user code modifies the Habitat Map used in the model according to this rotation. As a result, the modules get different sets of habitat dependent parameters at different times of the year.

tier calibration method, described by Voinov et al. (1999a). The calibration of the full model has been achieved in a step-wise process that started with the calibration of individual modules, moving then to spatial implementations of modules and groups of modules at several scales, until finally the full ecological model was calibrated for the whole watershed. The obvious benefit of this was a much simpler model to calibrate at each step. Clearly, the aggregate of several modules does not necessarily behave similarly to the individual modules taken separately. Therefore recalibration was needed every time we went from simple individual modules to their combinations, both locally and spatially. However, it was always much easier to fine-tune the already performing modules, than to do a full-scale calibration of the full model in its overall complexity.

We started with calibrations of the local hydrologic model. The input from other modules, primarily plants was imitated by fixed time series. For example, a time series was generated to represent the approximate dynamics of plants over a one-year time period. The model produced clearly different dynamics with and without plants (Fig. 7). Adequate data for local hydrologic calibrations was unavailable, since these processes are essentially spatial and it is hard to localize them and consider outside of the spatial context. Therefore the local hydrology was calibrated only in a “ballpark” fashion to make sure that the model behaves in a stable way in a variety of conditions. Similarly, we could provide only limited calibration of the local nutrient dynamics. This stage of local calibration was important to make sure that all the major fluxes, such as evaporation, transpiration, percolation, nutrient loading, and uptake, are within some reasonable values, that there are no inexplicable trends in the model. It was also important to run the sensitivity analysis and understand the effect of individual parameters on overall dynamics.

Most of the calibrations for these modules were done in combination with the module for spatial dynamics added within the SME context. The spatial model for hydrology and nutrients, or the water quality model has been calibrated for several subwatersheds in the Patuxent. We identified two spatial scales at which to run the model—a 200 m and 1 km cell resolution. The 200 m resolution was more appropriate to capture some of the ecological processes associated with landuse change but was too detailed and required too much computer processor time to perform the numerous model runs required for calibration and scenario evaluation. The 1 km resolution reduced the total number of model cells in the watershed from 58,905 to 2352 cells.

We did most of the preliminary calibrations for a small (23 km²) subwatershed of Cattail creek in the northern part of the Patuxent basin. Another small sub-
watershed that of Hunting creek, was located in the southern part of Patuxent, quite different in terms of soils and elevations. It also included an estuarine part that allowed us to test the second hydrologic algorithm that was designed for open water. The next larger watershed was the upper non-tidal half of the Patuxent watershed that drained to the USGS gage at Bowie (940 km²). And finally we examined the whole Patuxent watershed (2352 km²).

We staged additional experiments with the small Hunting creek subwatershed to test the sensitivity of the surface water flux. Three crucial parameters controlled surface flow in the model: infiltration rate, horizontal conductivity and the horizontal flow rate defined by path length on the link map over which water can travel per time step of the unit model. Riverflow peak height was strongly controlled by the infiltration rate. The conductivity determined river levels between storms and the link length modified the width of the storm peaks.

The results of surface water flow calibration have been reported elsewhere (Voinov et al., 1999a, b). They were in good agreement with the gage data, and what is most important, led us to several control parameters that were crucial to modify the patterns of the hydrographs in the way we needed. Whereas some individual peaks and situations were not always reproduced, the model worked well to represent the overall trends in the hydrologic patterns and gave a good estimate of the total outflow dynamics from the area.

Spatial nutrient dynamics were calibrated for data at several gaging stations on the Patuxent. Fig. 8 displays the calibration results for nitrogen concentrations measured at the USGS station at Bowie, which is in the mid-Patuxent watershed and accounts for dynamics in the upper half of the study area.

In contrast to water quality modeling, the plant module is less dependent upon spatial interactions. Therefore the unit model calibration in this case is more important. The calibrations were carried out for a series of parameter sets, representing the different habitat types and plant communities associated with them. We have considered a forest habitat, and a number of agricultural habitats, such as, corn, winter wheat, soybeans and fallow.

The data set that we used to calibrate the forest dynamics came from field monitoring over a 10-year time period at 12 forested sites located within the Eastern United States (Johnson and Lindberg, 1992). This provided mean flux rates and organic matter nutrient contents. Biomass and species composition were derived through the Forest Inventory and Analysis Database (FIA). The forest association used to select data was oak-hickory with 0.6% coniferous trees. For agricultural habitats, we have used data from the Maryland Cooperative Extension Agricultural Nutrient Management Program (http://www.agnr.umd.edu/users/agron/nutrient/home.html#homeplace), and other sources (Schroder et al., 1995).

It was most important to make sure that the available parameter set was sufficient to represent a variety of plant behaviors for different habitats and control factors. The overall pattern of growth, maturity and decay is similar for most of the plants; however, the dynamics of photosynthetic and non-photosynthetic biomasses varies for different plants. In Fig. 9, we represent the various growth curves for different habitats. The module producing these curves was the same plant module described above, only the parameter sets were different.

In another experiment, we have been testing the effect of various application rates of fertilizers upon the growth rates of a crop, soybeans in this case. The nutrient mod-

![Fig. 8. Spatial calibration of the water quality model for the gaging station at Bowie. The data available are quite sporadic and show considerable variability. It is not clear when the measurements were taken and how well they track the peak flows, when the nutrient content is the highest. Nevertheless, the model well represents the general trend and stays within the ranges of variations in the observed data.](image-url)
ule was used to generate the dynamics of available nitrogen, which was then fed into the plants module (Fig. 10). Two parameters were modified. In the first four scenarios, it was the amount of nitrogen fertilizer applied. In the fifth scenario, the dissolution rate for the fertilizer was decreased 10 times. Whereas the plain addition of fertilizers did not dramatically change the plant growth pattern, by decreasing the dissolution rate, we have significantly increased the amount of biomass produced. This may look somewhat contrary to the amounts of nitrogen available as shown in Fig. 10B. Apparently, the amount of nitrogen in the fifth scenario is the least. It requires the zoom-in in Fig. 10B to see that most important is the pattern of how the nutrient is delivered to the plants. By extending the dissolution time, we actually increased the amount of fertilizer that was made available for plant uptake. As a result, the production of photosynthetic biomass has jumped and consequently the non-photosynthetic gains also increased. This may be viewed as a Best Management Practice in which the fertilizers are applied in a granular form that is then slowly dissolved and infiltrated into the soil. The gain in the yield and biomass production turns out to be quite remarkable in this case. Once again, our purpose here is not to demonstrate model behavior in particular applications, but to show that individual modules, and their combinations produce meaningful output in a broad range of parameters and forcings, and can be used to test various hypotheses and scenarios.

Once the local modules were tested and precalibrated, they were translated and compiled by SME into a general spatial model that has been further applied to the full Patuxent watershed and its subwatersheds. The resulting model has then been used to run an extensive scenario analysis program (Costanza et al., 2002). By running these scenarios, we actually further test the model for an even wider range of parameters and forcing functions, which considerably increases our confidence in the model’s robustness and feasibility.

9. Conclusions

Somewhat in contrast to GEM, in the modular approach, we do not intend to design a unique general model. In this case, our goal is to offer a framework that can be easily extended and is flexible to be modified. A module that performs best in one case may not be sufficient in another. The goals and scale of a particular study may require a completely different set of modules that will be invoked and further translated by the SME into a working model. Though STELLA may not be perfect for all models and processes involved, by using it to describe the modules we can provide the transparency that is essential to reimplement modules in different contexts and environments.

There is a certain disparity between the software developer and the researcher views upon models and modules. For a software developer, a module is an entity, a black-box, which should be as independent as possible, and should be as easy as possible to combine with other modules. This is especially true for the federation approach to modular modeling and is well demonstrated by the web-based modeling systems. The utility of such
For a researcher, a model is predominantly a tool for understanding the system. By plugging together a number of black boxes, for which specifics and behavior is obscure and hardly understood, we do not significantly increase our knowledge about the system. The results generated are difficult to interpret when there is not enough understanding of the processes that are actually modeled. As noted above, this is especially characteristic of ecological and socio-economic systems, which are complex and allow much ambiguity in their formalization. The decomposition of such systems requires careful analysis of spatial and temporal scales of processes considered and is very closely related to specific goals of the model built.

We argue that in this context, the modular approach can be useful if the focus is shifted from reusability and “plug-and-play”, to transparency, analysis and hierarchical description of various processes and system components. With the modules being transparent and open for experiment and analysis, the researcher can better understand the specifics of the model formalism that is inherited. It is then easier to decide whether a module is suitable or if it should be modified and tuned to the specific goals of the particular study. It is mostly for this reason that, when possible, we offer the LHEM modules as STELLA implementations that provide the much needed transparency and openness.

There have been several attempts of collecting, documenting, and archiving environmental models (Fiddman, 2001; Noble and Davies, 1995; CEML, 1997), among which the Kassel University Register of Ecological Models is probably most noteworthy (Benz and Knorrenschild, 1997; Hoch et al., 1998). However, in our case, we seek quite a different goal and instead of collecting all the available models and approaches we tend to limit our scope to a minimal set of modules needed to represent a fairly wide variety of environments. In this respect, this approach can be compared to the Modular Modeling System (MMI, Leavesley et al., 1996), where the goal is not to collect and archive existing models, but rather present certain modules and models in a format that would allow recombination and modification to meet the user’s needs. This does not preclude expandability of the system. Additional modules are invited and can be added to the system, as long as they comply with a certain set of rules that would allow their integration into the system.

When applying the LHEM, or any other modeling library, the major complication for the user is to put together the modules in a meaningful and consistent way. In GEM, or in any other prefabricated model, the issues of scale consistency where taken care of by the model developers previously. Now with the modular approach, the challenge of combining the modules in such a way that they match the complexity of the modeled system and are mutually consistent becomes the task of the library user. Once again this added concern is the price that is paid for the added flexibility and optimality of the resulting models. In theory, we can envision modeling systems that would keep track of the scales and resolutions of the various processes involved, and automatically allow links with only such modules that would match these scales. In practice, with all the complexity and uncertainty associated with ecological and socio-economic systems, it may still be a while until such modeling tools appear. In the meanwhile, we think that the model transparency will be a very important prerequisite of modularity, especially if the modules are to be used in a research context.

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References


