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Non-spatial calibrations of a general unit model for ecosystem simulations

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Abstract

General Unit Models simulate system interactions aggregated within one spatial unit of resolution. For unit models to be applicable to spatial computer simulations, they must be formulated generally enough to simulate all habitat elements within the landscape. We present the development and testing of a unit model for the Patuxent River landscape in the state of Maryland, USA. The Patuxent Landscape Model (PLM) is designed to simulate the interactions among physical and biological dynamics in the context of regional socioeconomic behavior. The PLM is a tool for evaluating landscape change within the Patuxent watershed through simulation of ecological systems. A companion economic model estimates land development patterns and effects on human decisions from site characteristics, ecosystem properties, and regulatory paradigms. Landscape elements that are linked within the PLM are forest, agriculture and open water systems, and three levels of urban development. Urban developments are low and medium density residential areas (14.07% of the total watershed), and commercial, industrial and institutional area (5.7%). Forests are mixed populations of deciduous and evergreen species (45.11%). Agricultural areas (28.02%) are simulated through rotating crops of corn, winter wheat and soybeans within a cycle of two years. Open water (6.84%) represents the ecosystems within the rivers and streams where phytoplankton are the primary producers. In this paper we illustrate, how we gathered and formalized working models used within the Patuxent watershed for forests, agriculture urban settings and wetlands. Further, we show how we tested and merged the variety of models employed by scientific disciplines and created a general unit model to be used in the Patuxent Landscape Model (Pat_GEM). The Patuxent Landscape Model is built under the Spatial Modeling Environment.

Keywords: Ecosystem; Simulation; Complex; Calibration

1. Introduction

Watersheds are composites of landscape elements, which traditionally are not studied and managed in an integrated way. Foresters study forest, agriculture is the domain of farmers and

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agricultural scientists, and planners manage urban areas. At a landscape scale all these management objectives and scenarios for the individual landscape elements are linked.

Studying the workings of systems through scientific observation requires recognition and formulation of models for hypothesis testing. The underlying objective for landscape modeling is to create tools that allow a more integrated management of landscapes through simulation of interactions between landscape elements. To go from specialized management to a more integrated approach, the gap between the working models of observers specialized in single landscape elements and the entire landscape needs to be bridged (Fig. 1).

Computer landscape simulation is a logical method for the integrated approach between disciplines due to its ability to handle large amounts of data and information and to provide output aggregated for easy interpretation. The complexity introduced with large amounts of data and information very likely creates non-linear behavior, which in turn obscures the interpretation of the model output. Throughout this paper we present how confidence can be gained for simulation results from complex unit models.

1.1. General unit models

Landscape simulations require the formulation of general unit models for simulation of temporal processes (Fig. 2; Fitz et al., 1995). Dynamics for general models are by definition not habitat specific. Discrimination between habitats is accomplished by applying habitat specific initializations of stocks and parameters. General models in contrast to unique habitat specific models, ease the computational challenges in representing landscape dynamics at the higher resolutions (Fitz et al., 1995; Running and Coughlan, 1988; Running and Gower, 1991; Parton et al., 1994). Landscape models that do not make use of general models often are specialized for one habitat (e.g. forest models; Running and Gower, 1991; Band et al., 1991) or assume large aggregations of the landscape (Baker, 1989). The challenge is to create unit models that can easily be scaled to higher and lower resolutions in time and space.

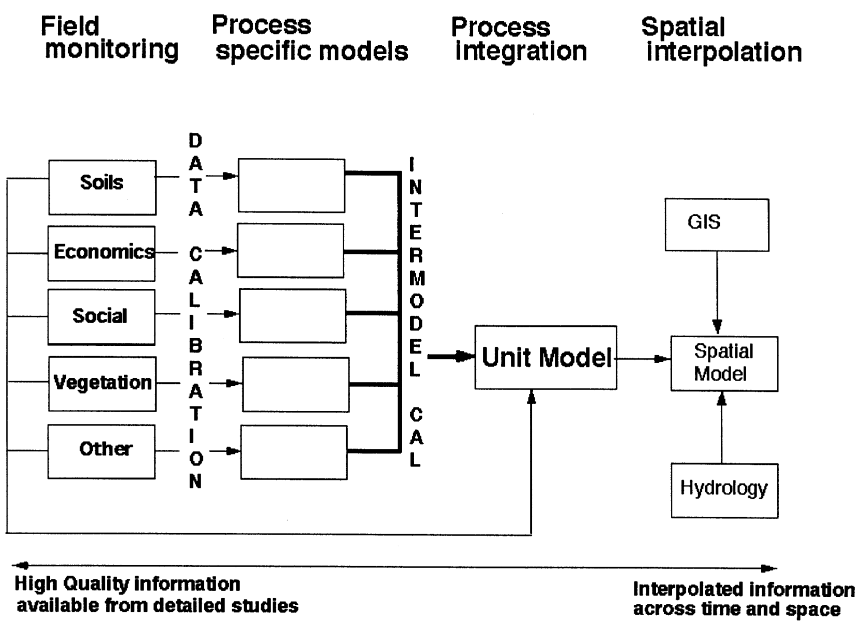

Fig. 1. Extrapolation of site-specific data derived from field monitoring to provide information at a larger spatial and temporal scale.

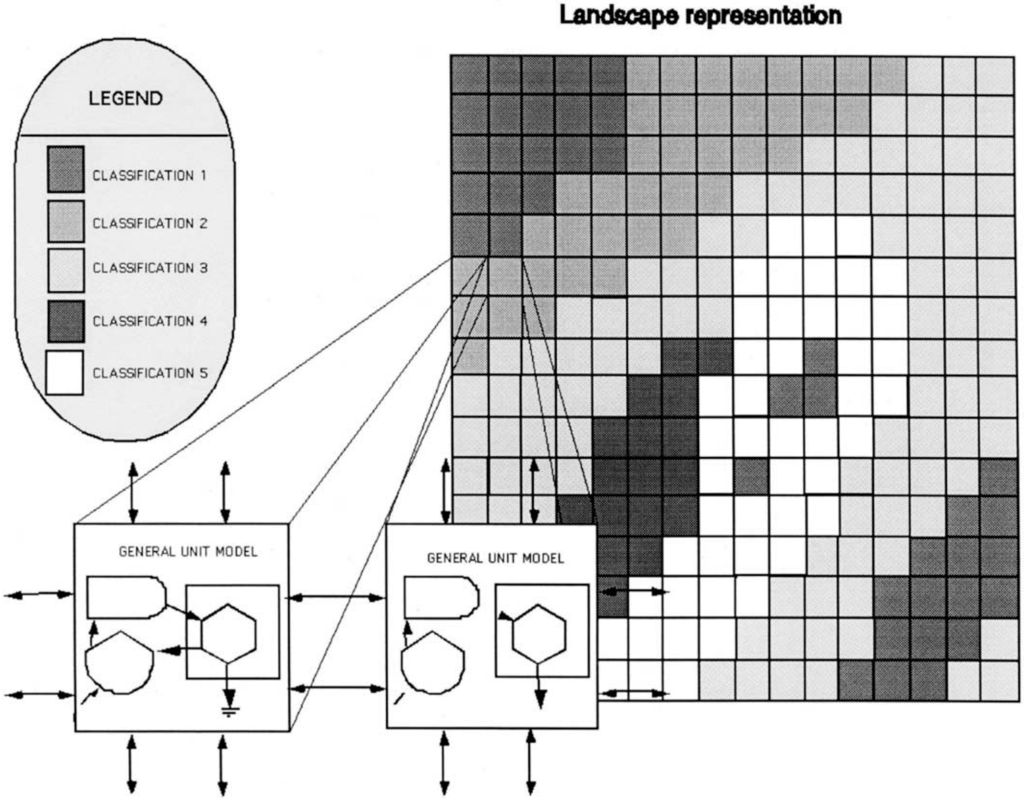

Fig. 2. Schematic of a landscape model.

1.2. Model description

Pat_GEM was developed to be the ecological model and non-spatial building unit for the spatial Patuxent Landscape Model (PLM). PLM covers ecological-economic dynamics of the 2500 km^2 Patuxent river watershed in Maryland and integrates data and knowledge over several spatial, temporal and complexity scales in order to aid regional management. The PLM effort is an outgrowth of a model first developed for Louisiana wetlands and later expanded and applied to the Florida Everglades (Costanza et al., 1990; Fitz and Sklar, 1999). PLM is the first implementation of the full ecological model in an upland setting and includes hydrology, nutrients, plants, animal populations, and human economic systems. The landscape is depicted as a grid of cells with a minimum cell size of 200×200 m^2 to allow adequate depiction of the pattern of ecosystem processes and human settlement on the landscape.

Pat_GEM includes modules for hydrology, nutrient movement and cycling, terrestrial and estuarine primary productivity, and general consumer dynamics (Fig. 3). The hydrology module of the unit model is a fundamental component for other modeled processes, simulating water flow vertically within the cell (e.g. infiltration, evapotranspiration). Phosphorus and nitrogen are cycled through plant uptake and organic matter decomposition, with the latter simulated in a sediment/soil dynamics module. The macrophyte module includes plant growth response to various environmental constraints (including water, light and nutrient availability and seasonal temperatures), changes in leaf canopy structure (influencing water transpiration), mortality and translocations of photosynthetic product. The principal dynamics modeled in Pat_GEM are:

plant and phytoplankton growth in response to available sunlight, temperature, nutrients, and water;
animal (consumers) growth in response to food sources;
dynamics in detrital matter;
dynamics in soil organic matter;
flow of water plus dissolved nutrients in three dimensions.

Feedbacks among the biological, chemical and physical model components are important structural attributes to the model. While the unit model simulates ecological processes within a unit cell, horizontal fluxes link the cells together across the landscape to form the full landscape model. These spatial fluxes are driven by cell-to-cell head differences of surface and ground water in saturated storage. Water fluxes between cells carrying dissolved and suspended materials for simulating water quality in the landscape.

1.3. Calibration/verification of unit models

Pat_GEM is a complex process-based simulation model. Models such as Pat_GEM are increasingly needed in predictive, site-specific environmental research (Band et al., 1993; Costanza et al., 1993; Wigmosta et al., 1994; Baron et al., 1998; Creed and Band, 1998). Increasing complexity causes the number of solutions within the parameter space to grow exponentially with the number of unknown parameters, and finding a unique solution through calibration at the complexity of Pat_GEM, with 21 state variables and 37 unknown parameters, is virtually impossible (Beven and Binley, 1992; Beven, 1993). Instead of narrowing down to one unique solution within the parameter space, we applied whole system tests for conservation of mass and robust behavior, and applied a newly developed Model Performance Index (MPI) (Fig. 4). We also utilized a set of exploratory techniques (Villa et al., 2001) to isolate multiple areas within the parameter-space that produce agreements between model simulation output and available systems information.

Theoretical problems with calibrating complex models is highlighted by Villa et al. (1998) who developed and applied a computer aided search algorithm for exploring model parameter spaces, and compared these explorations against more usual methods of calibration such as eyeballing,

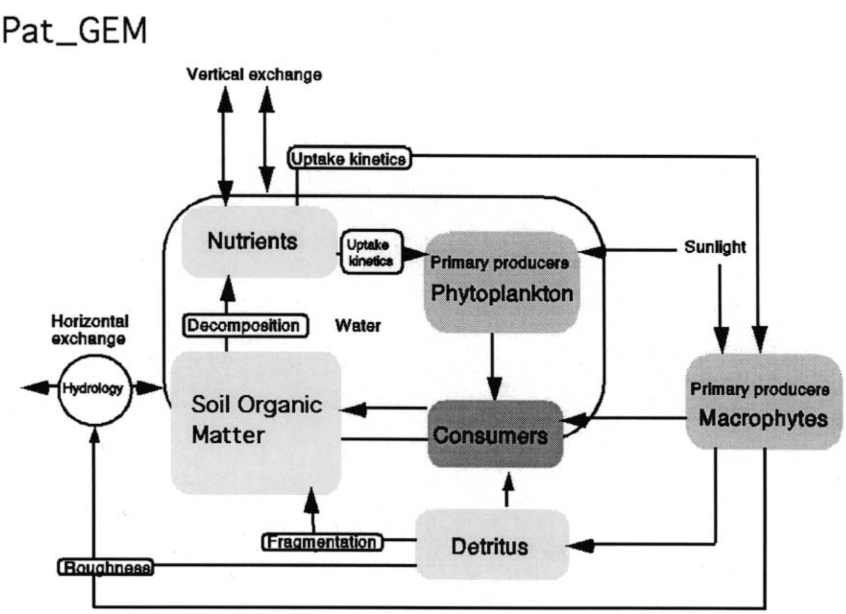

Fig. 3. Material flows between ecosystem components as modeled within a Pat_GEM unit.

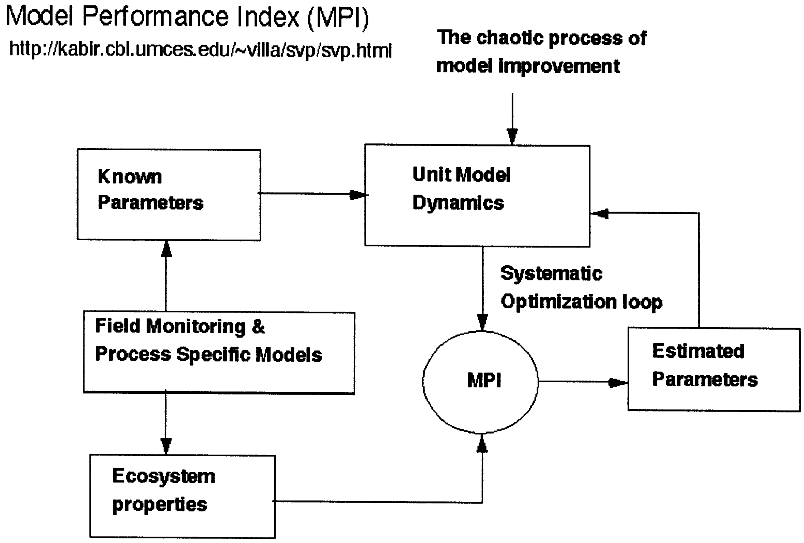

Fig. 4. Calibration process using MPI and systematic optimizations of unknown parameters to improve confidence in unit model performance.

hill climbing and Monte Carlo experiments. Villa et al. (1998) found that as the number of unknown parameters increases, the number of areas that can be discriminated within the parameter space to fit the same observed data is also increasing. When less is known of a modeled system, systematic calibration of complex models will reveal more potential solutions. Consequently, non-systematic calibrations, such as 'eye balling', have been inconclusive as methods for exploring the total potential parameter space.

2. Methods

2.1. Model applied

Pat_GEM was developed from the GEM model presented by Fitz et al. (1995). Development of the GEM was mostly for simulating wetland dynamics, emphasizing and elaborating on water column dynamics in mostly estuarine environments. With Pat_GEM we shifted focus to the dynamics of more terrestrial and human dominated habitats such as forests, agricultural lands and urban areas. This shift in focus not only required changes to settings of the parameter values, but also brought about more general approaches regarding how these parameters influenced the ecosystem properties. Applying the GEM model to additional alternative settings will continue this generalization process of modeling ecosystem processes.

The important objective after constructing Pat_GEM was to gain confidence in simulation outputs for mimicking the ecological, physical and biological processes that are of importance to the dynamics within the Patuxent watershed. Applying innovative strategies for unit model calibration, we learned about the limits of applicability and the range of behaviors exhibited by Pat_GEM, and we narrowed down the areas in the parameter space that are most likely to represent Patuxent watershed habitats. We discovered temporal scalability variations among variables and tested for conservation of materials.

2.2. Robustness

The unit model was tested for scalability across time (robustness). Pat_GEM simulations were executed at seven different time steps ranging from 2 h to 8 days. Model output from simulations diverting from the one-day time step for which the model was calibrated, were regressed against the one-day time step output (Table 1).

Poorly robust behavior in some of the state variables such as nitrogen did not cause similar poor behavior in state variables that track long term changes within a system such as soil organic matter in terrestrial ecosystems. Overall, state variables with low frequency dynamics were most predictable. Table 1 shows the results of the robustness tests for a selection of Pat_GEM state variables. Robust behavior varied between state variables and within state variables among landuses. For example, biomass in agricultural land uses could be reproduced at the higher resolution time steps (intercept 0, slope 1), but missed the day on which farmers planted crops at lower resolutions. The deciduous nature of the forest proved forest biomass to be time step sensitive due to the fast processes during the short periods of the year of greening up and litterfall. In comparison, urban lawns were more robust. The least robust was the biomass stock in open water habitat that is mainly modeled as phytoplankton, a biomass stock very sensitive to erratic behavior in surface water nutrient concentrations.

Interesting differences in robust behavior are illustrated by the two nutrients, nitrogen and phosphorous. While phosphorous behaves fairly robustly, nitrogen performed poorly. Pat_GEM recognizes the immobile stage of inorganic phosphorous in the soil, but not of nitrogen. Consequently, nitrogen concentrations are more sensitive to hydrologic events which are fast paced, in comparison to the buffered phosphorous concentrations.

2.3. Conservation of materials

Pat_GEM was tested for conservation of materials. Pat_GEM lumps organic carbon, nitrogen and phosphorous within the state variable 'biomass', while accounting separately for inorganic nitrogen and phosphorous. Conversions between organic and inorganic states are derived through assigning parameters for carbon to nitrogen to phosphorous ratios. Unless materials are represented by state variables through all configurations (e.g. inorganic and organic states), calibration of C:N:P ratios are required to balance material influxes, outfluxes and stocks to comply with the law of conservation of mass. In Pat_GEM, no state variables are assigned to variation in inorganic carbon, nor are the dynamics of oxygen and trace minerals included.

Calibrations carried out for forest simulations showed that nutrient ratio parameters could be found to ensure conservation of mass within an acceptable margin of error. After calibration, losses or gains never exceeded 0.0012% for phosphorous or 0.0002% for nitrogen at any time during a two-year simulation. Regrettably, these calibrated results were very sensitive to new settings in other areas of the parameter space so that re-calibration of the nutrient ratios is required for each new implementation of the model.

Although material ratios in phytoplankton are considered very stable (e.g. Redfield ratios) other systems have worked out mechanisms to concentrate nutrients in the living part of the organic matter while depleting the non-living part. For example, nutrients in trees are concentrated under the bark and in the leaves. When this tissue dies and becomes wood, nutrients are recovered for use by non-woody parts. A similar recapturing of nutrients takes place during coloring and shedding of leaves in the fall. From this example, we learn that when forests grow in age (more standing wood) nutrient to carbon ratios decline (Parton et al., 1988; Vitousek et al., 1988). Increase in nutrient ratios occur within the transformation from detritus to soil organic matter. Given the right temperature and moisture conditions the microbial organisms that carry out the decomposition will sequester the nutrients while respiring the carbon causing a change in nutrient ratios.

2.4. Exploration of the parameter space

Pat_GEM model's behavior was extensively investigated across its parameter space, representing four of the habitats commonly found within the Patuxent watershed. This exercise was to: (1) understand the limits of applicability and range of behaviors exhibited by the model with parameter change; and (2) reduce the dimensionality of the parameter space, pointing out the most sensitive

Table 1
Model output from simulations diverting from the one-day time step for which Pat_GEM was calibrated, were regressed against the one-day time step output [a]

DT	Biomass				Inorganic nitrogen				Inorganic phosphor				Soil organic matter			
Day	Intercept	SD	Slope	SD	Intercept	SD	Slope	SD	Intercept	SD	Slope	SD	Intercept	SD	Slope	SD
Agriculture																
0.125	0.19	−0.04	0.94	−0.02	10 698	−3360	−4.3	−8.9	0	0	0.81	−0.1	0.37	−0.03	0.96	−0.01
0.25	0.2	−0.04	0.96	−0.02	3759	−1040	−1.5	−2.8	0	0	0.82	−0	0.2	−0.03	0.98	0
0.5	0.19	−0.04	0.98	−0.02	610	−208	−0.2	−0.6	0	0	0.82	−0	−0.01	−0.02	1.01	0
2	0.07	−0.12	0.53	−0.08	9	−4	-2.0×10^{-3}	−0.01	0	0	0.31	−0.3	0.28	−0.03	0.96	−0.01
4					4	−2	-5.0×10^{-4}	−0.004	0	0	0.18	−0.7	−1.93	−0.06	1.26	−0.01
8					4	−2	-2.0×10^{-3}	−0.004	0	0	−0.07	−0.1	−1.51	−0.05	1.2	−0.01
Forest																
0.125	25.2	−1.71	0.16	−0.06	36 888	−12 000	-7.0×10^{-2}	−0.22	0	0	0.93	−0	2.03	−0.22	0.89	−0.01
0.25	13.5	−1.02	0.55	−0.03	13 117	−3800	-3.0×10^{-2}	−0.07	0	0	0.94	−0	0.78	−0.23	0.96	−0.01
0.5	4.23	−0.29	0.86	−0.01	2163	−748	-4.0×10^{-3}	−0.01	0	0	0.96	−0	1.05	−0.12	0.94	−0.01
2	39.21	−3.86	−0.3	−0.13	129	−48	-2.0×10^{-4}	−0.0009	0	0	−0.39	−0.3	4.1	−0.66	0.77	−0.04
4	41.7	−3.75	−0.39	−0.12	38	−18	-2.0×10^{-5}	−0.0003	0	0	−0.59	−0.4	−1.36	−0.8	1.08	−0.04
8	40.09	−3.48	−0.34	−0.12	16	−6	-3.0×10^{-5}	−0.0001	0	0	−0.82	−0.3	−2.53	−0.66	1.14	−0.04
Urban																
0.125	−0.01	−0.01	1.04	−0.04	14 765	−4790	−3.4	−8.03	0	0	0.8	−0.1	2.26	−0.08	0.9	0
0.25	−0.01	−0.01	1.05	−0.04	5291	−1520	−1.2	−2.55	0	0	0.8	−0.1	1.76	−0.06	0.92	0
0.5	−0.02	−0.01	1.13	−0.04	877	−302	−0.2	−0.51	0	0	0.82	−0.1	1.03	−0.03	0.95	0
2	−0.02	−0.01	1.06	−0.06	3.0×10^{12}	-3.0×10^{12}	-7.0×10^{8}	-5.3×10^{9}	0	0	0.9	−0.2	1.27	−0.08	0.94	0
4	−0.11	−0.02	1.85	−0.15	7	−3	5.0×10^{-4}	−0.01	0	0	1.35	−0.5	−5.29	−0.13	1.24	−0.01
8	−0.02	−0.01	1.1	−0.06	4	−2	-9.0×10^{-4}	0	0	0	−0.03	−0	−4.44	−0.13	1.2	−0.01
Open water																
0.125	0	0	0.01	−0.01	2.0×10^{-5}	-5.0×10^{-5}	1	0	0	0	1	0				
0.25	0	0	0	−0.01	2.0×10^{-5}	-4.0×10^{-5}	1	0	0	0	1	0				
0.5	0	0	0.01	−0.02	2.0×10^{-5}	-3.0×10^{-5}	1	0	0	0	1	0				
2	0	0	0.32	−0.46	2.0×10^{-3}	-3.0×10^{-4}	0.9	−0.01	0	0	0.99	0				
4	0	0	4.93	−1.61	3.0×10^{-3}	-4.0×10^{-4}	0.7	−0.02	0	0	0.98	−0				
8	−0.02	−0.01	42.4	−19.9	5.0×10^{-3}	-4.0×10^{-4}	0.2	−0.02	0	0	0.97	−0				

[a] Most robust variables show intercepts closest to 0 and slopes closest to 1.

parameters, to obtain maximal calibration efficiency and highlight feasible areas on which to concentrate investigation.

To carry on this investigation, we exploited the Model Performance Index framework described in Villa et al. (1998). This framework allows the definition of a model's parameters function (from now on called the objective function) expressing the agreement of quantitative data and semi-quantitative hypotheses about the model's expected behavior with the model's output. MPI-based objective functions are used to explore the parameter space under different viewpoints, from simple feasibility of the output to exact matching of particular data sets. A number of search techniques were used, from Monte Carlo exploration to global optimizations using genetic algorithms.

The sensitivity of the MPI scores for state variables to particular individual parameters is very dependant upon a total configuration of the objective function, and no general conclusion can be drawn about the effect of parameter changes without considering this overall objective function context. But simply knowing the proportion of cases that particular parameters were influential for changes to state variables for many configurations of the objective function is obviously important to the investigator. The influence plot in Fig. 5 shows this proportion for single parameter effects and two-way interaction effects. The effect of each parameter is detailed for each single variable. As the plot shows, most effects are significant only in a minority of cases, which further demonstrates the complex nature of the model's response. However, some parameters seem to influence the variables' MPIs in most cases. With the help of the influence plot, the experimenter can check at a glance whether a change in a parameter is likely to improve the MPI score for a variable, which other variables are likely to be involved, and which other parameters are likely to be involved in the effect. This proves to be essential in forming the next step in the calibration process. Parameters which do not seem to have an effect can be excluded from the next search to save on computational time, using their maximum likelihood estimates. Parameters and their interactions which appear to have an effect in the majority of cases can be further investigated until a better calibration point is found. This can be used as the initial guess for a new automated search cycle, maybe with redefined parameter boundaries and sensitivities to narrow the search space.

2.5. Calibration experiments

During the analysis of many search cycles, Exploratory Data Analysis (EDA) techniques and careful use of data reduction are useful to overcome the complexity due to the multivariate nature of the response surface. To help this process, we have designed a suite of tools, which quickly allow us to interactively generate specific plots according to specific needs. After determining that the combined effect of two parameters is worth exploring by looking at the influence plot, more quantitative knowledge about these particular effects can be sought by plotting the MPI values as a function of parameter value.

We explored the potential for subdivision of the parameter space to carry out multiple calibrations at reduced complexities. Subsets in the parameter space were identified, and parameters clustered around their most likely to be influenced variables. In addition, we separated those parameters that introduced the highest levels of complexity and gave them fixed values to simplify analysis of the remaining parameter space.

Initially, a large sample of 71 from the 128-dimensional PLM parameter space was selected for exploration. Parameter space dimensions that involved processes between cells (spatial parameters exclusively linked to hydrology), parameters designed for specific scenarios, and parameters involved in processes that are not likely to be within a forested habitat at the 200 m resolution were not explored. The 71 parameters were assigned maximum and minimum boundaries and subjected to an initial exploration for sensitivity using genetic algorithms (Wang, 1997). An additional 43 parameters were excluded when they proved to be insensitive on the overall modeling results.

After parameter space complexities were explored and reduced to manageable and influential proportions we applied the MPI search algorithms to fit the GEM models against measured data. As we explored a remaining 37-dimensional parameter space (Fig. 5; Table 2), we found macrophyte variables for Net Primary Productivity and Leaf Area Index (Fig. 6) most sensitive to parameter changes. Variables and test criteria selected are presented in Table 3. Least sensitive were material fluxes associated with mortality of photosynthetic and non-photosynthetic macrophyte biomass, the translocation of photosynthetic materials from the leaves to the roots, and the stock in non-photosynthetic carbon. Some sensitivity was observed for consumption of non-photosynthetic tissues.

We found that the Leaf Area Index in the PLM is most efficiently calibrated using single parame-

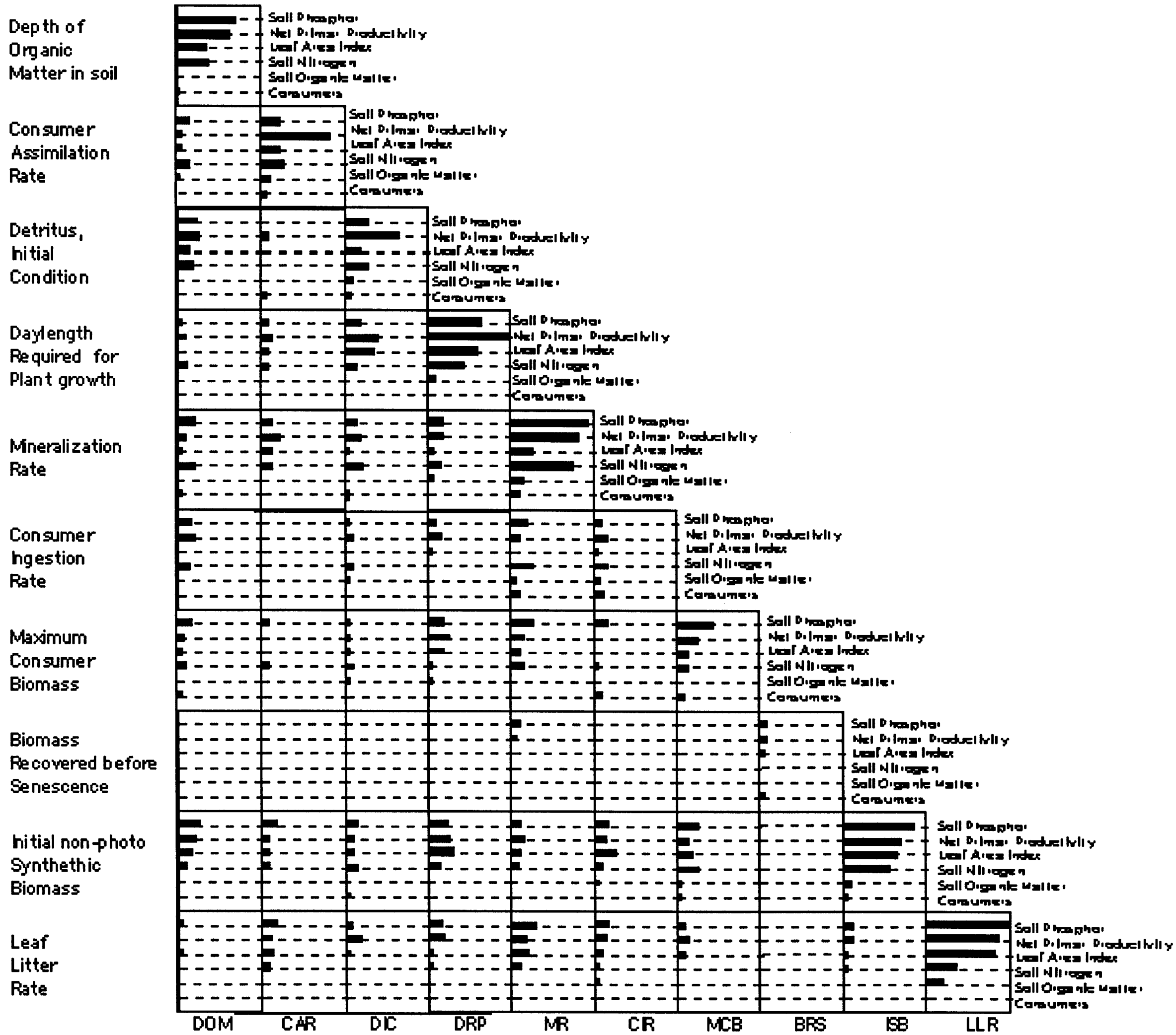

Fig. 5. Portion of the influence plot for the data calibration experiments. Each box contains a bar plot summarizing the proportion of significant effects found for a particular parameter or parameter interactions on each variable's MPI. The length of each bar is proportional to the number of search cycles where the second-degree polynomial regression of the variable's MPI versus the parameter value has been significant at the 95% level. Diagonal elements show single-parameter effects and sub-diagonal elements show two-way interaction effects between parameters. The plot has been generated with data coming from the *F* calibration experiments.

Table 2
Pat_GEM parameter values [a]

Parameters	Units	Initial value	Boundaries				Calibrated value
			Lower		Upper		
Consumer module							
Consumer assimilation rate	$1\ d^{-1}$	0.5	0	(o)	1	(o)	0.15
Maximum consumer biomass	$kg\ m^{-2}$	1	0.1	(c)	100	(c)	5.9895
Consumer ingestion rate	$1\ d^{-1}$	0.175	0	(o)	1	(o)	0.175
consumer mortality rate	$1\ d^{-1}$	0.014	0	(o)	1	(o)	0.003
Consumer respiration rate	$1\ d^{-1}$	0.03	0	(o)	1	(o)	0.03
Opt temperature for consumer activity	C	30	20	(c)	40	(c)	28
Detritus module							
Detrital decay rate	$1\ d^{-1}$	0.00015	0	(c)	1	(c)	0
Initial stock for detritus	$kg\ m^{-2}$	5	0	(o)	100	(o)	5
Rate in detrital shredding	$1\ d^{-1}$	0.01	0	(c)	1	(c)	1
Module for dissolved inorganic nitrogen in soils							
Concentration gradient	Dimless	0.3	0	(o)	1	(o)	0.8
Mineralization rate	$1\ d^{-1}$	0.2	0	(c)	0.5	(c)	0.5
NH4 porportion of the inorganic nitrogen	Dimless	0.5	0	(o)	1	(o)	0.5
Soil organic matter N:C ratio	Dimless	0.066	0	(o)	0.1	(o)	0.067
Photobiomass N:C ratio	Dimless	0.01	0	(o)	0.1	(o)	0.001
Module for soil dead organic matter							
Detrital biomass C concentration	Dimless	0.5	0.1	(c)	0.9	(c)	0.42
Initial value for organic matter porosity	Dimless	0.2	0	(c)	0.9	(c)	0
Initial value for percent organic matter in soils	%	0.5	0	(c)	0.9	(c)	0.05
Depth of the organic matter soil horizon	m	0.5	0	(o)	10	(c)	0.5
Hydrology module							
Initial soil moisture	%	0.5	0.1	(c)	0.9	(c)	0.3008
Maximum canopym conductivity	Dimless	0.5	0	(o)	1	(o)	0.5
Macrophytes module							
Biomass recovered before leaf litter fall	$1\ d^{-1}$	0.5	0	(o)	0.9	(c)	0.5
Daylength required for plant growth	h	13.5	0	(o)	24	(o)	9.42
Nitrogen uptake rate	$1\ d^{-1}$	0.2	0	(o)	1	(o)	0.15
Phosphor uptake rate	$1\ d^{-1}$	0.003	0	(o)	1	(o)	0.003
Light saturation point	Langleys	600	0	(o)	1000	(o)	600
Plant optimum growth temperature	C	31	20	(c)	40	(c)	21
Ratio above and below biomass	Dimless	35	10	(o)	50	(o)	40
Ratio photo to non-photo biomass	Dimless	0.5	0.1	(c)	0.9	(c)	0.5
Ratio above to below non-photo biomass	Dimless	3.6	0	(c)	10	(c)	3.6
Non-photosynthetic biomass	$kg\ m^{-2}$	30	0	(c)	100	(c)	23
Photosynthetic decomposition rate	$1\ d^{-1}$	0.0005	0	(c)	1	(c)	0
leaf litter rate	$1\ d^{-1}$	0.1	0	(c)	1	(c)	0.99
Module for soil phosphor							
Photobiomass P:C ratio	Dimless	0.0108	0.01	(c)	0.09	(c)	0.01
Concentration gradient	Dimless	0.3	0	(c)	0.9	(c)	0.3
Equilibrium conc. for mobile phosphor	$kg\ m^{-3}$	0.03	0	(o)	0.1	(c)	0.03
Initial concentration	$kg\ m^{2-2}$	0.003	0	(c)	1	(c)	0
Absorption rate for mobile phosphor	$1\ d^{-1}$	0.2	0	(o)	1	(c)	0.2

[a] Initial rates are hand calibrated values, boundaries are expected maxima and minima, while calibrated values were derived through the MPI search algorithms ($MPI = 0.29$) (Villa et al., 2001).

ters within the macrophyte module. We also found important parameter interactions between the consumer and macrophyte modules, soil organic matter and macrophyte modules, and among macrophyte parameters. Table 4 shows the frequency distribution of single parameters and parameter combinations.

Net Primary Productivity is sensitive to single parameters within the macrophyte, soil organic matter, consumer and nitrogen modules. Important parameter interactions occur between the macrophyte and consumer modules, soil organic

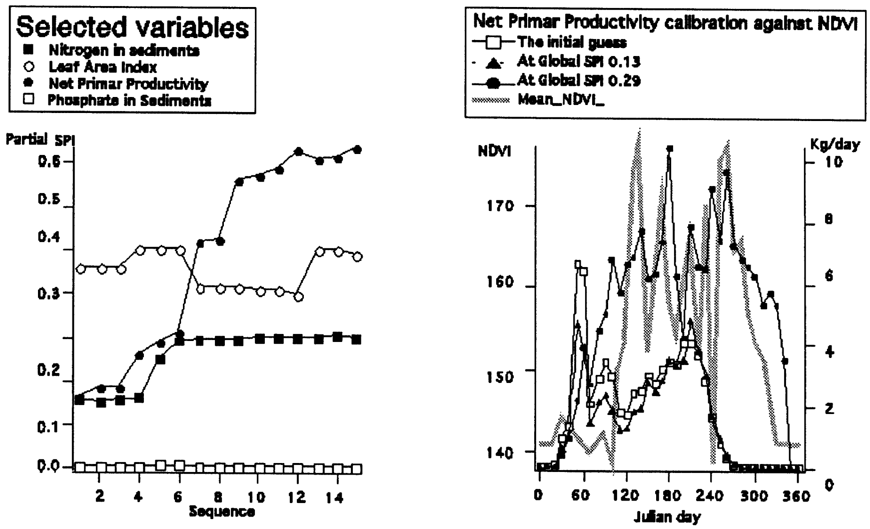

Fig. 6. Panel A shows the most successful parameter update sequence during the execution of the MPI search algorithm for Pat_GEM forest applications. Individual variable agreements with assigned test requirements (partial MPI) are evaluated against collective variable test agreement (global MPI). Panel B shows model agreement between NDVI values and Net Primary Productivity after eyeballing (the initial guess), after the most successful update sequence (MPI = 0.29), and after a less successful update sequence (MPI = 0.13).

Table 3
Variables, test criteria and data sources as the observation space for calibration of forest habitat within the Pat_GEM

Variable	Test assigned	Data	Reference
Detritus module			
Detritus biomass	Wbounds	Min = 0.3; max = 6.6	Johnson and Lindberg, (1992)
Module for dissolved inorganic nitrogen			
N in soil	Theil	Time series	McFarland, (1995)
Soil organic matter module			
Soil organic matter	Wbounds	Min = 7; max = 34	
Macrophyte module			
Leaf area index	Wbounds	Min = 0; max = 9	Johnson and Lindberg, (1992)
Non-photo biomass	Wbounds	Min = 2.5; max = 42	FIA database
Photo biomass	Wbounds	Min = 0.1; max = 3.5	FIA database
Net primar prod.	Freq	Time series	NDVI
Phosphor module			
P in soils	Theil	Time series	McFarland, (1995)

Table 4
Frequency distributions of single parameters and parameter combinations

10–19	20–29	30–39	40–49	50–60
N:C soil organic matter	Consumer assimilation	Nitrogen uptake	Organic soil depth	Plant daylength required
Consumer assimilation × mineralization	Initial detritis	Plant opt growth temp	Initial soil moisture	Mineralization
Consumer assimilation × initial soil moisture	Initial detritis × plant daylength required		Initial OM porosity	Non-photo biomass
Initial detritis × organic soil depth	Max consumer biomass		Phosphorous uptake	Leaf litter
Initial detritis × initial OM porosity	Initial OM porosity × initial soil moisture		Detrital C	
Plant daylength required × nitrogen uptake	Decomposition of photo materials			
Plant daylength required × non-photo biomass				
Mineralization × photobiomass N:C ratio				
Mineralization × initial soil moisture				
Mineralization × initial OM porosity				
Mineralization × plant opt growth temp				
Mineralization × leaf litter				
Consumer ingestion × organic soil depth				
Consumer ingestion × mineralization				
Consumer ingestion × initial soil moisture				
Consumer ingestion × non-photo biomass				
Max consumer biomass × plant daylength required				
Max consumer biomass × mineralization				
Max consumer biomass × initial soil moisture				
Max consumer biomass × initial OM porosity				
Max consumer biomass × non-photo biomass				
Photobiomass N:C ratio				
Consumer mortality				
Opt temp for consumers				
Initial soil moisture × plant daylength required				
Initial soil moisture × nitrogen uptake				
Initial soil moisture × phosphorous uptake				
Max canopy conductivity				
Initial OM porosity × plant daylength required				
Initial OM porosity × plant opt. growth temp				
Initial OM porosity × non-photo biomass				
Detrital C × initial OM porosity				

matter and nitrogen modules, detritus and hydrology modules, and among macrophyte module parameters.

2.6. Pat_GEM calibrations for four habitats within the Patuxent watershed

PLM land uses are aggregated into six separate categories of which three are within different urban settings. Unit model calibrations explored the parameter space to represent characteristics found in forest, agriculture, open water and urban settings. The paper presents only examples carried out for forests. Data sources upon which we have based our assumptions for correct model behavior are presented in Table 2. Explorations on relevant areas in the parameter space of the Pat_GEM model for agricultural urban areas and wetlands are within various stages of completion (Fig. 7). Development and calibration of General Ecosystem Models runs parallel to the advancements that take place within the various fields of science dedicated to individual habitat types. Changes in paradigms will lead to the adjustment of General Ecosystem Model dynamics, while new observational information on parameters will further narrow our unknown parameter space. New observations in time and space will expand the test criteria that are available for calibration.

3. Discussion

We presented methods and results that were designed to help increase and report the confidence in output from models that are too complex for

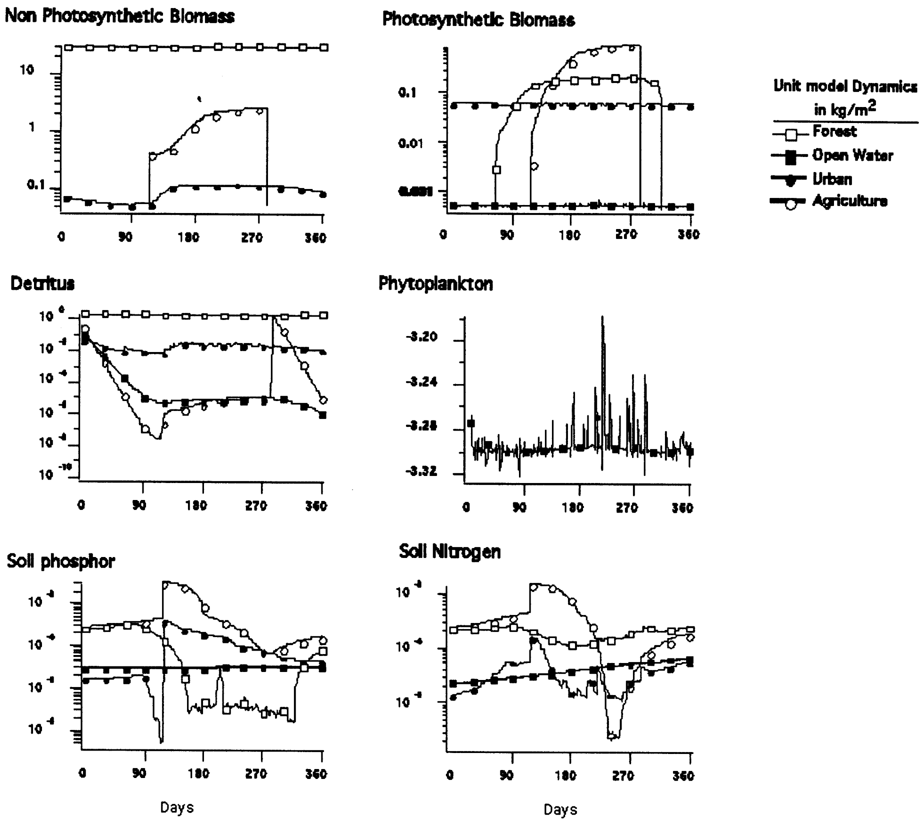

Fig. 7. Pat_GEM unit model output for six state variables and four habitat types. Outputs in kg m^{-2} for all variables are seasonal dynamics at one-day time steps over a 365 day period.

applying conventional means of calibration and verification. Our model, derived from less complex models based upon careful observation of time and space specific phenomena, is intended for simulating ecological processes in the Patuxent watershed. The attempt to cover within one model, all potential habitats under all conditions not only caused expansions in the unknown area of the parameter space, but also reached levels of complexity and non-linear behavior such that conventional techniques for means of building confidence were inappropriate. Through our experiments, invaluable information was gathered on how to improve complex model calibrations and report the results objectively.

Confidence levels remained low after applying the tests on conservation of mass. Pat_GEM is intended for use in spatial modeling, where each pixel in the landscape represents a unique combination of parameters. Additional calibration to have each unique combination meet conservation of mass requirements is cumbersome. The question is raised as to whether the computational benefits expected from lumping the organic nutrient fractions in the biomass weights justify the calibration efforts that are needed to satisfy the law of conservation of mass. The error can be noted but ignored assuming the existence of a non-modeled nutrient pool that functions as capacitor. A likely candidate for the function could be the non-modeled microbial biomass.

Confidence gained from the parameter search routines was subject to pre-calibration conditions of the availability and quality of the information and data available for testing. Reporting this subjectivity provided the means upon which confidence levels between complex models can be compared. Before testing a complex model such as Pat_GEM, an observational space will need to be defined. Testing output against observations is the most powerful means to gain confidence in model predictions. The Pat_GEM model potentially can be tested against 76 different categories of observations (total sum of stocks and fluxes) and most confidence would be gained when all stocks and fluxes would agree with data from observations. Unfortunately, for a large subset of the 76 stocks and flows in the Pat_GEM, there were no observations, no data from observations, or no compatible data from observations. Good agreement on a few categories of observational data could give a false sense on the complete goodness-of-fit when other properties of the model were not tested at all.

A calibration specific formulation of the MPI is defined within an a priori observational space, not only in quantity, e.g. how many of the stocks and flows are being tested, but also in quality. Quality statements are for the individual fluxes or stocks and are imbedded when a particular statistical test is assigned, as well as in the weighting of the test results in the ultimate index. For example, more confidence is gained when one of the model outputs is able to track a time series expressed in compatible units, measured at time intervals similar to the model time step (thiel test), than when a particular model output is not exceeding boundary conditions (boundary test). On the other hand, if the data quality of the time series is questionable while the boundary conditions are firm, more confidence should be assigned to the results of the boundary test.

3.1. The narrowing of the parameter space

Confidence can be gained for complex simulation models when the objective function can be reduced to only the most important dimensions. Villa et al. (1998) found that with increasing numbers of unknown parameters the number of potential areas in the parameter space for fitting the model output to the observational space also increased. Although this opens up an important discussion on how natural phenomena classified similarly through observation can have very different underlying dynamics and building confidence in the model output requires systematic narrowing of the parameter space before calibration. How the parameter space is narrowed is important information for judging calibrations. As in defining the observational space, the a priori explanation of the quality and quantity of the known parameter space and how non-relevant and insensitive parameters are identified create yet another dimension to the confidence level expectancy.

Confidence was gained when the Pat_GEM parameter space, reduced for forests, showed no surprises for the remaining parameters and parameter variable interactions with respect to the literature on forest dynamics (Gholtz et al., 1994; Reichle, 1981; Vitousek et al., 1988). After assigning values to 34 parameters to be known of no consequence to either forest or non-spatial dynamics, we were still left with 37 unknown parameters. Because Villa et al. (1998) found in the complex model they explored, a maximum allowable number of nine unknown parameters, we searched the records on the successful hill climbing attempt for those parameters that were most influential for improving upon the overall MPI score (Fig. 5). Different definitions of the observation space undoubtedly will expose different sets on influential parameters. Extra confidence is gained when calibrations for observational spaces, defined within habitat, bring forward tendencies in parameter variable interactions that can be recognized by habitat experts.

4. Final conclusion

More detailed classification through hierarchical schemes applied to landscape models (Mitsch, 1992; Lavorel et al., 1995; Michaelsen et al., 1994) will have to be followed up with more specific calibrations of complex unit models. Not only will we want a calibration for a generic forest; eventually we will want to know about available observations, objective function reductions and attainable MPI scores for deciduous and coniferous forests.

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