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Research Article

Impacts of Spatial Partitioning in Hydroecological Models: Predicting Grassland Productivity with RHESSys

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Abstract

Environmental models constructed with a spatial domain require choices about the representation of space. Decisions in the adaptation of a spatial data model can have significant consequences on the ability to predict environmental function as a result of changes to levels of aggregation of input parameters and scaling issues in the processes being modelled. In some cases, it is possible to construct a systematic framework to evaluate the uncertainty in predictions using different spatial models; in other cases, the realm of possibilities plus the complexity of the environmental model in question may inhibit numeric uncertainty estimates. We demonstrate a range of potential spatial data models to parameterize a landscape-level hydroecological model (RHESSys). The effects of data model choice are illustrated, both in terms of input parameter distributions and resulting ecophysiological predictions. Predicted productivity varied widely, as a function of both the number of modelling units, and of arbitrary decisions such as the origin of a raster grid. It is therefore important to use as much information about the modelled environment as possible. Combinations of adaptive methods to evaluate distributions of input data, plus knowledge of dominant controls of ecosystem processes, can help evaluate potential representations. In this case, variance-based delineation of vegetation patches is shown to improve the ability to intelligently choose a patch distribution that minimizes the number of patches, while maintaining a degree of aggregation that does not overly bias the predictions.

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1 Introduction

Evaluating the performance of environmental models is necessary to judge their development progress and their suitability for given tasks. This can involve comparisons to measured responses, inter-comparisons of models, and sensitivity analysis to evaluate uncertainty and the relative importance of different parameters. When an environmental model incorporates a spatial domain, extra complexity is introduced in that the form of the spatial data model itself could impact the predictions of environmental behaviour on the landscape. This general issue in spatial environmental modelling is not treated very often in the literature. If the choice of spatial representation does not have significant effects on the predictions, there is no need to be overly concerned with the choice – in fact, any arbitrary scheme would be suitable. However, for many environmental processes there are likely to be important spatial effects, as a function of some combination of: (1) spatial interactions between many of the processes, and (2) the effects that aggregation of input conditions in any particular spatial representation may have on the ability to predict environmental function.

Ecophysiological models generally attempt to scale observations at a site to some concept of a larger region. There is a range of possibilities to accomplish this, from considering the entire region as one aggregate unit (e.g. for productivity models, the world can be modelled as one big leaf), to dividing up the region into as many individual model units as are needed to represent the site scale (possibly going down to modelling individual objects such as actual plants or leaves), with a range of strategic partitioning methods in between (Rastetter et al. 1992).

Considering the extreme cases first for illustration, one could divide the study region into as many small units as needed for them to be considered similar to the individual objects or sites in a research project, and then examine an aggregated (or distributed) prediction. In this approach, it is perhaps tempting to simply overlay a very large, fine mesh over the region, in effect running a large number of site models and aggregating. However, this will normally be undesirable in terms of practicality (computing power, data volumes), or due to the associated uncertainty in the parameters. As computing power increases, the issue returns because previously impractical approaches become possible. Despite changes in computational practicality, however, it is unlikely that the model parameters are known for all the locations in the grid, so some method of estimation must be used. It has been argued in the past (e.g. Lammers 1998, Handcock et al. 1999), and will be further demonstrated here, that the uncertainty in this estimation can be considerable and non-intuitive.

Returning to the first extreme, it could be feasible to use spatially large, highly aggregated regions. This leads to two areas of concern: (1) will the loss of variability in the aggregated inputs limit the ability of the model to predict relevant output patterns within reasonable bounds, and (2) is it possible to measure ecosystem parameters at scales that correspond to these spatial units? For example, one cannot measure with any certainty some of the quantities we want to predict, such as mineralization rates, photosynthetic activity, or total nitrogen runoff across large areas (such as those typically dealt with in environmental management), and this contributes to prediction uncertainty (Aber et al. 1993).

For a given prediction problem, a suitable compromise between these extremes is needed. This presents a significant challenge in two ways: determining how many modelling units are required, and how they should be located. The entire range of possible realizations of a partitioned landscape are typically unmanageable (i.e. as many as $M^{(N-1)}$-1 where N = number of original units (pixels) and M = number of partitioning units) (Csillag and Kabos 1997, 2002), but some basis for choosing an appropriate method is far preferred over arbitrary choices (White and Running 1994, Lammers 1998, Handcock et al. 1999, Mitchell and Csillag 2000, Handcock and Csillag 2002). Alternatives to select an appropriate combination could range from a "blind guess" (completely arbitrary choice) to an adaptive method which conforms to the distribution of the data, or an exploratory analysis (which may build upon an adaptive solution) incorporating knowledge about the environment (e.g. representative patch sizes, or relationships of the modelled entities to landscape features such as aspect, catenary position, etc). The goal is to capture the landscape patterns that are created (or governed by) the processes of interest.

We present an analysis to find a suitable combination of spatial units to capture the pattern and processes of concern across a landscape. We will show the sensitivity of productivity, predicted by the RHESSys hydroecological model, to spatial definitions of vegetation patches derived from a range of choices, including arbitrary tessellations and adaptive methods, and demonstrate how exploratory techniques can be used to select a particular scheme. A specific application, predicting regional productivity in Grasslands National Park, Saskatchewan, will be used to test the model. Our objectives are to determine:

1. How does our prediction of ecosystem function depend on the chosen spatial representation?
2. Can we develop general conclusions or guidelines for either this modelling environment or spatial environmental modelling in general?

1.1 Background

The uncertainty of predicting landscape response based on knowledge gathered at relatively fine resolutions, or small extents, is a well recognized phenomenon (e.g. Jarvis and McNaughton 1986, Rastetter et al. 1992, Biondini and Grygiel 1994, Fuhlendorf and Smeins 1996, De Pury and Farquhar 1997, McNulty et al. 1997, Lammers 1998, Chen et al. 1999, Hansen and Jones 2000, Wirtz 2000, van Noordwijk 2002), but strategies to deal with the problem are varied. Despite increasing evidence that prediction uncertainty is important (e.g. Csillag 2000, Mackay and Robinson 2000), attempts to control or account for spatial accuracy in environmental analysis often seem to be missing or undervalued (Chrisman 1999, Mowrer 1999).

Some of this apparent reluctance may stem from the fact that the uncertainty in predictions from already complicated process models can stem from a very large range of sources. Individual models have uncertainty associated with assumptions in mathematical or algorithmic representations of natural processes that are derived from our current imperfect understanding of these systems. This physical science perspective is perhaps the classical view of modelling uncertainty. Ecosystem models are usually an agglomeration of "sub-models" taken from various sources, meaning that the individual pieces were developed for different purposes and may have conflicting assumptions; this source of uncertainty has been termed "semantic error" (Mackay and Robinson 2000). In parallel with these issues surrounding the physical science are those that might be classified as being in the GIS or geostatistical domains. Uncertainty in parameter and input values also contribute to model uncertainty. There are two issues here. The first concerns uncertainty associated with the measurement or estimation/calibration of individual input or parameters values for a given spatial unit. Beven and Binley (1992) discusses numerous examples of parametric uncertainty and offers strategies for addressing this type of uncertainty. Once the models are distributed across space, the method used to aggregate inputs can also impact model predictions. The spatial structure of a model or how it partitions the landscape into discrete units contributes to model uncertainty since the implications of landscape tessellation are rarely quantified.

Rastetter et al. (1992) reviews the problems encountered when moving between modelling scales. Perhaps the most fundamental concept to environmental modelling is that if a relationship developed at a relatively fine scale is not linear, when that relationship is applied at a coarser scale with more aggregation of input conditions, the prediction will always be biased. There are methods to correct or at least minimize this effect. One of the most popular approaches is spatial partitioning, which aims to minimize heterogeneity of input conditions within each modelling unit. Partitioning aims to reduce aggregation error rather than correct it, by reducing the set of fine-scale components into a manageable number of units such that within each of the partition units the variability among the aggregated fine-scale units is minimized (Rastetter et al. 1992). In other words, each partition unit should represent as homogeneous an area as possible in terms of the distribution of model inputs. The response of the entire area can then be taken as a weighted average of all of the partition units, while the aggregation error is minimized. However, even if the need for such strategic partitioning is recognized, the huge number of potential combinations of partitioning schemes means that it is practically impossible to evaluate all possibilities, or derive an optimum solution.

There is a significant literature on the impact of aggregation on the modelling of ecosystem response. The implications of scaling vary with research questions being asked, the associated scale of available input data and the types of ecosystem processes involved. Numerous studies have investigated the impact of spatial resolution for global (or general) circulation models (Harvey 2000) as well as for models of continental vegetation dynamics such as BOREAS (Chen 1996), FIFE (Friedl et al. 1995) and VEMAP (VEMAP Members 1995).

For most environmental management problems, however, the scale of interest is more intermediate, focusing on areas still considerably larger than field research plots (or individual forest stands, rangeland paddocks, etc.), but much smaller than continents. At this mesoscale, there seem to be fewer integrated modelling efforts and only limited or very specific analyses of error or uncertainty caused by aggregation issues. There are isolated examples of this type of research, such as the ability to identify landforms at different scale and with different terrain models (Mackay et al. 1992), scaling insect population dynamic observations to regional behaviour (Fleming et al. 2002), and impacts of the aggregation of temporal data (Holman-Dodds et al. 1999, Mitchell and Csillag 2001). There seem to be more examples in the domain of hydrological modelling, perhaps due to the importance of terrain characteristics on hydrologic flows, and the sensitivity of terrain measures such as slope and aspect to the models and resolutions selected to represent the terrain (e.g. Band 1993, Band et al. 1995, Higy and Musy 2000, Kirkby 1997). Results from these primarily hydrologic models, however, have implications for coupled models that examine feedbacks between hydrology and vegetation growth and biogeochemical cycling (i.e. soil moisture controls on evapotranspiration, photosynthesis, nitrogen cycling, etc.) over spatially variable terrain. This is especially important in semi-arid areas such as in Grasslands National Park, where water availability has strong controls on plant growth.

Band (1993) explored the effect of spatial aggregation on water balance and photosynthesis with an early version of RHESSys. This experiment varied the level of complexity of the input parameterization and the hydrologic sub-model, and demonstrated that significant prediction bias resulted from lumped representations of surface resistance, and that vapour and heat fluxes were significantly sensitive to soil water distributions, particularly in dry environments. Band (1993) cautioned that many of his findings may have been caused, or at least amplified, by the high topographic relief in the study area, and called for further experiments across a range of environments. White and Running (1994) examined scaling effects with RESSys (a precursor to RHESSys which had less emphasis on hydrology), in order to test whether or not the model's predictions would scale well (linearly) in complex terrain when changing resolution from Landsat TM (30 m) through AVHRR (1 km) resolutions. Their predictions of photosynthesis and above-ground NPP remained stable across scales; however, evapotranspiration predictions were affected by changes in the hydrological modelling at different scales. Since we know that grasslands are very sensitive to moisture availability, it is reasonable to assume that if their study were repeated in Grasslands National Park, it would be more difficult to scale net productivity.

Zhu and Mackay (2001) looked at the effect different levels of detail had on predicted streamflow and photosynthesis using RHESSys, and found that detailed spatial soil information and distributed parameterization were important when there was moisture stress, but not at other times. Mackay and Band (1997) and Creed and Band (1998) both demonstrate examples (also using earlier versions of RHESSys) where small pockets in the landscape that are disconnected hydrologically can produce very different dynamics from their surroundings, and that this behaviour is significant within the context of the landscape, but the ability to capture it is lost with aggregation that averages out the local soil water content. Beven and Franks (1999) show that two different partitioning schemes can lead to identical predictions from a SVAT model, and introduced the term "functional similarity" to describe this phenomenon.

All of these studies demonstrate specific instances where issues of aggregation or details about landscape representation can have important impacts on the ability to predict ecosystem dynamics. Many of these are a factor of, or can potentially be controlled by, how the landscape is partitioned into modelling units, and we focus on this aspect of the modelling process.

Although the objectives of the partitioning are clear, there is a wide range of approaches to the task. The size, and shape of the partition units, or the location of boundaries between them, can be arbitrary or a function of something distributed across the landscape. The specific tradeoffs between increasing the number of modelling units and decreasing bias in the predictions will be unique to the models and landscapes being studied. This is not necessarily a simple relationship, either. One perspective on these interactions is to look at the relationship between residual variance of the output variable against the number of partitioning units, as shown in Figure 1. We know that this will be a more or less monotonic function (Rastetter et al. 1992, Lammers 1998), but the actual shape of the function depends on the landscape pattern which controls the processes. In the extremes, if the landscape was a checkerboard pattern of two values, nothing would happen to the variance:resolution function until the last (finest resolution) step in the partitioning, whereas if the landscape was divided into two

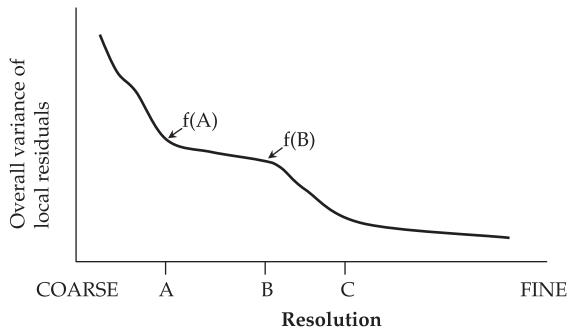

Figure 1 The relationship between the bias caused by aggregation and the degree of aggregation may take many forms. The most obvious target for selecting modelling units is to find areas where the trade-off between the number of units and the bias in predictions has identifiable changes in behaviour; for example, on the curve in this graph there is a relative plateau between the resolutions A and B. Between these points the bias does not decrease significantly with finer resolution (f(A) is similar to f(B)). Therefore, there is little advantage in choosing a partitioning level anywhere from point A until the bias/resolution relationship becomes steep again (between B and C)

contiguous internally uniform halves, all variance would be taken care of in the first split. Intermediate cases will lead to curves like the hypothetical one in Figure 1, which demonstrates that more than one partitioning of the landscape can result in similar or equal residual variance. For many datasets, two possible spatial arrangements of input data show functional similarity and can lead to the same overall residual variance. In this case, the more parsimonious scheme should be chosen to increase computatational efficiency and reduce the need for input estimation.

Partitioning methods can be classified according to topology, use of terrain information, and scalability. Figure 2 illustrates the two methods used in this study. The uniform grid is the same structure used in raster data models, i.e. a regular tessellation of uniform-sized rectangles (usually squares) with an arbitrary origin. This has the advantages of simplicity and easy computation or comparison of multiple data sets with the same grid system, but there is no enforced relationship between the partitioning units and the landscape pattern.

Quadtrees are a good example of variance-based partitioning, directly addressing the purpose of partitioning as one way to reduce aggregation error (Rastetter et al. 1992). Variance-based partitioning refers to dividing up data by comparing the relative variance of various subsets of the data. Other examples include many image classification methods, regression trees, or any other statistical technique based on ANOVA.

Quadtrees share an arbitrary rectangular tessellation and coordinate system with regular grids, but the size of each unit is variable, allowing different levels of "interest" in spatially distributed data (Csillag 1996). Simply put, the algorithm used to build the quadtree on a 2-dimensional dataset first divides the region of interest in four equal-sized squares (called "leaves"), then examines the data falling into each of these leaves to find the one that contains the most residual variance, and that leaf is itself split into four smaller units. This process is repeated until either the total number of leaves reaches a defined maximum, or the average residual variance is reduced to an acceptable level.

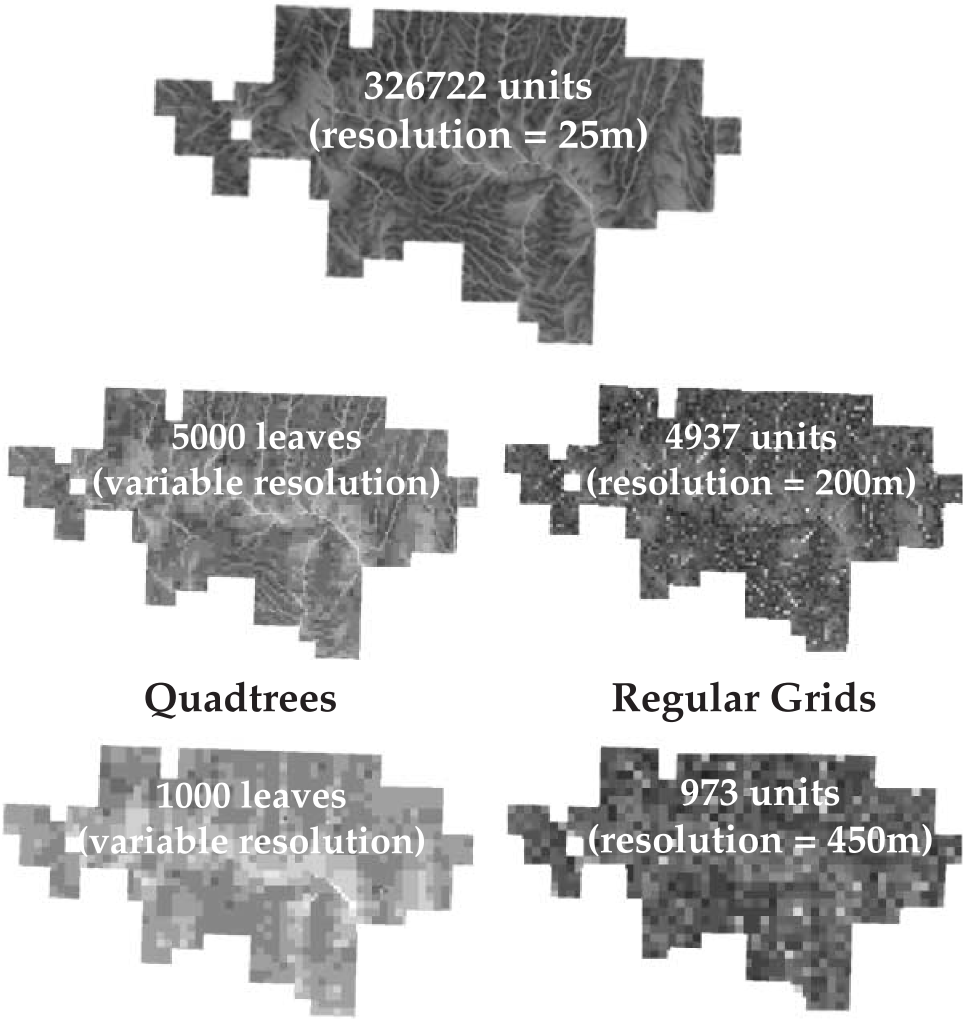

Figure 2 Examples of a landscape (west block of Grasslands National Park) partitioned using two levels of quadtrees and regular grids. The original data is the TOPMODEL wetness index, at 25 m resolution. The quadtree algorithm described in the text was used to create the quadtrees with 1,000 and 5,000 leaves. The regular grids were created by aggregating the original data at 200 m and 450 m resolutions, to create grids with approximately the same numbers of units as the quadtrees. The same procedures were used to define vegetation patches within each hillslope in the test area for this study

This represents one particular approach to the trade-off between data complexity and error due to aggregation. Because of the variance-based targeting of leaf splits, one ends up with the smallest units in areas with the highest variability of the underlying data. It is a top-down "steepest descent" approach, and there is no guarantee of reaching a global optimum. A more detailed explanation of the properties and theory behind the tool used to construct quadtrees in this study can be found in Csillag (1996, 1997), Csillag and Kabos (2002), and Kertész et al. (1995).

Even with just the sampling of methods presented above, there is a prohibitive number of possibilities to test exhaustively. Many of the possibilities will have negligible differences, however, either because small differences in the size or number of partitions does not significantly change the distribution of variance, or because different realizations may have similar effects to model predictions. The latter possibility can occur when different distributions of model units exhibit functional similarity even though they are geometrically or cartographically different. It is reasonable, then, to approach the problem by exploring a range of potential methods and thresholds, using knowledge of the dominant controls on the processes of interest and reasonable judgment about the relevance of details to the questions being addressed and the acceptable costs of both uncertainty and tractability of computer time and realistic parameterization demands.

To explore the implications of a range of partitioning strategies and associated thresholds, we use RHESSys (Regional Hydro-Ecologic Simulation System) version 4 to model a range of hydrologic (i.e. soil moisture, ET) and ecosystem (photosynthesis, LAI) processes. We will examine the sensitivity of these processes to systematic variation in both the method used to partition the landscape and the degree of spatial partitioning.

RHESSys is a process-based spatially distributed hydro-ecologic model that couples models of vertical and lateral soil moisture redistribution with ecosystem models of carbon and nitrogen cycling. Details of RHESSys hydrologic and biogeochemical cycling sub-models are described in Tague and Band (2004). Overall model structure and implementation within a GIS system are discussed in Band et al. (2001). For the purposes of this paper, it should be emphasized that as a coupled hydro-ecological model RHESSys models the dynamic feedback between vegetation water use, biomass (expressed as LAI) and soil moisture conditions.

RHESSys was developed in forested ecosystems, and had to be adapted to grasslands prior to this experiment. The necessary modifications are the scope of a separate manuscript, but are summarized here:

- potential photosynthesis is constrained as a function of soil moisture,
- a more detailed phenology model delays green-up as a function of soil moisture and accumulated degree days, and
- separate photosynthetic mechanisms are used for cool-season (C_3) and warm-season (C_4) grasses.

The range of choice for representing space in RHESSys is somewhat more constrained by the hierarchy imposed by its spatial database structure (Figure 3). The landscape hierarchy, from coarsest to finest nested elements, consists of basins, hillslopes, elevation zones, patches, and vertical strata within the patches. Operationally, for each level of the nested hierarchy except the stratum, a spatial partition definition must be chosen. Basins and hillslopes are normally delimited using standard GIS watershed delineation tools. Basins are used primarily for output aggregation, and hillslopes to organize lateral redistribution of soil moisture between patches. Zones – which are spatial units within hillslopes – control meteorological (including radiation) inputs. For this study, zones and hillslopes were defined using the same spatial partition, since in this area there is relatively little relief, so the meteorological forcing is assumed constant. Patches are the fundamental modelling unit within RHESSys (canopy strata have the same horizontal spatial definition as patches but include vertical subdivision). All biogeochemical cycling

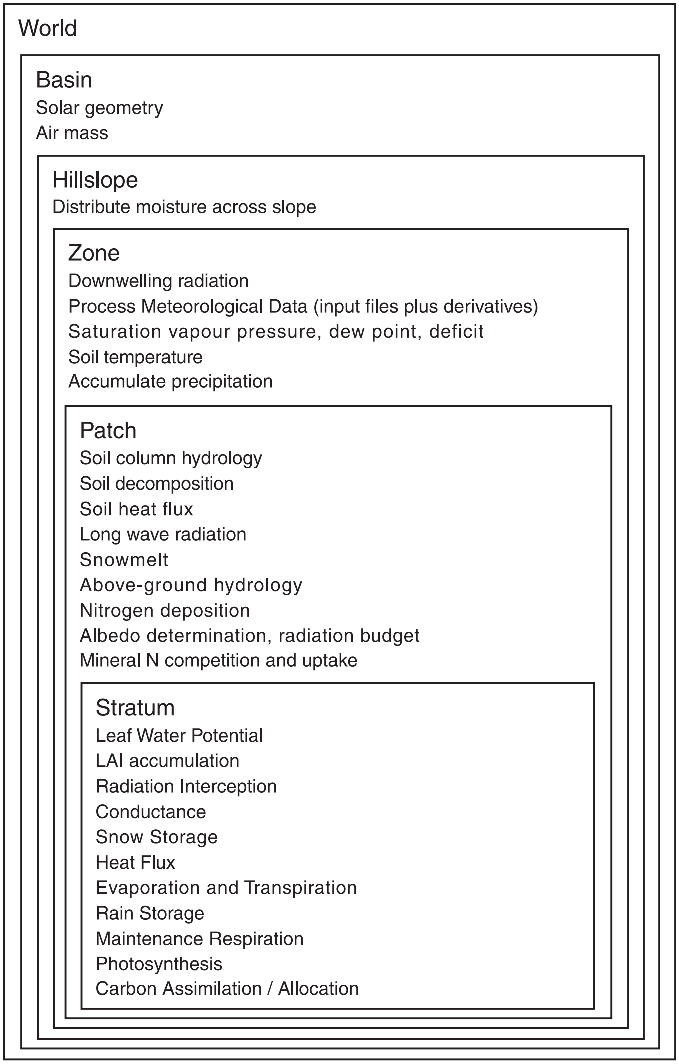

Figure 3 Spatial hierarchy in RHESSys and relationship between sub-process models and the spatial level

and vertical soil moisture processes occur at the spatial resolution defined by the patch. In addition, lateral soil moisture redistribution occurs between patches. This study focuses on possible patch definitions.

1.2 Study Site

Globally, grasslands play an important role in the carbon cycle, covering approximately 20% of the Earth's surface and containing about 30% of global carbon stocks (Ojima et al. 1996, Parton et al. 1996). They are also economically important, containing much of the grain growing capacity of the world (Burke et al. 1989). The grassland biome is largely defined by moisture availability (Aber and Melillo 1991); most natural grasslands (excluding areas maintained by heavy grazing pressure) are in areas with constrained or highly variable precipitation, making them potentially sensitive to climate change. Consequently, there is a need to monitor and predict changes to grassland dynamics under changing climate and future scenarios.

The study area, Canada's Grasslands National Park, has been the focus of a series of experiments studying strategies to predict productivity and the uncertainties involved in these predictions (Mitchell and Csillag 2001, Mitchell et al. 2002, Mitchell 2003). This is a relatively new park, with continuing land acquisition that started in 1984, and a purpose to protect a representative portion of the Prairie Grasslands Natural Region of Canada (Parks Canada 2002). It is situated near the northern edge of the mixed prairie, which makes it the limit of the continental distribution of vegetation that uses the C_4 photosynthetic pathway. The two functional groups (C_3 and C_4, also referred to as cool- and warm-season grasses, respectively) have important differences in adaptive strategy and competitive abilities, and consequently distinct potential productivity for given temperature and moisture combinations. It is important to determine relative affinities of C_3 and C_4 plants to expected climate and atmospheric changes, in order to evaluate potential impacts on species distributions, and global carbon and nitrogen budgets (Peat 1997). Such work helps answer questions about functional group dynamics across large regions such as the North American prairies, as well as addressing important issues specific to regions experiencing changes to vegetation communities. There are many remaining questions on the controls on relative productivity and distributions of these groups (see Epstein et al. 1997 for example), therefore this is a priority area for further modelling and field work.

2 Methods

A study area was chosen using a well studied test basin within Grasslands National Park plus six adjacent basins, forming an area of approximately 1.7 km^2 with a range of upland, sloping, and valley bottom areas of varying sizes. RHESSys was parameterized using the same basin, hillslope and zone boundaries throughout, varying only the patch definitions (Figure 4). Vegetation and all other model parameters were defined using grasslands defaults developed earlier (Mitchell and Csillag 2001, Mitchell et al. 2005), but 100% cover of cool-season (C_3) plants was assumed throughout to reduce computational load. Patch definitions included the following possibilities, all within the standardized hillslope definitions (full details of the experimental design showing each partitioning used in the experiment are provided in Table 1):

- regular grid: with resolutions between 25 and 750 m, plus additional realizations with a redefined origin of the grid, shifting the lattice arbitrarily within the sub-cell resolution (hereafter called "shifted grids"),
- quadtrees: with targeted numbers of leaves between 10 and 13,312, and
- "full hillslopes", where each hillslope contains only a single patch.

The quadtrees were built using the algorithm described above (section 1.1), decomposing the variance of the area by creating successively smaller leaves in the areas of maximum variance at each step, until a specified maximum number of units (in this case, vegetation patches) was reached. We experimented with different inputs for assessing

Table 1 (a) Patch distributions for regular grids, and (b) patch distributions for quadtrees. NA means that a quadtree could not be built for the specific target due to software limitations. Average patch sizes are expressed in m^2

(a)

Grid resolution (m)	Resulting # of patches	Average patch size (m^2)
25	26,748	625
50	7,218	2,316
75	3,442	4,856
100	2,074	8,060
125	1,381	12,018
150	1,018	16,421
175	812	20,588
200	611	27,360
250	472	35,418
300	353	47,358
350	285	58,657
400	239	69,947
500	171	97,763
600	138	121,141
700	114	146,644
750	112	149,263

(b)

	NDVI		DEM		NDVI + DEM		WI	
# quadtree leaves targetted	# patches	Avg patch size	# patches	Avg patch size	# patches	Avg patch size	# patches	Avg patch size
13,312	10,748	1,555	8,950	1,868	NA	NA	NA	NA
7,172	6,611	2,529	5,827	2,869	6,623	2,524	2,979	5,612
3,456	3,693	4,527	3,214	5,201	3,647	4,584	1,628	10,269
3,072	3,307	5,055	2,864	5,837	3,271	5,111	1,511	12,026
2,048	2,282	7,326	1,890	8,845	2,286	7,313	1,125	14,860
1,408	1,634	10,144	1,261	13,257	1,631	10,250	880	18,997
1,024	1,225	13,647	871	19,193	1,220	13,703	699	23,916
768	954	17,524	613	27,272	950	17,597	539	31,016
640	819	20,412	463	36,107	822	20,338	478	34,974
512	694	24,089	335	49,903	694	24,089	409	40,874
384	553	30,231	342	48,882	558	29,960	337	49,607
256	407	41,074	315	53,071	405	41,278	260	64,298
128	259	64,546	235	71,138	256	65,303	164	101,936
64	164	101,936	171	97,763	171	97,763	122	137,029
45	142	117,728	140	119,411	146	114,503	107	156,238
25	120	139,313	120	139,313	107	156,238	90	185,750
10	85	196,676	88	189,972	88	189,972	77	217,110

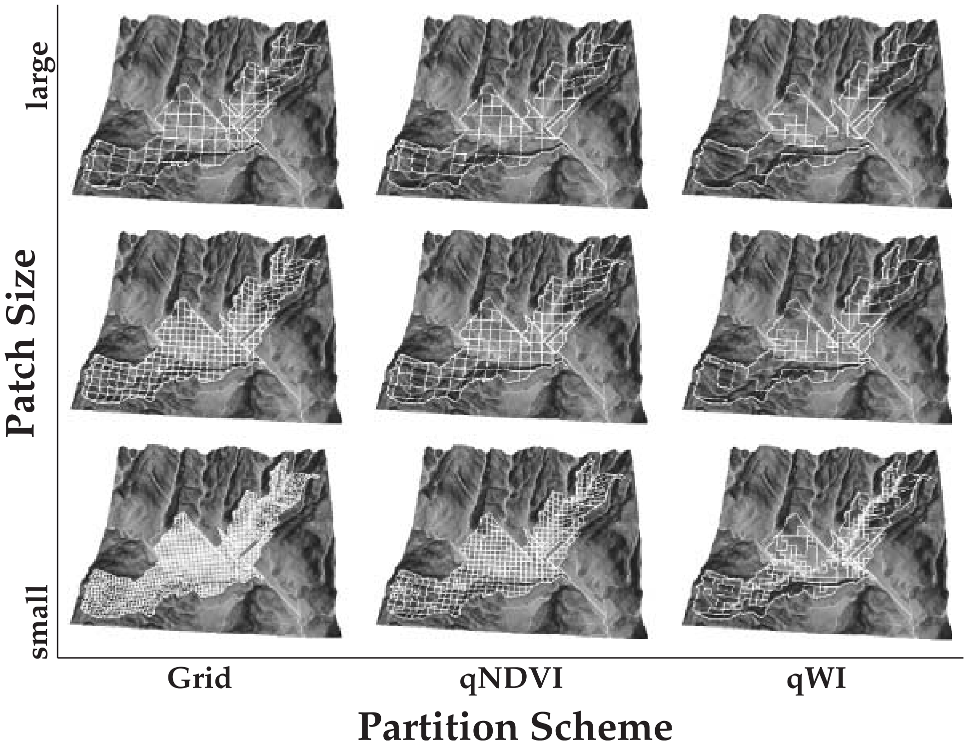

Figure 4 Examples of patch partitions using a range of thresholds and a regular grid, a quadtree built based on the variance of NDVI ("qNDVI"), and another quadtree built based on the variance of wetness index ("qWI"). In all cases, the background colour draped over the terrain is based on the wetness index for this area, plus illumination for visualisation purposes

the variance being decomposed as the quadtree was built. Using elevation and wetness index (WI) to determine patch definitions represents a "typical" strategy for RHESSys because of the importance of topography in soil moisture estimates using TOPMODEL (Tague et al. 2001). We also used an NDVI image for the area from 28 August 1998, to see if a snapshot of vegetation conditions would prove useful, as well as the combined effect of NDVI and elevation. For multiple input decompositions, at each stage whichever input contributes the highest within-leaf standardized variance is used.

The wetness index (WI) was calculated as in TOPMODEL, where it is used as an index of hydrological similarity (Beven 1997), and can be thought of the likelihood of water accumulation:

$$WI = \ln \frac{A}{\tan \beta} \tag{1}$$

where A indicates the accumulated upslope area, and β is local slope gradient.

The NDVI (Normalized Difference Vegetation Index) image was calculated using Landsat TM imagery from 28 August 1998, which was converted to reflectance and corrected for atmospheric effects using the 6S (Vermote et al. 1997) atmospheric transfer modelling software, and then the index was calculated as the normalized difference between Landsat TM band 4 (TM4), or near-infrared reflectance, and Landsat TM band 3 (TM3), red reflectance:

$$NDVI = \frac{TM4 - TM3}{TM4 + TM3} \tag{2}$$

Processing these partitioning alternatives resulted in RHESSys databases with various numbers of patches, because of the unique combinations of intersecting boundaries across the hierarchy. At the coarse extreme, the "full hillslopes" approach with 1 patch on each of the two hillslopes per basin, resulted in 14 patches, with an average size of 1,190,638 m^2.

Differences in outputs are a result of variable levels of aggregation of input distributions, therefore relationships between aggregation and key input statistics were explored. Statistical tools within GRASS (GRASS Development Team 2002) were used to collect average values of elevation, slope, aspect, wetness index, and NDVI within each of the partition maps. The links (Bivand 2000) between GRASS and the statistical software R (Ihaka and Gentleman 1996) were used to collect the distribution of input data underneath each potential vegetation patch, and calculate the means and variances of these patch averages for comparison and to graph the results. The use of open source GIS and statistics packages allows uniform scrutiny of the analysis methods and provides an archive of the procedures used along with the datasets, enhancing the chances that analyses are not misused (Mitchell et al. 2002).

RHESSYs was run on the resulting spatial definitions using the parameterization developed in previous work (Mitchell et al. 2005). For the purposes of comparison, predictions of annual net productivity and daily leaf area index, unsaturated storage, evaporation, and transpiration were collected from each run.

3 Results

3.1 Inputs

Examining the aggregation of various inputs allows us to evaluate key differences in the partitioning methods. Figures 5 and 6 present the variability of patch means of key model inputs (i.e. the "captured variance", or amount of variance in the input data that is preserved by the partitioning) under various methods. Figure 5 compares the variability of inputs under the regular grids and under a quadtree built based on the DEM ("DEMquad"). As expected, the variance of aggregated elevation decreases as the patch area increases, due to greater spatial averaging, under both regular grids and quadtrees. Under quadtrees this trend can be divided into two relatively linear sections with contrasting slope, and the degree of aggregation at which this change in behaviour occurs (at an average patch size of about 7 ha) indicates a potentially important change in the scaling behaviour of this variable which could be used to guide partitioning choices.

The effect of shifting the origin of the arbitrary grid is remarkable, since it can cause such large (~20%) changes in the amount of captured variation with the same size, shape, and number of units. The effect of aggregation changes according to whether or not the boundary of the grid cell cuts across abrupt changes in the distribution of inputs. For example, when aggregating an elevation surface, the average and variability in the aggregate units will be much different if the cell boundaries line up with a ridge in the surface than if they cut across it and in effect smooth the peak.

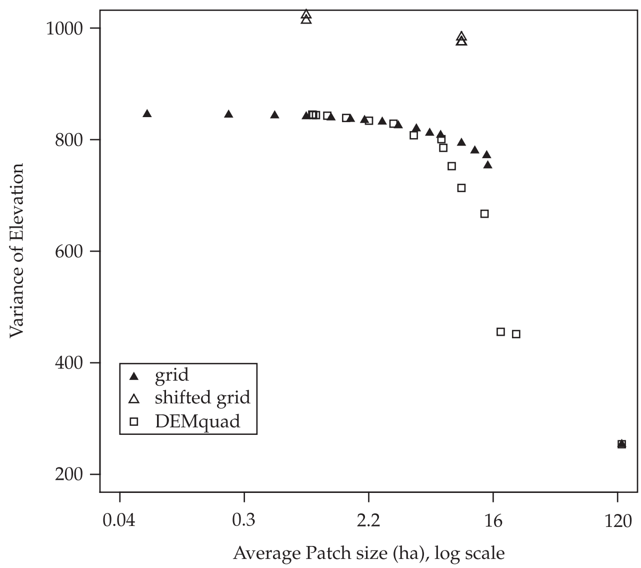

Figure 5 Variance of patch means of elevation for patches defined by regular grids of various resolutions, some examples of the same grids with their origins shifted, and a quadtree built based on the variability of elevation. The grids and the quadtree converge on the largest patch size in the bottom right, which represents one patch per hillslope (the most aggregation possible for a given basin delineation)

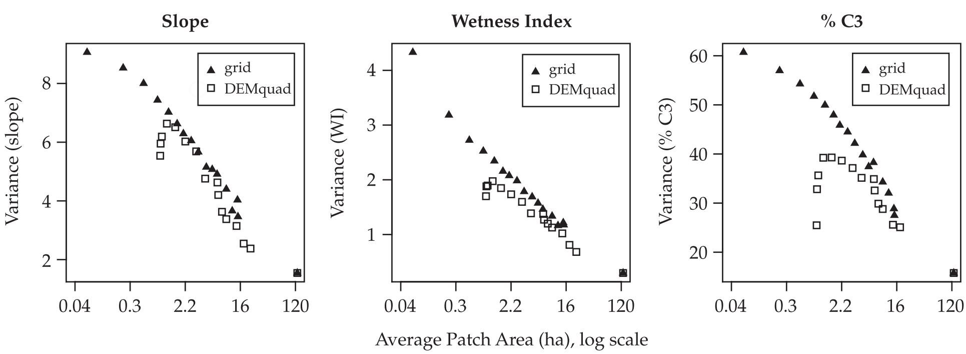

Figure 6 Variance of patch means of slope, wetness index, and proportional C_3 vegetation cover for patches defined by regular grids of various resolutions, some examples of the same grids with their origins shifted, and a quadtree built based on the variability of elevation

Figure 6 shows the captured variance of three other potentially important inputs: slope, wetness index, and proportion of C_3 vegetation, under the same regular grids and DEMquad. For the quadtrees, instead of a monotonic decrease in patch variance, we see a "humped" curve, indicating a transition between local and global controls on the variance. When the partitioning is based on variation of a particular input, there is an

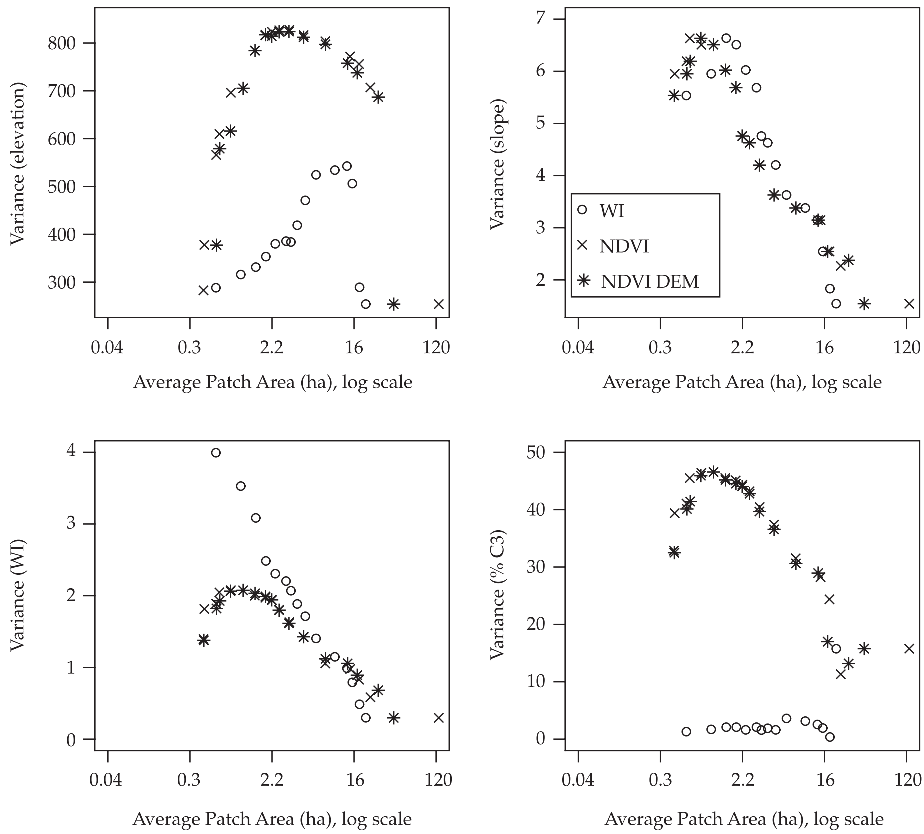

Figure 7 Variance of patch means of elevation, slope, wetness index, and proportional cover of C_3 vegetation under quadtrees built according to variance of NDVI, a combination of NDVI and elevation ("NDVI DEM"), and wetness index ("WI")

expectation of decreasing variance with smaller patches; however, these other inputs do not have the same spatial distribution as elevation, leading to different patterns of aggregation. In each curve, the final point on the right indicates the maximum aggregation, of one patch per hillslope.

Figure 7 shows the average patch variance of the same four inputs under a quadtrees built based other variables: the NDVI image ("NDVIquad"), and the NDVI image plus the elevation model ("NDVIDEMquad"), and wetness index ("WIquad"). The NDVIquad and NDVIDEMquad curves are very similar, reflecting the fact that in most locations the variance of NDVI was higher than that of elevation, and therefore controlled the quadtree pruning (this may also reflect a strong correlation between the spatial structure of NDVI and both wetness index and the DEM). In terms of plant growth, it is particularly important to preserve variability of wetness index because that will create differences in local moisture availability. The bottom left graph pane shows that WIquad preserves inter-patch variability of wetness index much better than the other partitions for smaller patch sizes, whereas all quadtrees have similar small differences above a patch size of about 6 ha.

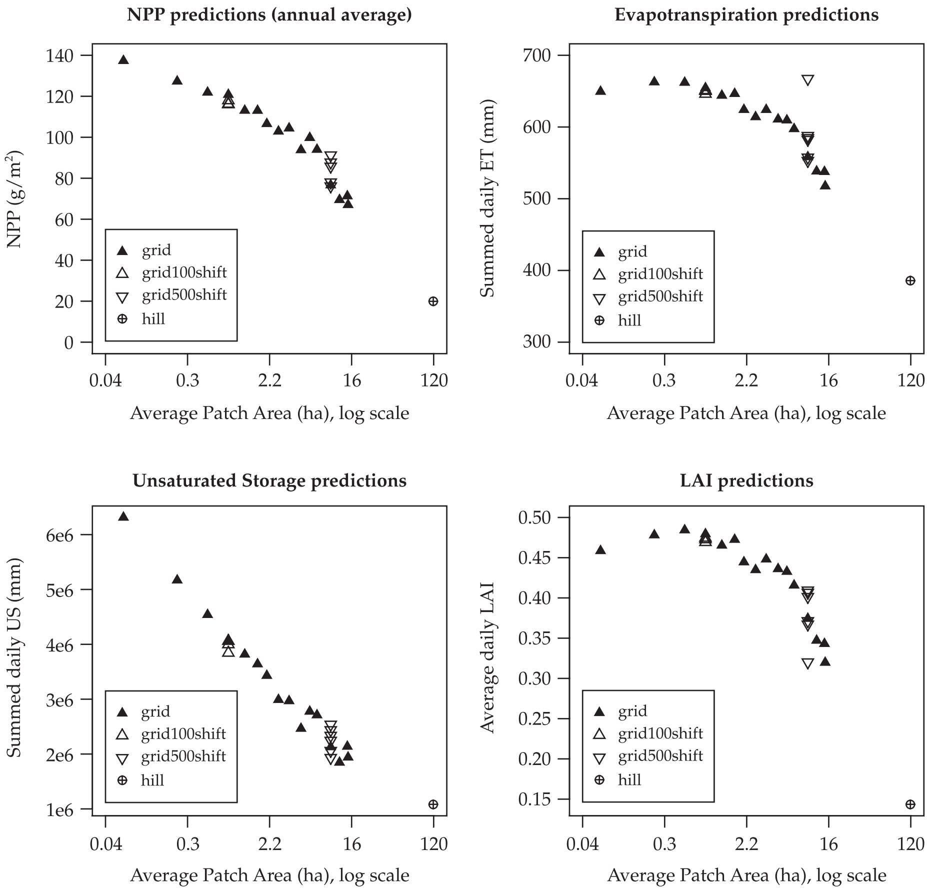

Figure 8 Aggregated values of predicted NPP, evapotranspiration, water storage in the unsaturated zone, and LAI under regular grids of different resolutions and some samples with shifted origins (grid100shift is the 100 m grid with different origins, grid500shift is shifts of the 500 m grid). The "hill" point represents the maximum aggregation of one patch per hillslope. In all cases, the prediction shown represents the total (for evapotranspiration and storage) or average (annual NPP and daily LAI) of predictions between 1995 and 1998

3.2 Outputs

Figure 8 shows predictions of NPP, evapotranspiration, unsaturated moisture storage (an analogue of soil moisture) and LAI under regular grids, while Figure 9 shows the same quantities under the quadtrees. We have concentrated on average annual productivity as a primary diagnostic of the predictions. In all cases, predicted NPP (the top left graph of both Figures 8 and 9) shows at least a 50% decrease moving from the smallest to the largest patches used in this study, under all partitions. There is an even further reduction, down to only ~20 g/m^2/year, if only one patch is used per hillslope (the point marked as "hill" in the legend). This follows similar trends in daily predictions of evapotranspiration and unsaturated storage and is mirrored by average daily LAI.

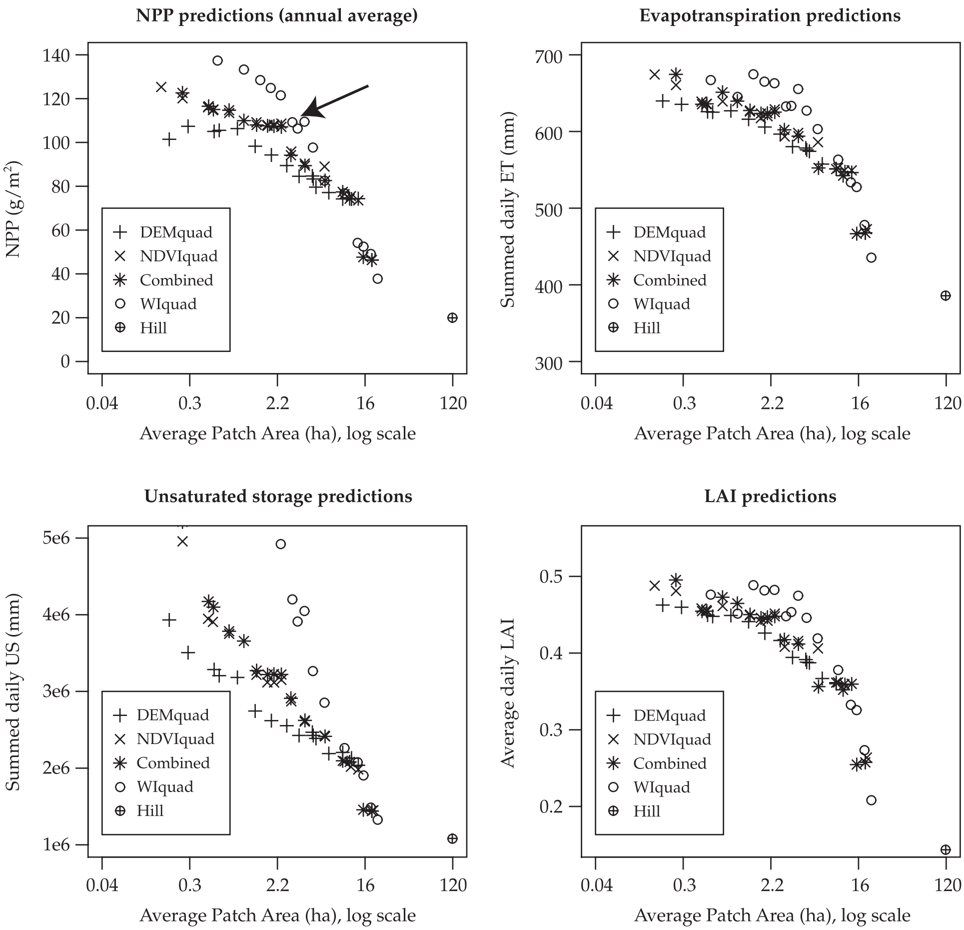

Figure 9 Aggregate predictions from 1995–1998 (as in previous figure) for NPP, evapotranspiration, unsaturated zone water storage and LAI under quadtree partitions with varying numbers of leaves, built based on elevation (DEMquad), NDVI (NDVIquad), the combination of these two (Combined), and wetness index (WIquad), plus the hillslope aggregated patch ("Hill"). The arrow in the NPP plot (upper left) indicates the general area where the response of model predictions to spatial aggregation levels off, as discussed in the text

Based on these trends and the analysis of input aggregation, we conclude that predictions are negatively biased at larger patch sizes because in this low moisture environment, key pockets of moisture availability are smoothed out. It is possible to argue that the hydrological model was calibrated at a different scale and could be recalibrated to accommodate larger areas. This would still neglect the high variability of moisture availability across the landscape, however, ignoring any potentially important dynamics between the local patterns of water availability and the resulting ecosystem function.

These plots also show the advantage of variance-based partitioning – i.e. the quadtrees still exhibit the smoothing effect, but it is much closer to a linear decrease and is therefore scalable. As suggested by the plots of input variability, the WIquad partition maintains higher aggregate moisture availability at larger patch sizes, and this is realized by the modelled vegetation as higher net productivity and LAI.

The predictions made under WIquads were consistently different from all other combinations, and the nature of how pockets of soil moisture and therefore primary productivity were captured is consistent with expectations of the actual environmental behaviour. This creates a basis for choosing the WIquad over other partitions. Since the patch definition in RHESSys should capture areas of relatively homogeneous vegetation and soil conditions, a suitable patch delineation could be created by combining the boundaries of the vegetation and soil surveys with a delineation based on wetness index. This provides a distribution of patches that acknowledges the trade-off between number of units and the distribution of variance of wetness index. While we do not have a systematically-defined optimum partition to use, the exploration of model behaviour across a range of possible patch sizes can be used to guide selection of the appropriate patch definition.

In this study area, the curves of input variability or aggregate predictions often showed key changes in behaviour of WIquad around patch sizes of 2.2 to 6 ha: it was around this range that the inter-patch variability of wetness index became higher than all other quadtrees, and all predictions under WIquad show steep declines at larger patch sizes, whereas for NPP, LAI and evapotranspiration at least, smaller patches than this show less difference. Based on these observations, an overlay of the soil and vegetation survey boundaries with the WIquad targeted at 1,024 leaves has been selected for further work.

4 Conclusions

The choice of partitioning method and associated parameters changes the aggregation of inputs to a spatial environmental model, and was shown to have significant consequences on the predictions of ecosystem response. Although the range of possibilities is too broad to test exhaustively, a "common sense" approach utilizing knowledge of key controls and a range of possible parameters can help narrow the field. Variance-based partitioning is a useful tool for this type of work because it explicitly addresses the trade-off of the number of modelling units versus acceptable representations of variability of inputs. Regular grids, while efficient both computationally and in terms of effort to construct, have no relationship with the distribution of the data and therefore the eventual modelling uncertainty; moreover, simple small changes to the origin of the grid can radically change model predictions. Quadtrees share the geometric regularities and therefore the computational advantages of regular grids, but also are sensitive to the variance of inputs across space. This important difference enables setting the objective of the partitioning to a desired number of homogeneous patches. Other variance-based strategies may prove useful, with different compromises between the benefits of a variance-based strategy and computational or implementation efficiency.

The same techniques used to demonstrate differences between partitioning strategies were used to choose improved data models for future prediction projects in the study area; the quadtrees based on wetness index captured input variability such that important local differences in hydrologic parameters and consequent primary productivity were retained at intermediate numbers of modelling units. A specific partition was chosen for further work based on these comparisons.

The important feature of this partitioning scheme for this application was a combination of the variance-based approach to control aggregation-induced bias, and the selection of appropriate driving variables for the quadtree generation. The appropriateness of wetness index as a constraint was not surprising due to the assumptions in this model regarding the role of topography in controlling moisture distribution. The performance of NDVI-based partitioning was interesting since this application of RHESSys does not use any inputs from remote sensing data in either the parameterization or setup of the data model (some versions of the submodels in question use proscribed LAI obtained through satellite data, but here LAI is "freely" predicted according to modelled daily carbon allocation). This suggests that NDVI has captured a combined effect of the controls on productivity, in essence independently capturing the important moisture limitations on growth. There may be interesting roles for NDVI data in more intelligent parameterization or regional validation exercises, and this will be the focus of further research.

In general, for modelling environmental function where aggregation error has the potential to be significant, the definition of the spatial database can have critical implications on prediction uncertainty (Harvey 2000, Rastetter et al. 1992). The recommended approach coming from this experiment is to identify key controls on the processes of concern, and use as "intelligent" a strategy as possible to define modelling units that retain important characteristics of the distribution of those controlling inputs. If a regular grid is chosen with a completely arbitrary origin and resolution, no such intelligence is used in the spatial model definition. On the other hand, a combination of coarser "known" spatial units and a variance-based partitioning of finer-grain distributed inputs will lead to a feasible model setup that can yield more confident predictions. GIS has enhanced our ability to improve environmental research using biogeochemical models by creating an environment in which to explore the range of possibilities for spatial representation; open-source systems have expanded these possibilities even further by allowing us to examine and potentially change the assumptions and methods used in the spatial representation.

We demonstrate that the preparation of data and parameters for making predictions with RHESSys is very important, and it will probably remain the most time and effort consuming part of all potential use of the model within an area. However, once the problems and range of appropriate questions for the model are mutually understood, and the spatial database has been constructed, systems could be designed that tie the model-geographic information system combination together with a query-based interface. This would allow managers to request further scenario-based questions as they become relevant, or focus the questions on specific sub-regions of interest. One such system (called Knowledge-Based Land Information Manager and Simulator, or KBLIMS) has been demonstrated with an earlier version of RHESSys (Robinson and Mackay 1996), and similar projects could be a logical extension of this work.

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