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Development of a decision framework to identify appropriate spatial and temporal scales for modeling N flows

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Abstract

Decision makers need to know the effects of alternative watershed management strategies on export of nitrogen (N) to coastal waters. They use this knowledge to reduce undesirable effects of excess N in coastal waters. Various models exist to predict the effects of watershed management on export of N. This paper describes a decision framework to identify the appropriate spatial and temporal scales for using N flux models. The framework is developed for existing models that predict N export from large watersheds and the contribution of N sources and N sinks to this N export. With this framework, modelers can identify the appropriate scale for model predictions and independently scalable model parts. The framework bases the appropriateness of model scales on indicators, which are to be specified by the modeler and which are associated with four criteria. The four criteria require modeling scales to correspond with (A) data, mitigation options, and scenarios, (B) model assumptions, (C) available resources for modeling, and (D) requirements of prediction users. A successful application of the framework is illustrated for a global model of dissolved inorganic nitrogen export from watersheds to coastal waters. Ranges of appropriate scales are determined for model output and five independently scalable model parts, which model the (1) surface N balance, (2) point sources, (3) N flux in sediments and small streams, (4) retention in dammed reservoirs, and (5) riverine retention. Appropriate model scales were found, if the four criteria were not set too strict. We conclude that the decision framework can contribute substantially to selecting the appropriate modeling scales in a balanced and comprehensive manner.

Keywords: nitrogen cycling, surface water quality, decision support, models, scale

1 Introduction

Many different large scale watershed N flux models exist [Andersen et al., 2003]. These models have in common that they simulate processes related to horizontal movement of nitrogen through large drainage networks of river basins. An important property of such models is their modeling scale. Modeling scale can be viewed as the combination of support, extent, and stream order of independently scalable model parts, and model outputs. Model support is the temporal or spatial range in which modeled processes are assumed to be homogeneous. Model extent is the total range of time or space within which processes are modeled. The spatial extent of N flux models is typically a basin or a group of adjacent basins. The temporal model extent is usually between a few months and a few decades. Modeling scale affects many important properties of N flux models such as the processes that can be described, the required input data and the size of watersheds that can be modeled. A model may only make good predictions if the scale of application is the same as the scale at which validation provided good agreement. This is because existing models for N export from river basins are nonlinear to some degree and, hence, scale specific.

N flux models relevant for environmental impact assessments often require predictions for specific river basins. Such models can have different spatial and temporal supports and extents. For example, the Riverstrahler model [Billen et al., 1994] has been applied with various temporal supports on watershed surface areas ranging from 100 to 100000 km^2 and with spatial model supports ranging from 1st to 5th order upstream basins ranging in area between 1 and 5000 km^2 [Sferratore et al., 2006].

The reason for selecting a particular modeling scale is usually not explicitly reported, and the appropriateness of a particular modeling scale is therefore difficult to judge. Modelers have no clear guide for selecting appropriate spatial and temporal modeling scales for predictions of N fluxes in large river basins.

The purpose of this paper is to present a comprehensive framework to identify the appropriate spatial and temporal scale for N flux models. The framework is developed for models that predict N export from large watersheds and the contribution of N sources and sinks to this N export. With this framework, modelers can identify appropriate scales for model predictions, and for independently scalable model parts. This decision framework may also assist in reporting the rationale behind the scale of a model application. The framework focuses explicitly on existing N flux models that serve as predictive tools. In this paper an application of the framework to a global N flux model is summarized.

2 Description of decision framework

Here we describe a decision framework aiming to assist model users in identifying appropriate modeling scales in a well balanced and comprehensive way. The framework aims at minimizing the prediction bias by ensuring sufficient validity of model assumptions, while simultaneously ensuring feasibility of model application, agreement with scales of data and scenarios, low scaling error, and useful predictions.

Four criteria are used to assess the appropriateness of modeling scale. These four criteria require modeling scales to correspond with; (A) data, mitigation options, and scenarios, (B) model assumptions, (C) available resources for modeling, and (D) requirements of prediction users. For each criterion, indicators are used, that serve as a basis for the evaluation of appropriateness of support, extent and stream order of a scalable model part. The indicators to be used are selected by the user of the framework. Table 1 gives an overview of possible indicators. The framework is developed such that scales for which indicator values are found that exceed a threshold (specified by the user of the framework) are considered appropriate.

The output of the decision framework is an indication of appropriate ranges of up to six measures of spatial and temporal modeling scale (S). These are spatial support (sup_s), temporal support (sup_t) spatial extent (ext_s), temporal extent (ext_t), minimum stream order (so_{min}) and maximum stream order (so_{max}).

Here, sup_s and sup_t are the average size and duration, respectively, of areas and times assumed to be homogeneous by the model, and ext_s and ext_t are the total area and duration, respectively, within which the model is applied. Variables so_{min} and so_{max} are measures of the minimum and maximum sizes of river reaches, respectively, to which a model component is applied [Strahler, 1964]. Appropriate ranges of S are estimated for a number of scalable model parts (SMPs). We define an SMP as a part of a model that simulates at a unique scale S. In this paper, an SMP is a crucial element in the decision framework.

The decision framework identifies appropriate S for each SMP selected. This is done in five steps: (1) selection and identification of SMPs to be considered by the framework, (2) estimation of indicator values, (3) estimation of fulfillment of criteria, (4) estimation of appropriateness according to each criterion, and (5) estimation of appropriateness according to all criteria.

2.1 Step 1: Selection and identification of scalable model parts (SMPs) to be considered by the framework

As a first step, a user of the framework will have to decide on the model parts to be considered. It is almost impossible to consider all instances[1] and all N sources and sinks[2] described by an SMP, due to the complexity of most N flux models. Therefore a model user may limit the application of the decision framework to a restricted set of instances, sources, and sinks represented by an SMP. Similarly, the user may want to consider only a subset of all SMPs.

There are several motivations to consider only a particular part of the model in the application of the framework. For instance, one could consider only those model parts that are relatively important in the modeled N transport. To calculate the contribution of all such important instances, sources and sinks the model must distinguish various pathways of N through locations, times and environments in the river network. All pathways converge to one single location in a river, or the outlet in the coastal zone. Depending upon instances, sources and sinks affecting the N flux, some parts of this pathway network may be more important than others for identifying the appropriate modeling scale. Their importance can be determined by their expected contribution to outlet N flux, and potential for mitigation.

Before application of the decision framework it is necessary to set the upper and lower limits of possible SMP scales (S) for which the appropriateness is to be identified. The framework only identifies appropriate scales of SMPs used in representative existing model applications or default applications. Figure 1 is an example of a representation of possible SMP delineations and SMP scales.

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[1] An instance is defined as a part of an SMP receiving input for an area, time or stream order range that is assumed to be homogeneous.
[2] Examples of possible N sources described by an SMP are fertilizer or sewage; Examples of N sinks described by an SMP are riparian zones or lakes.

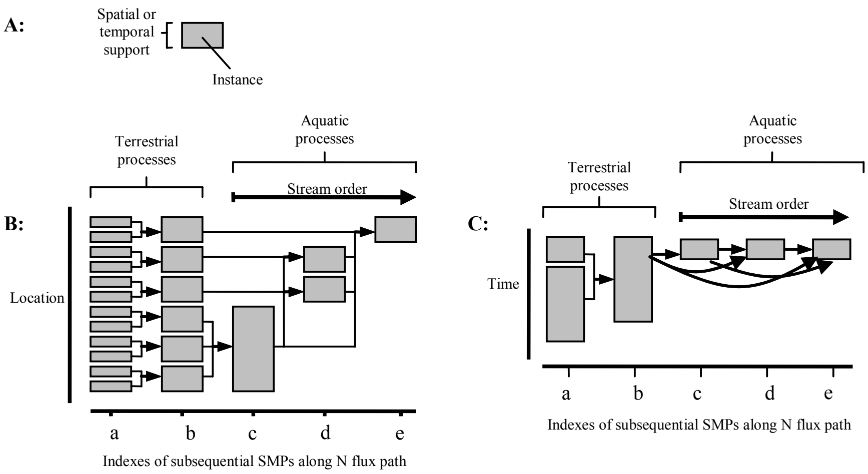

Figure 1 Possible delineation of SMPs, SMP instances, and their relations in an N flux model. Grey rectangles are SMP instances. Arrows indicate the flow of information. Bold arrow indicates stream order. A: legend. B: Possible delineation of SMPs and their relative location and spatial support. C: same as B, but for relative time and temporal support.

2.2 Step 2: Estimation of indicator values

In the second step, the user of the framework will have to select indicators to be used, and to estimate their value. Indicator values can be estimated as:

$$f_{c,j}(S) = \sum_{i=1}^{N_j} w_{j,i} \cdot I_{j,i}(S) \qquad (1)$$

where:

$f_{c,j}(S)$ – is a value of indicator j that depends on S (0 to 1),
$w_{j,i}$ – is a weight to indicate relative importance of indicator function $I_{j.i}$ for $f_{c,j}(S)$,
$I_{j.i}$ – is indicator function i of indicator j which value (0 or 1) depends on S,
N_j – is the number of instances of $I_{j.i}$ used in the calculation of $f_{c,j}(S)$.

Indicator j is used to test the fulfillment of criterion c, $c \in \{A,B,C,D\}$, being indices for the four criteria used in the framework. For our framework we suggest three possible indicators to test the fulfillment of criterion A, 6 for B, 2 for C, and 4 for D (Table 1). Only the relevant indicators listed in Table 1 need to be used. A user of the framework may add user-specific indicators. An indicator function can only be 0 or 1 [Folland, 1999]. Weights $w_{j,i}$ may be defined by the user using methods prescribed by the framework.

Table 1 Description of criteria A, B, C, and D (*c*) and indicators (*j*) that can be used in the decision framework. Indicators are listed below the criterion for which they can test the fulfillment (see Section 2.3).

c	*j*	Description of criterion or indicator
A		Requires SMP scale to correspond with that of data, mitigation options, and scenarios
	1	Degree to which artifacts in available input data facilitate model representation of process variability
	2	Measure of the fraction of spatial or temporal variability of relevant mitigation options that can be represented by the considered SMP
	3	Measure of the fraction of the spatial or temporal variability of anthropogenic influences described in scenarios that is represented by an SMP
B		Requires that the SMP scale is such that model assumptions are valid
	4	Measure of the fraction of actual N flux variability on the scale of the considered SMP that is accountable to drivers of N flux variability described by the considered SMP
	5	Measures of the degree to which an SMP with one or more calibrated coefficients describes processes occurring on the scale for which it uses input.
	6	Measure of the fraction of N emitted by a source described by the SMP that is able to reach the prediction location within the duration of sup_t or ext_t in case of a steady state or dynamic model, respectively. When this indicator has low values there may not be sufficient relation between modeled N source emissions and outlet N flux during the time of prediction.
	7	Measure of the validity of the common assumption that flow of N from a terrestrial N source enters the drainage system on the location were it was emitted
	8	Measure of the fraction of total input variation caused by error
C		Requires that available resources are sufficient for modeling, given the SMP scale
	9	Indication of the effort needed for downscaling to obtain inputs from other SMPs, and provide input to other SMPs
	10	Measure of the resources required for an SMP to use input for areas, depending on the range of stream orders that dominates in these areas
D		Requires that the prediction scale is such that model predictions are sufficiently useful
	11	Measure of the usefulness of predictions for known impact studies
	12	Measure of the usefulness of predictions for yet unknown impact studies
	13	Measure of the usefulness of river N export predictions and predictions of source and sink contributions for a fundamental scientific objective of the modeler
	14	Measure of the usefulness for policy makers of river N export predictions and predictions of source and sink contributions

2.3 Step 3: Estimation of fulfillment of criteria

Fulfillment of criteria can be estimated using indicator values. This can be summarized as;

$$F_c(S) = \sum_{j=1}^{N_c} v_j \cdot f_{c,j}(S) \tag{2}$$

where:

$F_c(S)$ – is the fulfillment of criterion c for scale S (0 to 1),
v_j – is a weight indicating the relative importance of indicator j for $F_c(S)$,
N_c – is the number of indicators that is used to calculate the fulfillment of criterion c.

The weights v_j are to be defined by the user of the framework.

2.4 Step 4: Estimation of appropriateness according to each criterion

Estimation of appropriateness according to each criterion can be summarized as;

$$a_c(S) = I(F_c(S) > T(c)) \tag{3}$$

where:

$a_c(S)$ – is the appropriateness of modeling scale S for criterion c (0 or 1),
I – is an indicator function,
$T(c)$ – is a threshold for appropriateness according to criterion c.

Appropriateness $a_c(S)$ takes the value of 1 if S is appropriate for criterion c and 0 if S is inappropriate for criterion c. Threshold $T(c)$ is user defined and indicates the relative importance of criterion c for the user.

2.5 Step 5: Estimation of appropriateness according to all criteria

Appropriateness according to all four criteria is estimated as;

$$A(S) = \prod_{c=A}^{D} a_c(S) \tag{4}$$

where:

$A(S)$ – is the appropriateness of scale S for all four criteria (0 or 1).

Here, $A(S)$ is 1 for appropriate scales S and 0 for inappropriate scales S. Appropriateness values $a_c(S)$ (0 or 1) according to each of the four criteria are multiplied.

If there are no ranges of sup_s, sup_t, ext_s, ext_t, so_{min}, or so_{max} that are appropriate according to the framework, then this may be an indication that the considered SMP is not adequate given the research question and available data, or that thresholds $T(c)$ for one or more criteria are set too strictly by the modeler.

3 Application of decision framework

This section illustrates the decision framework by using it to identify the appropriate scale for SMPs of an existing model for river export of dissolved inorganic nitrogen (DIN) to coastal zones of the world [Dumont et al., 2005]. This model, called NEWS-DIN, takes into account both diffuse and point sources. When this model was used by Dumont et al. (2005), its equations were applied on three different spatial supports: surface N balance equations had 0.5 × 0.5 degree gridcell specific variables, equations for dammed reservoir retention had subbasin specific variables, and equations for riverine processes and point sources had basin specific variables (Table 2). Model predictions were obtained per coastal zone. Each coastal zone prediction involved upscaling from 0.5 × 0.5 degree SMP outputs to basin support, upscaling from subbasin-specific SMP outputs to basin support, and upscaling of basin-specific SMP outputs to coastal zone support.

Table 2 Average scale (*S*) and data connections of five scalable model parts (SMPs) and model predictions distinguished in NEWS-DIN when applied by Dumont et al. (2005).

SMP index	1	2	3	4	5	n.a.[a]
Modeled process	Surface N balance	Point source emissions	N flux in sediments and small streams	Dammed reservoir retention	Riverine retention	Flux to coastal zones
sup_s (km)	55	150	150	135	150	2200
sup_t (y)	3	10	10	10	30	10
ext_s (km)	globe	globe	globe	globe	globe	globe
ext_t (y)	3	10	10	10	30	10
so_{min}	0	0	0	5	6	6
so_{max}	0	0	5	10	12	12
Receives input from	Datasets	Datasets	SMP 1, and datasets	Datasets	SMPs 3 and 4, and datasets	SMP 5
Provides output to	SMP 3	SMP 5	SMP 5	SMP 4	SMP 6	Prediction user

a Model prediction.

The framework is applied to all SMPs of NEWS-DIN because this is feasible due to the limited complexity of this model. All indicators of the framework (Table 1) are used. As an example of indicator estimation, only the estimation of Indicator 6 ($f_{B,6}(S)$) for SMP 1 is described here. SMP 1 of NEWS-DIN models the surface N balance. In SMP 1, Indicator 6 measures the fraction of N emitted by sources modeled by SMP 1 that reaches the coastal zone within the duration of sup_t (Table 1). Sources modeled by SMP 1 are located on land surfaces. Values of sup_t for SMP 1 with low values of Indicator 6 are expected to cause insufficient relation between modeled land surface N emissions and N flux to coastal zones during the time of prediction. Values of $f_{B,6}(S)$ for SMP 1 are higher if a larger fraction of N emitted at land surfaces reaches coastal zones within the duration of sup_t. Indicator 6 is determined for an exhaustive number of sup_t values between one day and 100 years. Here, $f_{B,6}(S)$ for SMP 1 is a function of various N residence times between the land surface and the coastal zone (Table 3). Residence times in different N stores are distinguished. The relative importance ($w_{6,i}$) of such an N store in the calculation if $f_{B,6}(S)$ is the expected fraction of N reaching the coastal zones that has flown through this particular N store.

Five pathways of N from land surfaces to coastal zones are distinguished for the calculation of $f_{A,6}(S)$. Each pathway has a different N store in the land surface system modeled by SMP 1, being either (1) forest biomass, (2) humus, (3) peat, (4) fine textured mineral soil or (5) coarse textured mineral soil. Downstream of the system represented by SMP 1, each pathway is assumed to encounter the additional N stores in the same ratio. This assumption leads to estimated residence times of 203, 103, 107, 43, and 4 years for pathway 1, 2 3, 4, and 5, respectively.

Table 3 Values used when estimating the value of Indicator 6 ($f_{A,6}(S)$) for SMP1: Estimated residence times of N in temporary N stores in, and downstream of the system modeled by SMP1, and their relative importance ($w_{6,i}$) in the calculation of $f_{A,6}(S)$.

N store	Estimated residence time (y)[a]	$w_{6,i}$[a]	SMP that models this N store[b]
Forest biomass	200	0.05	SMP 1
Humus	100	0.10	SMP 1
Peat	10^4	0.05	SMP 1
Fine textured mineral soils	40	0.4	SMP 1
Coarse textured mineral soils	1	0.4	SMP 1
Groundwater	10	0.285	SMP 3
Overland flow	$1.4 \cdot 10^{-3}$	0.14	SMP 3
Through flow	0.011	0.57	SMP 3
Dammed reservoir	0.25	0.25	SMP 4
River surface water	$2.7 \cdot 10^{-3}$	0.91	SMP 5
River sediment	0.5	0.09	SMP 5
Seawater circulations	0.083	1	SMP 6

a Expert judgment

b Weight $w_{6,i}$ is estimated as the expected fraction of N reaching the coastal zones that has flown through the considered N store.

c See Table 2.

Values of sup_t below 4 years have an $f_{A,6}(S)$ of zero because none of the N entering land surfaces is expected to reach the coastal waters within the duration of such small sup_t. Values of sup_t between 4 and 43 years have an $f_{B,6}(S)$ of 0.4, being relative proportion of N entering land surfaces that is expected to reach the coastal zones in a time period between 4 and 43 years. We expect that this is the case for land surfaces of coarse textured mineral soils. Values of sup_t between 43 and 100 years have an $f_{B,6}(S)$ of 0.8, being relative proportion of N entering land surfaces that is expected to have reached the coastal zones in time periods between 43 and 100 years. We expect that this is the case for land surfaces of either coarse or fine textured mineral soils. The inertia of 4 and 43 years that we expect for coastal zone responses to land surface processes resulting from coarse and fine textured soil storage, respectively, are in line with those found by Grimvall et al. (2000).

Table 4 Values of Indicator 6 (fB,6(S)) for supt of SMP 1 between 1 day and 100 years. Within this supt range three sub ranges can be distinguished having different values of fB,6(S).

Sup_t range (y)	$f_{B,6}(S)$
0.003 - 4	0
4 – 43	0.4
43 - 100	0.8

In the following steps (Steps 3-5), Equations 2 to 4 are used to combine the values of Indicator 6 with those of other indicators to find the appropriate scales for SMP 1 (Table 5). First values of Indicator 6 are combined with those of Indicators 4, 7, and 8 in Equation 2 to find $F_B(S)$.

This fulfillment of Criterion B is then inserted in Equation 3 to identify $a_B(S)$, which is inserted in Equation 4 to identify $A(S)$. These steps are also taken for the other SMPs resulting in the appropriate SMP scales reported in Table 5.

Table 5 Ranges of appropriate scales for SMPs of NEWS-DIN as identified by one of the model builders using the decision framework described in Section 2 of this paper (preliminary results).

SMP index	1	2	3	4	5	6
sup_s (km)	42–194	10–67	42–244	10–133	42–244	42–300
sup_t (y)	1.1–10	$3{\cdot}10^{-3}$–26	1.1–10	0.28–17	$3{\cdot}10^{-3}$–0.27	$3{\cdot}10^{-3}$–0.8
ext_s (km)	$3{\cdot}10^{3}$–$3{\cdot}10^{4}$	$2{\cdot}10^{3}$–$3{\cdot}10^{4}$	30000	$1.3{\cdot}10^{4}$–$3{\cdot}10^{4}$	$2.4{\cdot}10^{4}$–$3{\cdot}10^{4}$	$1.3{\cdot}10^{3}$–$3{\cdot}10^{4}$
ext_t (y)	10^{2}–10^{3}	10^{2}–10^{3}	unclear	23–10^{3}	47–10^{3}	23–10^{3}
so_{min}	0	0	unclear	<8	<10	>8
so_{max}	0	0	unclear	>7	>8	12

The largest differences between SMP scales appropriate to the framework and those used by Dumont et al. [2005], were found for sup_s of SMP 2 and sup_t of SMP 6, where the scales appropriate to the framework are approximately a factor 8 smaller (Table 5 versus Table 2).

4 Discussion and Conclusion

This paper describes the development of a decision framework to identify appropriate spatial and temporal scales for modeling N flows. It is based on four criteria, which in turn are fed by 14 indicators. A central concept in the framework is the scalable model part. Scalable model parts are distinguished in the framework to be able to fully account for all aspects of model scale.

The decision framework is applied to, NEWS-DIN, an existing model for river export of dissolved inorganic nitrogen to coastal zones. Ranges of appropriate scales were identified for all scalable model parts. However, Indicator 8 could not be used due to insufficient information on spatial and temporal autocorrelation of input error. Further applications have to show the qualities of this indicator in the nearby future.

Application of the decision framework requires profound knowledge of input data production, model development and characteristic scales of processes in the study area. Also the application of the decision framework for all scalable model parts of a model is only feasible if the model is relatively simple. Otherwise a selection of scalable model parts must be made.

We conclude that now we have been able to systematically and transparently address the issue of scale selection for N flux models. This attempt appears to be generic and general and is a useful basis for improved application of NEWS-DIN and many other N flux models.

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