Metamodels, Response Functions, and Research Efficiency in Ecological Economics

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ABSTRACT

Analysis of alternative environmental policies often requires execution of computer simulation models of the ecological or economic phenomena involved. This paper explores efficiencies to be gained by using these simulation models in a program of constructing metamodels. Constructing a metamodel involves statistical modeling of a simulation model's output—creating a model of a model. Metamodeling produces response functions that characterize relationships implied by the structure of a simulation model relating variables that appear to be important to policy evaluation. We first make the case for the research efficiency of metamodeling by discussing an integrated policy evaluation system designed for herbicide pollution policies (CEEPES) that could not have been constructed without metamodels. Next, we illustrate the metamodeling concept by describing a particular metamodel from the system.

METAMODELS, RESPONSE FUNCTIONS, AND RESEARCH EFFICIENCY IN ECOLOGICAL ECONOMICS

Introduction

Analysis of the economics of agricultural issues has always involved the task of characterizing relationships between inputs and outputs of biological processes through which food and fiber are produced. Such a characterization of "agricultural technology" is a part of the solution of even the most basic questions of agricultural economics. The work of conceptualizing and giving empirical content to such characterizations of agricultural technology is the subject matter of agricultural production economics. But the traditional subject matter boundary of production economics is being strained by a growing need to characterize technologies that are only incidentally related to agricultural production, such as the processes by which agricultural production can result in unwanted side effects of pollution or other environmental degradation. By analogy to narrowly defined agricultural technologies, these physical, chemical, and biological processes can be regarded as technologies of the environment, and their effects must increasingly be incorporated into analyses of agricultural production decisions.

The need to incorporate the technology of the environment into analyses of agricultural production decisions also strains the methodological boundary of production economics, in at least two ways. The first is the need to characterize the best available scientific knowledge about processes that are, in principle, not available for observation. While this difficulty applies to some processes of agricultural technology, it is pervasive in processes of the technology of the environment. This impossibility of directly observing relevant attributes of important processes can arise because the time scale of the process exceeds the time available for analysis and decision making, or because experimentation with the process may cause unacceptable harm to the environment. In either event, efforts to characterize the unobservable process will require methods other than those based on experimentation and direct observation, which are the traditional methods of production economics.

The second methodological difficulty raised by the need to model the technology of the environment is that models of the effects of agricultural production decisions must encompass a broader range of processes, which may be very dissimilar in structure. For example, the CEEPES illustration discussed later is concerned with the consequences of agricultural production decisions regarding weed control strategy, not merely for production and cost, but also for fate and transport of multiple herbicides in groundwater, surface water, and through the air over both short and long range. This need to incorporate a broad range of diverse processes implies more parsimonious characterizations of the diverse set of technologies that must be included.

An attractive response to the first methodological issue (the need to model processes that are not available for direct observation) is the use of structural simulation models of the relevant processes. This approach is not new to production economics [Johnson and Rausser (1977)] but, for the reasons outlined here, is likely to become more prominent. While this approach may be the best way to glean the state of scientific knowledge of processes not available for direct observation, it would appear to conflict with the need for parsimony dictated by the possibility of many such processes that must be modeled in order to understand the consequences of a single agricultural production decision.

This paper offers a practical means to integrate multiple simulation models of diverse structure into a unified environmental-agricultural economic system. Our proposal rests on the concept of metamodeling through statistical response functions.[1]

Because of these considerations, as well as declining natural resource research budgets and time constraints [see Day and Ruttan (1991)], metamodels and response surface methods are becoming increasingly attractive. Essentially, metamodeling starts by experimenting with and observing outcomes from a simulation model. The method then proceeds by the conventional practice of estimating relatively simple parametric forms to approximate a restricted set of outcomes of the simulated processes. This allows us to abstract from detail not needed for policy evaluations, and to use interpolation to estimate outcomes for experimental conditions that were not simulated with the process model. The parsimonious specification provided by response functions allows us to integrate the logical implications of diverse models and evaluate the consequences of alternative policies without having to return to the original process models for every possible combination of input conditions.

The paper first provides a general discussion of the concept of metamodeling. We next illustrate our point by describing the current configuration of the Comprehensive Environmental

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[1]Box and Draper (1987) is a very broad text on response surface methods. Smith (1982) surveys economic applications of response surface methods using process models.

Economic Policy Evaluation System (CEEPES) for the analysis of policies concerning the use of atrazine in corn and sorghum production. Comprehensive analysis of issues surrounding this policy question requires scientific input regarding plant growth processes and their response to alternative weed control practices, soil and meteorological conditions, fate and transport of various agricultural chemicals through hydrological and meteorological processes, and the economic processes that determine the behavior of producers and markets. CEEPES uses physical process simulation models incorporating state-of-the-art from the various scientific disciplines to elicit relevant input. The accomplished integration of scientific information of diverse sorts would not be possible under normal limitations of time and computational resources without the use of.metamodels.

Finally, we present a specific example of a response function from this configuration of CEEPES. STREAM [Donigian et al. (1984)] transforms runoff estimates from the groundwater model RUSTIC [Dean et al. (1989)] into estimates of surface water concentrations suitable for policy analysis. Discussion of the metamodel estimation for STREAM illustrates the use of a metamodel to achieve a parsimonious analytical specification for a very unwieldy physical process model. The estimated response function includes all parameter estimates significant at levels of .001 or better, and results in an R^2 for the regression of .90.

The Role of Metamodels and Response Surfaces in Agricultural and Environmental Economics

Costanza et al. (1990) point out that adequately predicting impacts of human intervention in ecosystems requires sophisticated computer simulation models that represent the current state of knowledge on how these complex systems behave. Given sufficient resources for computation, we could use such simulation models to directly estimate any indicators relevant to policies under consideration. This approach would require executions of simulation models for each alternative combination of policy instruments to be considered, and for input conditions appropriate to each element of the relevant geographical space under study. Such an approach might not be a problem with narrowly specified policy alternatives for a relatively site-specific problem such as a unique ecosystem (e.g., a specified wetland) or a single farm [see, for example, Andréasson (1990)]. Most policy analysis questions, however, are addressed to larger and more diverse areas, require analysis of a relatively broad range of policies, and involve alternative policy regimes that generate relatively complex impacts on the system under study, requiring the linking of more than one simulation model and knowledge of simulated outcomes over a large number of input conditions. In such a case, this "hammer and tongs" approach of simulating every conceivable combination of inputs to the natural system may not be possible, and is very unlikely to be an efficient use of a limited computation budget.

Consider a system of simulation models designed to evaluate I policies p_i from a discrete set P, where policies will have effects in J discrete geographic areas g_j from the set G. Geographic areas differ in several relevant respects. They differ in agricultural productivity due to differences in climate, soil properties, land improvements, the stock of capital equipment dedicated to agricultural production in the area, and the skills of local producers. They differ in attributes relevant to environmental processes peripheral to agricultural production, such as the processes that determine fate and transport of potential pollutants, and in the extent of damage caused by a particular concentration of a pollutant in a given medium within the area because of considerations such as population density downwind or extent of shallow groundwater use. Geographic areas must be small enough to allow homogeneity within the area with respect to each of these parameters, so the minimal number of geographic areas, J, determines the number of input parameter combinations. If the simulation models are completely deterministic, policy analysis will require IJ executions of the relevant simulation models. If expected values of some indicators are to be calculated, for example by integrating over an empirical distribution of K annual weather possibilities, IJK executions will be required. For nontrivial problems this can involve a very large, perhaps prohibitive, number of executions. The metamodeling approach exploits similarities among input conditions to reduce the required number of simulation executions.

A metamodel is a statistical model relating inputs and outputs of the actual simulation model. The concept of a metamodel arises from a hierarchical modeling approach where, from a complex and "messy" real phenomenon, we proceed to a well-structured simulation model and then to modeling the relationship between inputs and outputs of the simulation model. Figure 1 illustrates this general concept as it applies to the processes of weed competition, which are central to understanding the effect of different agrichemical strategies on the environment. The simulation model is taken as characterizing the current state of knowledge of the processes that determine growth of individual plants and their competition for water, nutrients, and light, all within specified management and environmental conditions.

Given an appropriate simulation model, the first phase in metamodel development involves selecting parameters whose values may change in the policy evaluations being considered and selecting of outcome measures to be modeled. Parameters whose values may differ regionally or

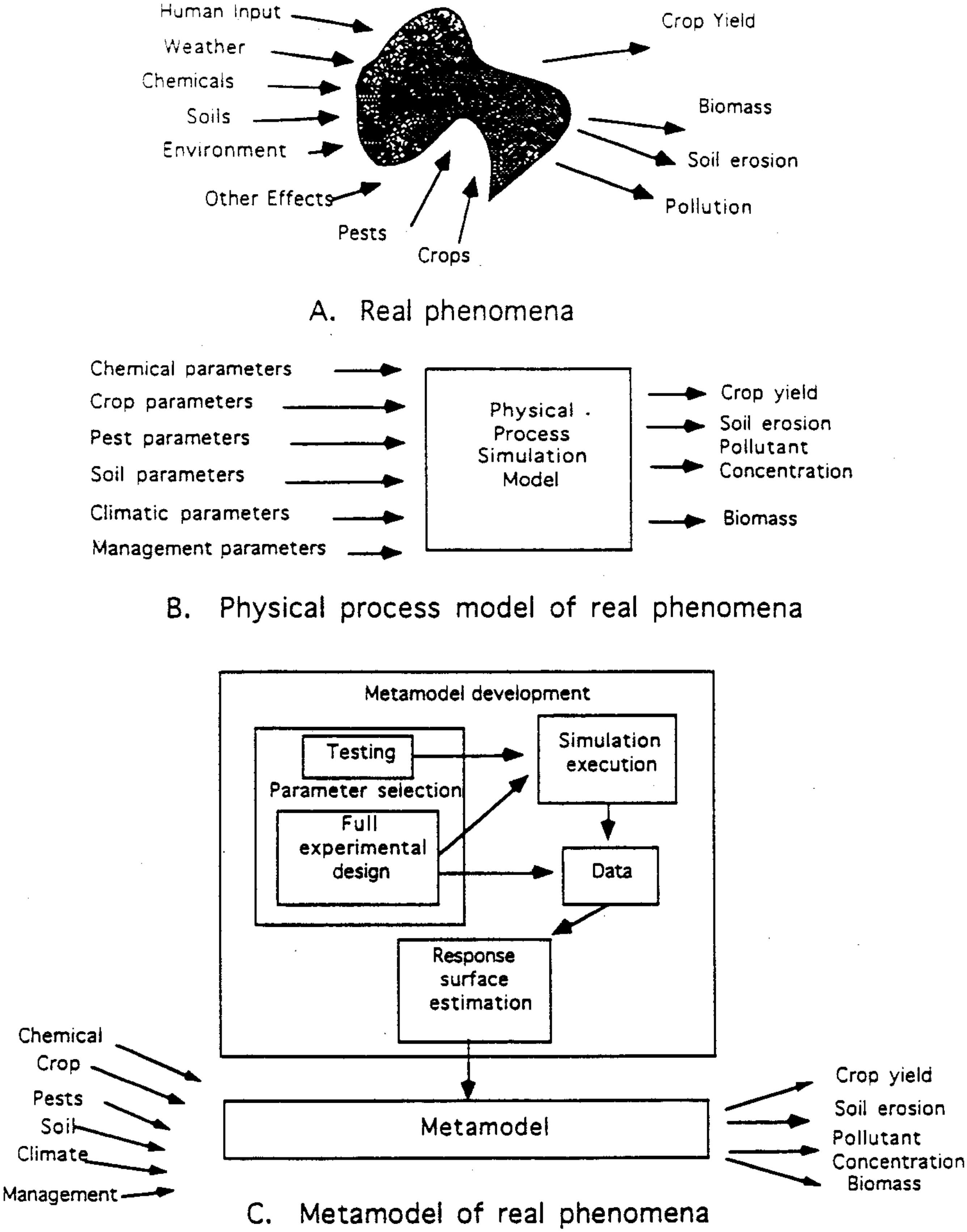

Figure 1. Metamodels in relation to physical process models and real phenomena

differ due to anticipated policy changes are regarded as the inputs of the metamodel. Parameters of the simulation model that will not vary over conditions being modeled can be regarded as constants of the simulation model unless they are subject to important uncertainties and will be varied for sensitivity analysis. Selection of outcome measures is dictated by the purpose for which the metamodel is being constructed. The outcome measure may be a final product of the modeling effort or an intermediate output that will be used as an input to another metamodel.

In either case, outcome measures must be selected carefully and may greatly reduce the dimensions of the metamodeling task. For instance, execution of a plant growth simulation model might produce a daily time series of 365 observations of plant biomass per unit area for each year. With 50 years of weather data, this amounts to 18,250 biomass observations for each combination of soil properties, tillage practice, climate, and other factors that can be modeled by the simulation. Depending on the policy analysis being conducted, the appropriate outcome measure might be expected value of end of growing season biomass.[2] If so, construction of the appropriate outcome measure reduces simulation output of dimension 18,250 to a single number, in the process ignoring the simulation model's rich (but irrelevant for the purpose at hand) characterization of the relationship between weather and plant growth to focus on the single relevant outcome measure.

After choosing the parameters to be varied and the outcome measures of interest, the metamodeling task is to approximate the relationship between these variables implied by the simulation model. The full experimental design phase identifies the values of the chosen parameters for which the simulation model is to be executed, and the outcome measures recorded. The experimental design determines the number of simulation executions that will be required, and must be undertaken with a view to the cost and time required for each execution of the simulation model. The experiment should call for computationally intensive simulations for only the most informative specifications of input variables. Finally, the last step of metamodel development consists of estimating response functions for the outcome measures of interest such as crop yield, plant biomass, and chemical concentration.

In reality, the outcome measure of interest, y (such as crop yield, average or peak chemical concentration, biomass), is determined by an unknown process, $y = f^{u}(x_1, x_2, \ldots x_k)$. Controlled simulation experiments allow the specification of a metamodel f^{m} based on relatively few parameters

[2]Although metamodels can be used for predicting time series of multivariate responses of simulations models, they are typically applied to individual mean system responses [see Kleijnen (1987); Rotmans and Vriez (1990)].

u_i, $i = 1, \ldots, n < k$. The number of parameters in the unknown true model is greater than the number of parameters in the metamodel for at least two reasons. First, as suggested, some parameters in the simulation model may be constant for the purposes at hand, and are then regarded as internal constants of the simulation that need not be included in the metamodel. In this case, the metamodel is best regarded as a simple parametric approximation of a very complex, but deterministic, unknown process. Second, the outcome measure of interest may be a statistic of the distribution of a random outcome measure formed by stochastic choice of some parameters of the simulation model. This is so in this case when the outcome measure is taken to be the mean over the distribution of end of season biomass values generated by choosing weather variables from the joint distribution implied by a specified climate. In this case, the outcome measure can be regarded as resulting from integration over a distribution of values of some parameters of the simulation model, with the variables of integration not appearing in the metamodel. In any case we then estimate $y = f^m(u_1, \ldots, u_n, \epsilon)$ where ϵ is an error term.

The metamodel is used to predict outcomes, essentially replacing the simulation model and the real process studied with a relatively simpler parametric form. This replacement is limited, of course, by the outcome measures, input parameters, and experimental ranges of the input parameters dictated by the experimental design. In a complex system like CEEPES, a network of process models is replaced with a network of linked metamodels allowing outcomes in a chain of influence to be approximated with a number of calculations many orders of magnitude smaller than would be required by direct execution of the simulation models.

The method of estimating simple response functions to approximate outcomes of complex process models is a powerful means of simplifying computation necessary for two types of integration often required by policy evaluation systems. One type of integration occurs when parameters of a simulation model vary over geographic areas in a way that can be described by a distribution function. The other is the integration of diverse models of the various phenomena that must be considered for policy analysis. Directly linking nontrivial simulation models together is normally a very large programming task, often tantamount to rewriting the code for the various models. By giving thought to selection of parameters to be varied and definitions of outcome measures for metamodels to be constructed, linking the resulting metamodels only requires forming indicated composites of the various response functions. Further, from the point of view of organizing interdisciplinary research, there is an intrinsic advantage in the response function method's requirement of careful specification of functional relationships that one work group will derive, and others will rely on, for further analysis. This advantage comes from being explicit about what outcome measures are needed from each model, from knowing what input conditions will be allowed to vary in response to policy changes, and by using statistical methods to approximate the model's performance in this narrowly prescribed domain, neglecting all the model's other unneeded capabilities.

Metamodeling in the CEEPES/Atrazine Project

Background

Atrazine accounts for 12 percent of all pesticides used in the United States, often topping the list of pesticides detected through groundwater or surface water monitoring. Atrazine detection is 10 to 20 times more frequent than the next most detected pesticide [Belluck (1991)]. In a survey of 150 sampling sites in 10 midwestern states, Goolsby and Thurman (1990) report detection in 90 percent of samples taken before the crop year's application date, and 98 percent of samples collected during periods of runoff immediately following application. The U.S. Environmental Protection Agency currently ranks atrazine as a Group C (possible human) carcinogen based on the incidence of mammary tumors in female rats [Belluck et al. (1991)].

CEEPES is a system of simulation models, linked together to form an integrated evaluation system to estimate indicators of both market and nonmarket consequences of alternative policies. We have configured CEEPES to evaluate the trade-offs of alternative policies to restrict atrazine use in agricultural production. We evaluate policy alternatives relative to the status quo and take into account the site-specific nature of fate and transport, agricultural production, and damage mechanisms. We simulate a farmer's substitution among herbicides, other inputs, crops, and agricultural practices in response to a specified policy. Simulated ecological damages occur through multiple media, with the possibility of interregional transport. Figure 2 is a schematic representation of the evaluation system.

CEEPES has four major components:

Policy Specification. Alternative atrazine policies are specified in a form suitable for subsequent economic modeling to determine choices of agricultural practices, including patterns of herbicide usage. Classifying sets of alternative policies is a crucial step in the design of simulation experiments and linkages among models. Policy options include bans, quantity constraints, and timing restrictions.

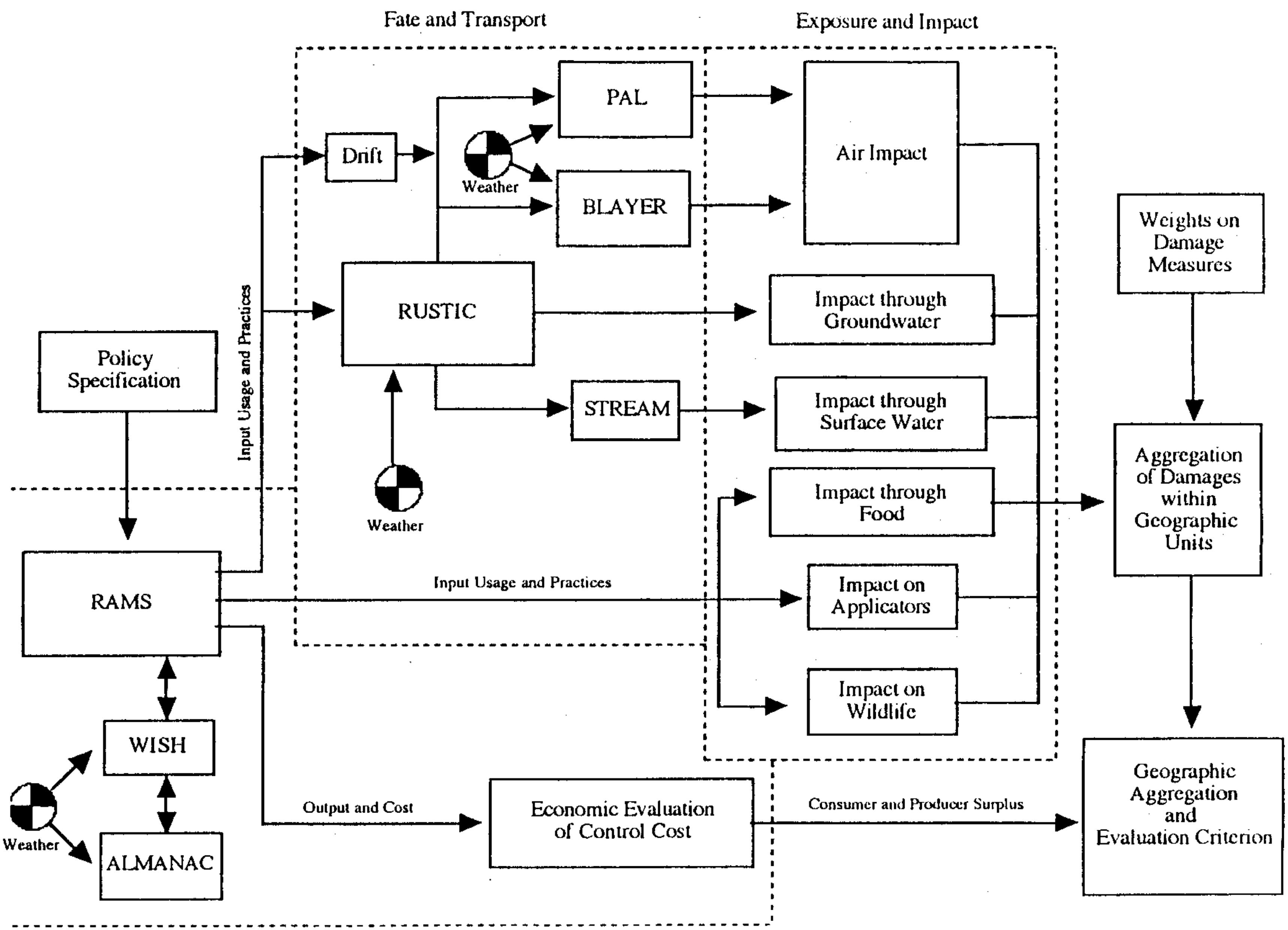

Figure 2. Production decisions and economic consequences

Agricultural Decision. This component models the choice of agricultural practices under alternative policies. The outcomes to be determined include acreage planted, rotation, tillage practice, chemical regime, yield, and cost of production for each geographic unit in the study area. The model uses profit maximization rather than cost minimization as the objective function, allowing more realistic modeling of government agricultural programs.

Fate and Transport. These models use information on agricultural activity in each geographic unit to produce damage-relevant concentration measures for (a) each damage category, (b) the geographic unit where the chemical was applied, and (c) other geographic units that may be affected by pollutant transport. For example, given an agricultural activity in a rural central Corn Belt geographic unit, the fate and transport components estimate shallow groundwater concentrations for domestic wells, surface water concentrations in the area, and contributions to air concentrations in Chicago. The component transforms a vector describing agricultural activity in all geographic units into a vector of ambient concentration measures for each medium in all geographic units. The concentration measures can include expected values, information on the probabilities of various concentrations, or the distributions of concentrations over time. Outcomes of greatest interest are 24-hour peak concentrations for acute toxicity and annual average concentrations for long-term exposure.

Exposure and Impact. These algorithms estimate physical measures of impact from concentrations reported by the fate and transport component. These models incorporate such considerations as the population distribution over the geographic units, chemical toxicity given concentration level, and the distribution of behavior, which translates ambient concentration into damage measure, such as drinking water from a shallow rural domestic well, breathing polluted air, or eating foods containing herbicide residuals. Damage measures take the form of risk indicators such as expected excess of various types of morbidity or mortality for each geographic unit.

Response Function for STREAM

As an example to illustrate the practicality of metamodeling and response function methods, we focus on STREAM from the fate and transport component [Donigian et al. (1984)] STREAM is a graphic methodology used to estimate pesticide concentrations in surface water due to runoff from agricultural applications. STREAM was developed by applying HSPF, a comprehensive watershed hydrology and water quality model, to representative watersheds in each of the four agricultural regions—Southeast, Mississippi Delta, Eastern Corn Belt, and Western Corn Belt. Cumulative frequency distributions of pesticide concentrations and loadings were developed for each crop in each region. Given the pesticide application rate and three pesticide parameters (KOC, organic carbon partition coefficient; KS, soil/sediment decay rate; and KW, solution decay rate), the user of STREAM can obtain pesticide loadings and concentrations for the crops and regions of interest.

STREAM is not a computer model, but a graphic presentation of sensitivity runs of HSPF. Donigian and Carsel (1987) describe a method of using only the in-stream component of STREAM to transform independently generated loadings into surface water concentrations. Figure 3 presents a simplified version of this procedure, ignoring pesticide and regional parameters.

Starting with a loading (lower vertical axis), we determine the percentage of time that STREAM expects this loading value to be exceeded (right horizontal axis). The STREAM loading curve is a cumulative frequency distribution of loadings from the HSPF runs from which STREAM was constructed. Following Donigian and Carsel (1987), assume that this percentage exceedance also applies to the level of surface water concentration associated with the initially chosen level of loading. Finding the associated level of solution concentration (top vertical axis in Figure 3) amounts to inverting STREAM's cumulative frequency distribution for solution concentration implied by the Donigian and Carsel (1987) procedure. Donigian and Carsel used a manual lookup version of this procedure that involved many references to graphs in Donigian et al. (1984) and frequently required interpolation within and among graphs. This manual approach did not allow the integration between STREAM and RUSTIC sought for CEEPES, but metamodeling reduced the graphic procedure to evaluation of a simple parametric form. This approach allows a fully automated integration of two simulation models that each represent the state of scientific knowledge regarding one facet of the policy question at hand.

The process of Figure 3, extended to take account of pesticide and regional parameters, was used to generate a data set of 429 points chosen to cover the relevant ranges of pesticide parameters, loadings, and concentrations.[3] Preliminary analyses, as well as theoretical consideration, indicate that a linear model on the log-transformed concentration loadings and pesticide parameters would adequately represent the relationship between concentration and the remaining variables. A linear, multiple regression model was fitted to the data, and ordinary least square methods were used to

[3]The 429 points arise from a factorial design with 2 regions, 4 levels of KOC, 3 levels each for KS and KW, and 6 levels of loading with 3 missing observations.

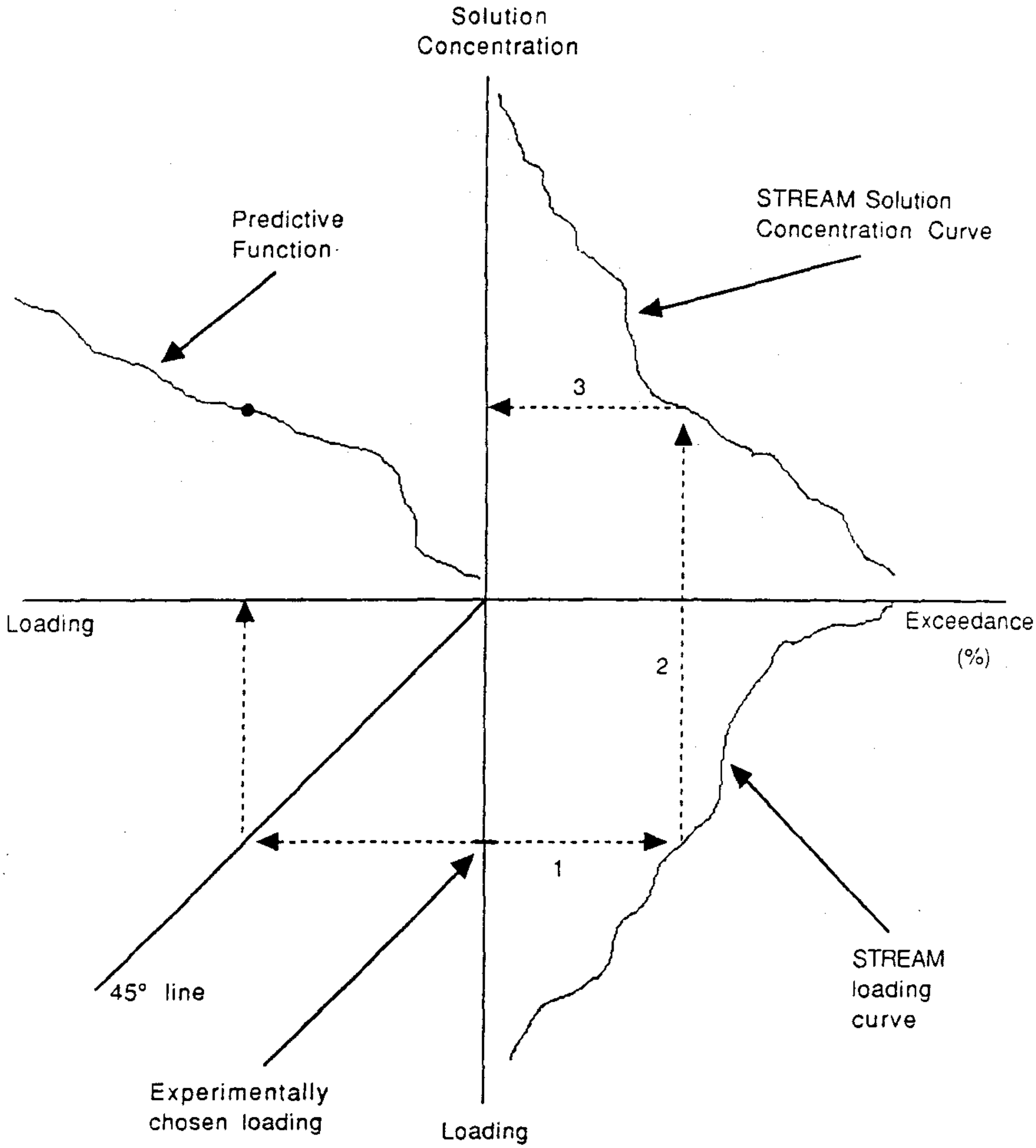

Figure 3. Simplified version of STREAM

estimate the unknown parameters in the model. Solution concentration was taken to be the dependent variable, and pesticide parameters, loading, region, plus all possible region by pesticide parameter and loading interactions were the independent variables in the model.

A test for multicollinearity among the independent variables in the model indicated that pesticide parameters and loading were uncorrelated ($p \geq 0.20$), with the exception of the pair of variables KS and loading, which exhibited a moderately high negative correlation ($r = -0.19$, $p \leq 0.01$). A dummy variable was included in the model to account for potentially different responses of concentration on pesticide parameters and loadings in the two regions: Eastern and Western Corn Belt. The estimated responses for each of the two regions are:

Eastern Corn Belt

$$C = \frac{1590(0.821)^{KW}(L)^{0.366}}{(KOC)^{0.455}(KS)^{0.263}}$$

Western Corn Belt

$$C = \frac{1590(0.516)^{KW}(L)^{0.448}}{(KOC)^{0.374}(KS)^{0.138}}$$

where

C:	estimated solution concentration	(ppb)
L:	pesticide loading	(kg/ha^{1})
KW:	solution decay rate	(day^{-1})
KS:	soil/sediment decay rate	(day^{-1})
KOC:	organic carbon partition coefficient	(mil/g).

A test for the hypothesis, H_o: $B_i = 0$ vs H_a: $B_i \neq 0$, was performed for each of the parameters in the model. In all cases, the null hypothesis was rejected at a $\mu \leq 0.0005$ confidence level. The R^2 for the model was 0.90, indicating that the variables in the model helped to explain 90 percent of the variation in concentration in these data. Usual residual diagnostics suggested that these data satisfied the model assumptions of normality and homogeneity of variances. No outliers were detected.

Concluding Comments

The goal of the CEEPES system is to explore both the environmental and economic consequences of alternative policies through simulation of producers' economic choice of inputs and technology, and through simulation of fate and transport of herbicides applied. The problem of integrating a large number of diverse and individually complex models becomes critical when simulating the consequences of alternative agricultural and environmental policies. The approach we suggest is to construct metamodels using response function methods. Although CEEPES is still evolving, enough has been accomplished to give some confidence in the general approach. In particular, the response function described in this paper allows STREAM to be closely integrated with other models that form adjacent links in a chain of reasoning, also streamlining application of the model sufficiently to make it feasible to integrate over the distribution of heterogeneous input conditions.

While metamodeling through response functions is by no means a panacea, nor is it applicable to all natural resource modeling problems, it does hold promise for integrating models that would otherwise be too unwieldy or inappropriately specified to operate together. In addition, metamodeling allows numerical integration over a distribution of heterogeneous input vectors in cases that would be computationally infeasible if every evaluation of the function required execution of a complex numerical simulation. Using metamodels can increase research efficiency, allowing integration of the state of knowledge from the various disciplines that each hold a piece of the puzzle of anticipating the diverse consequences of alternative agricultural and environmental policies.

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