Why Bayesian inference?

George Arhonditsis
Ecological Modelling Laboratory
Department of Physical & Environmental Sciences
University of Toronto

Bayesian Approach

In modelling context:

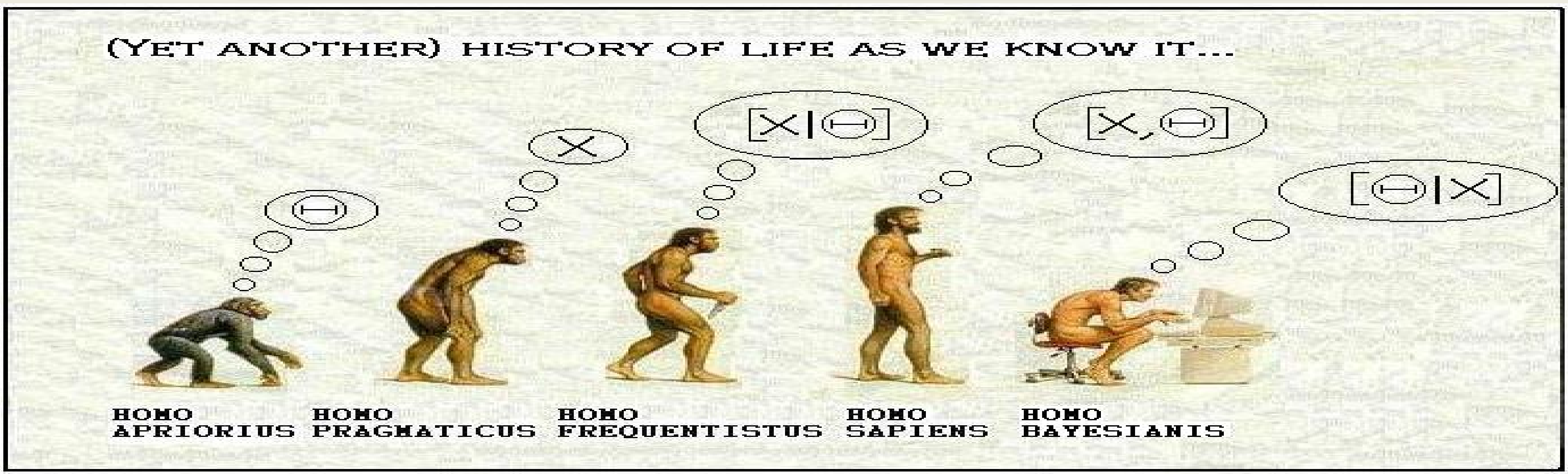
$$P(Model|Data) = \frac{P(Data|Model)P(Model)}{P(Data)}$$

$$\propto P(Data|Model)P(Model)$$

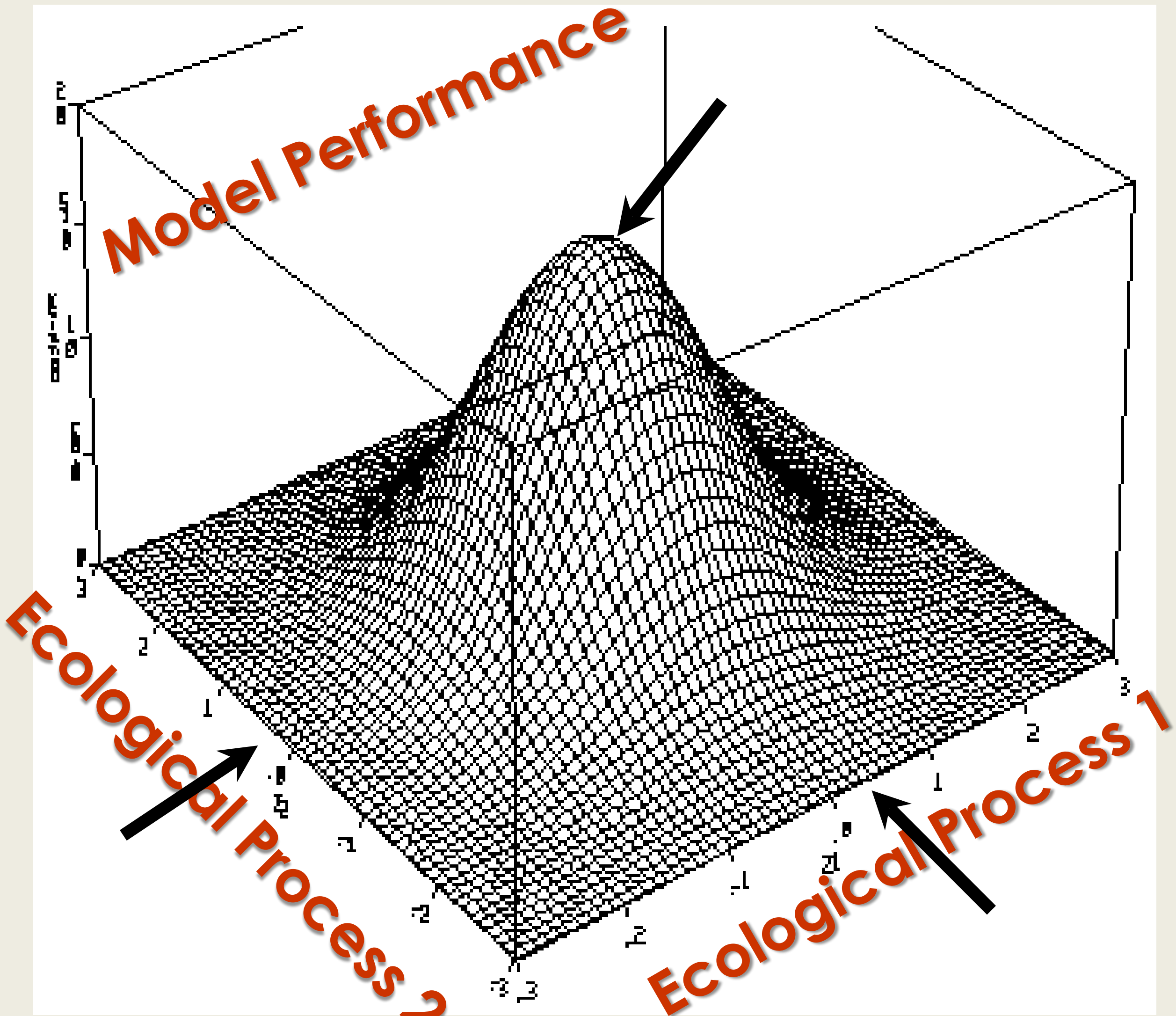
Future = $P(Model|Data)$

Present = $P(Data|Model)$

Past = $P(Model)$



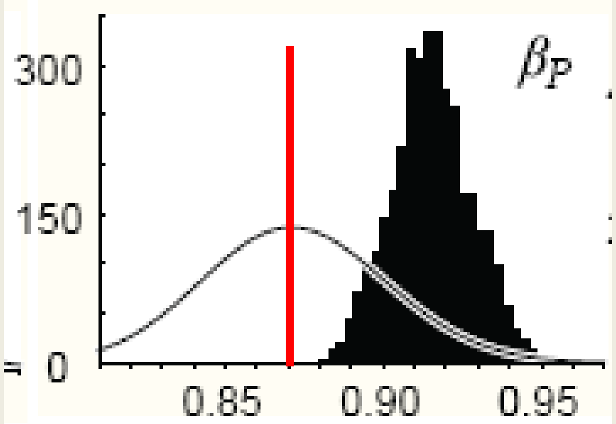
Basic Concept of the Bayesian Approach



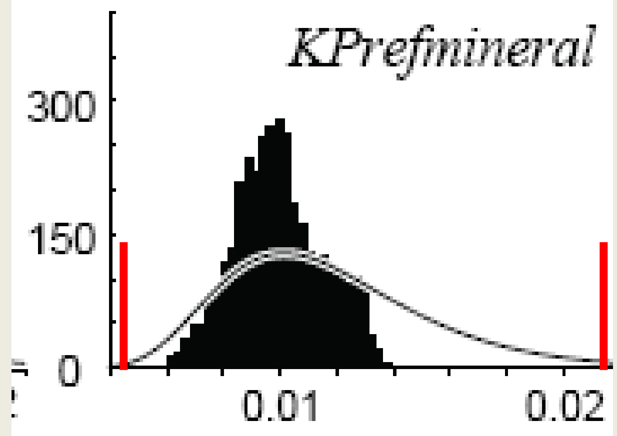
We do not care just for the tip of the "mountain" BUT for the entire "mountain", i.e., the likelihood of every single model realization associated with model inputs, data uncertainty, and exogenous forcing!!

How much can we learn about the magnitude of the ecological processes when we consider the data from the modelled system?

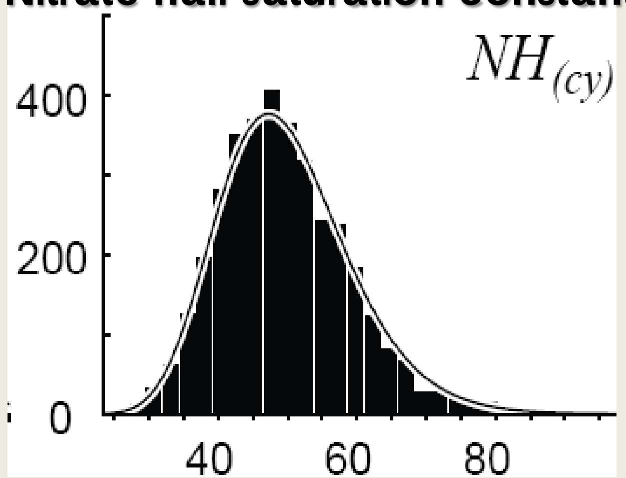
Sediment release rate



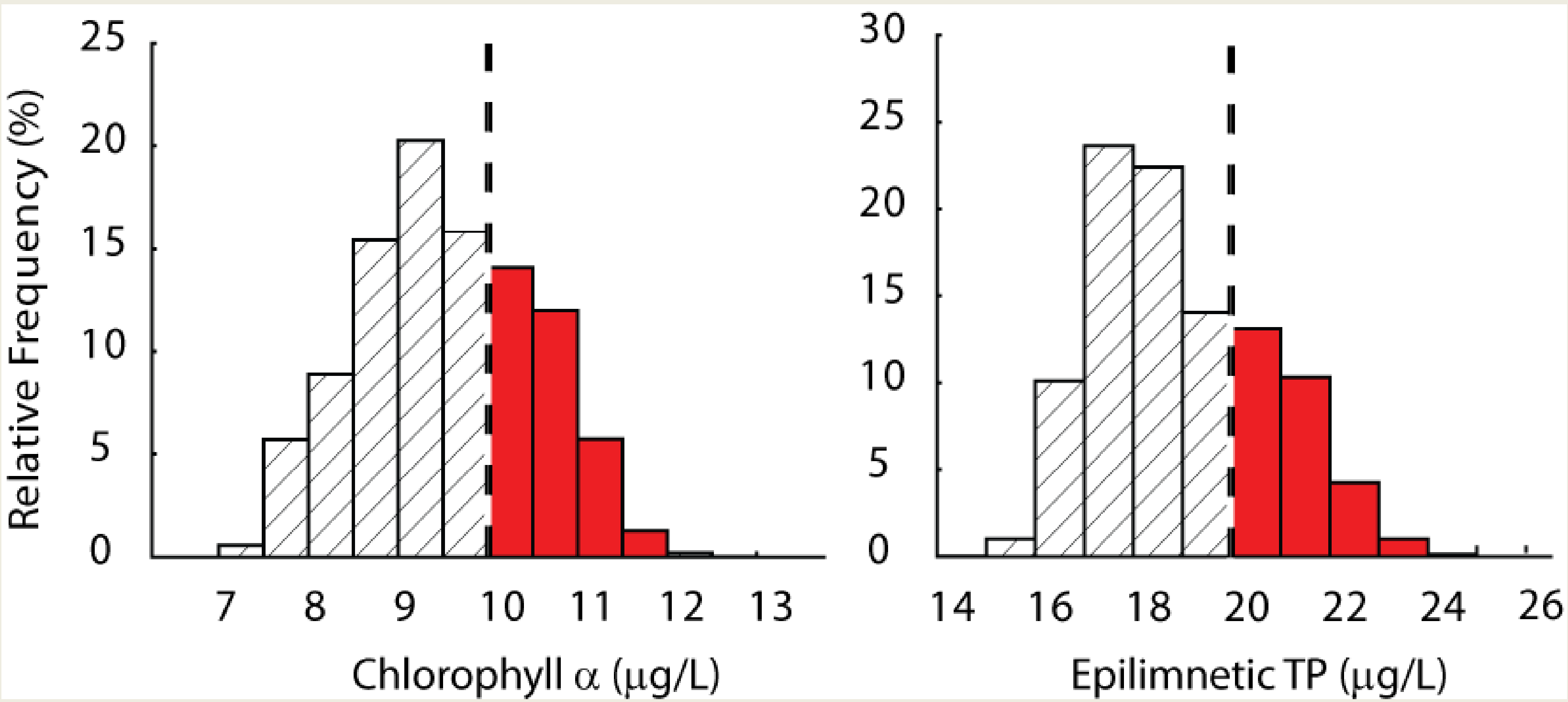
Mineralization rate



Nitrate half saturation constant



Realistic Uncertainty Estimates of the Ecological Forecasts

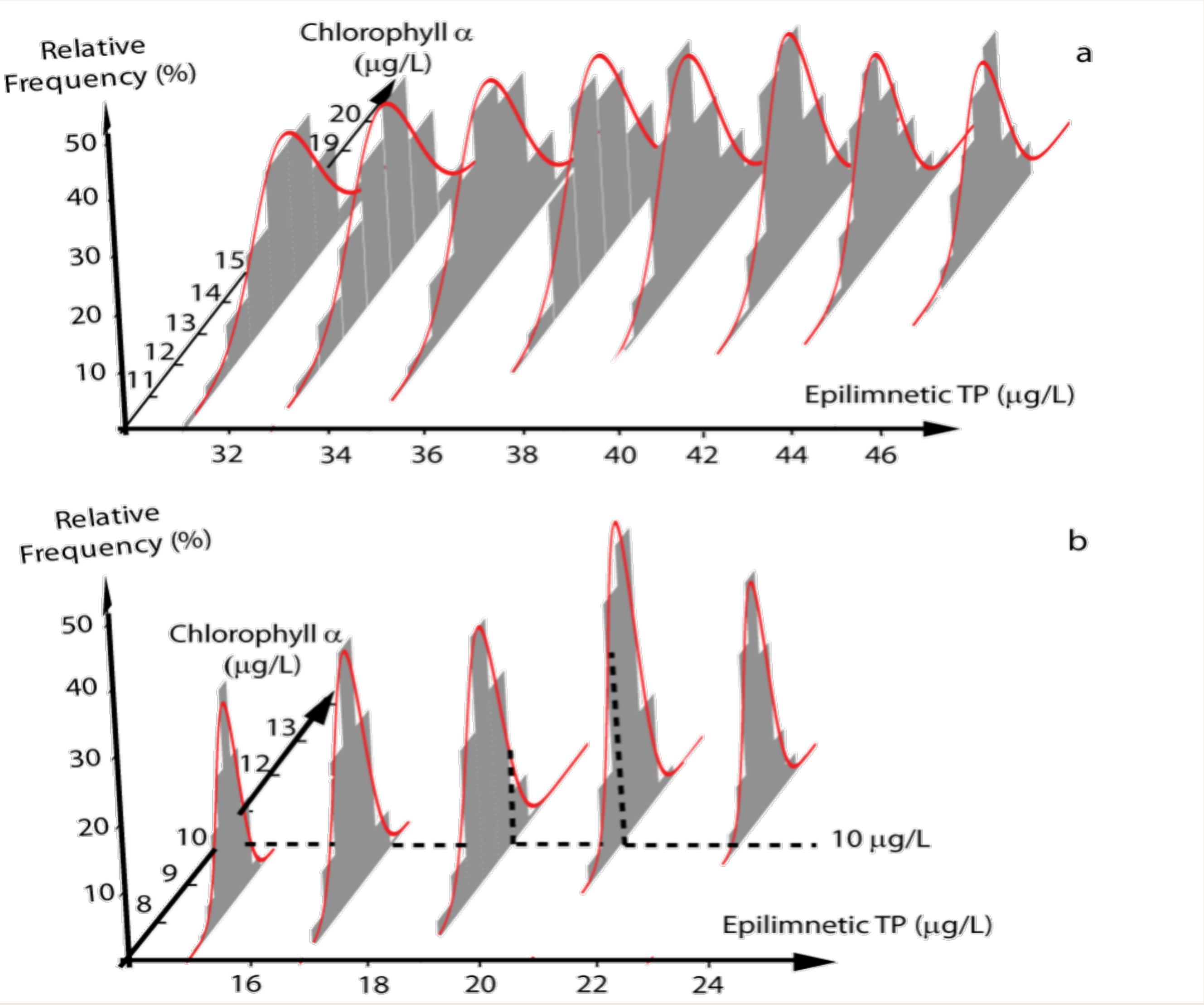


Probabilistic projection of system response to nutrient loading reduction strategies

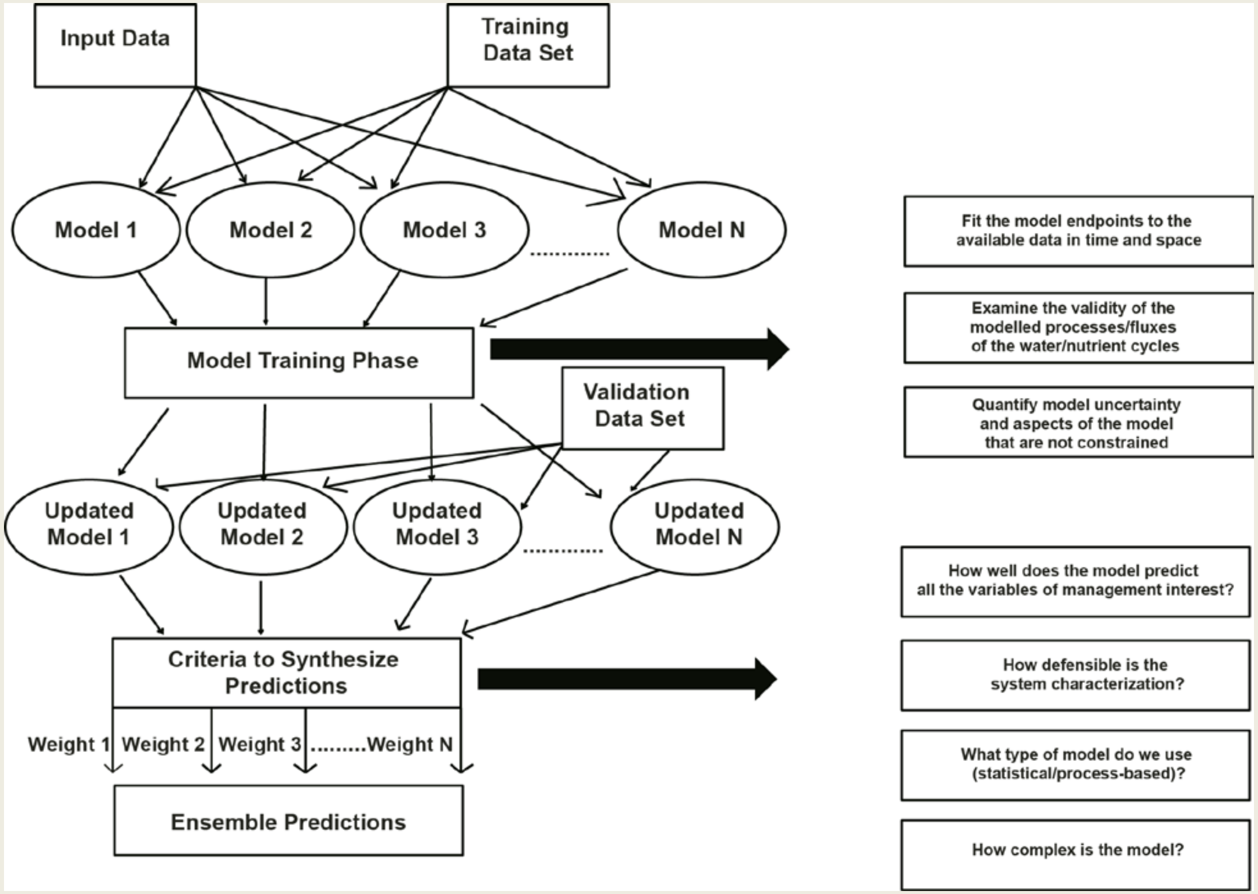
Chlorophyll *a* Predictive Distributions for Different Levels of Total Phosphorus

Present loading conditions

Nutrient loading reduction

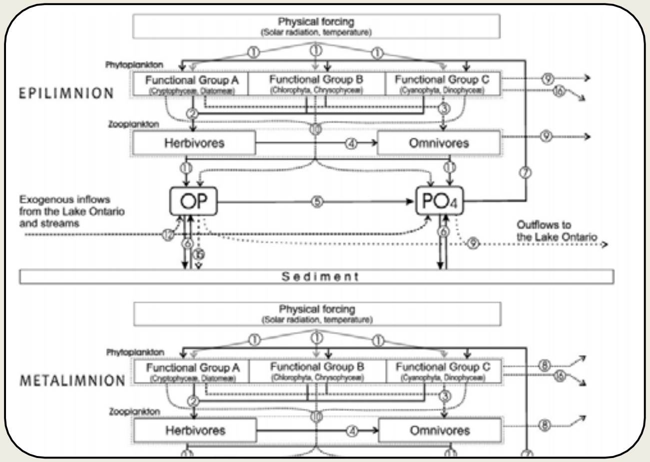


Ensemble Environmental Modelling



Ensemble modelling is the process of running two or more related but different models with respect to their conceptual/structural characterization and input specification, and then synthesizing the results into a single score or spread in order to improve the accuracy of predictive analytics and data mining applications.

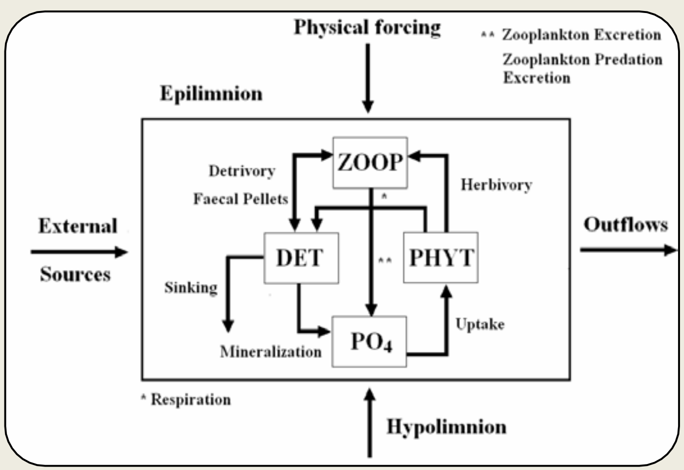
Complex Model

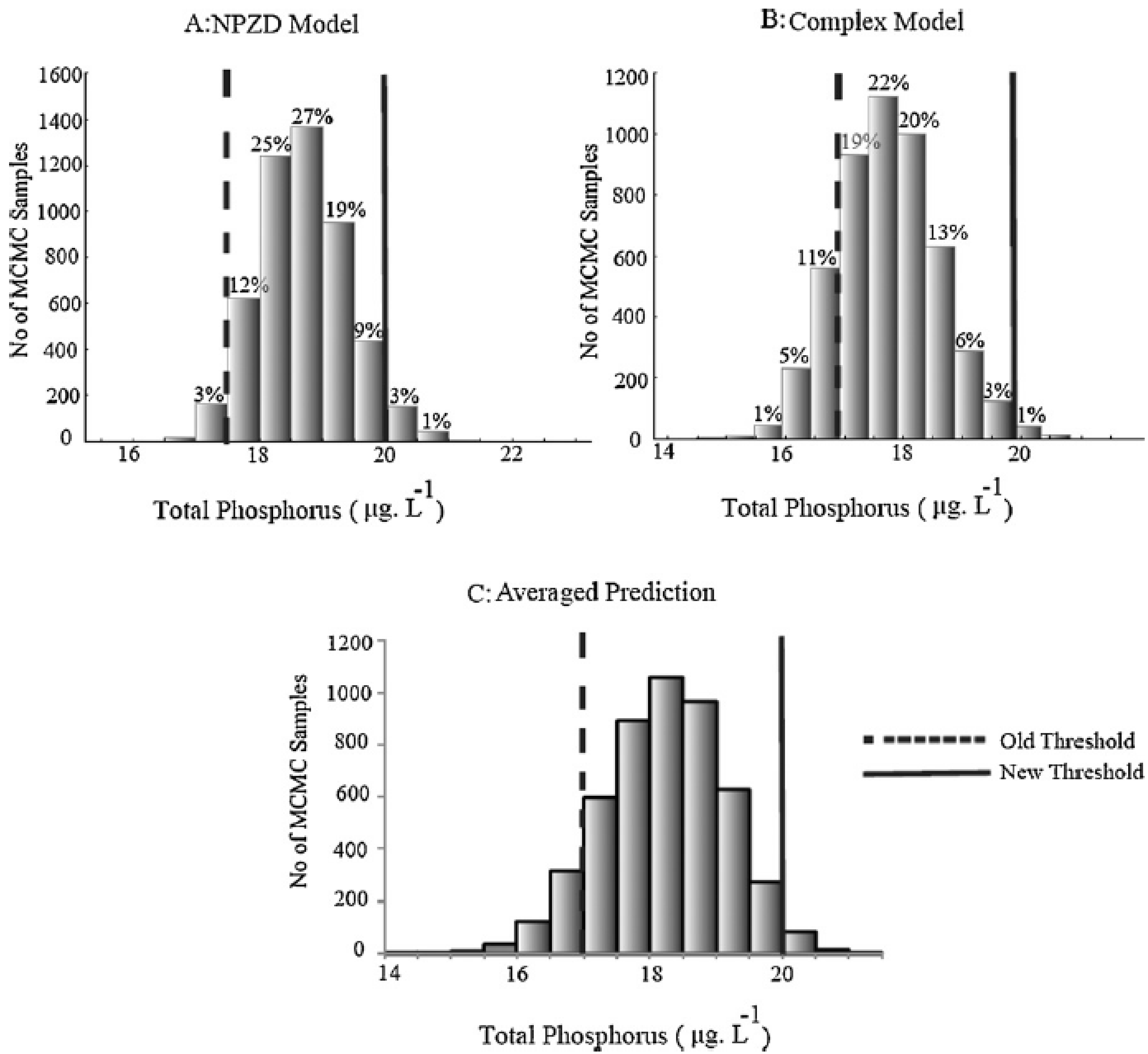


"…Because the goal of predictive limnology is predictive power, its advance is measured by decreased uncertainty of prediction and its controversies are resolved by comparing the ability of alternative approaches and theories to make the required prediction…" R.H. Peters (1986)

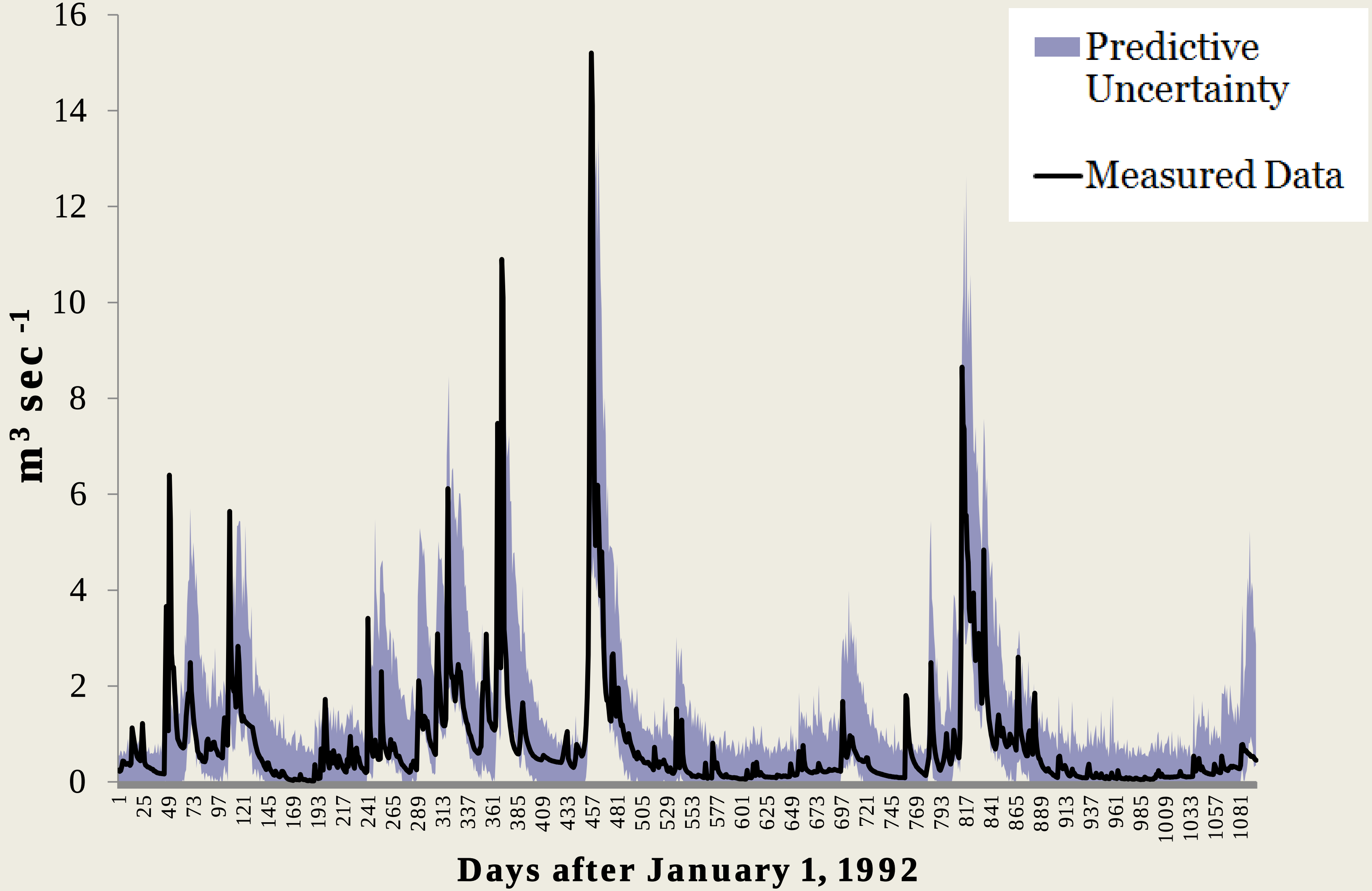
Bayesian Averaging

Simple Model

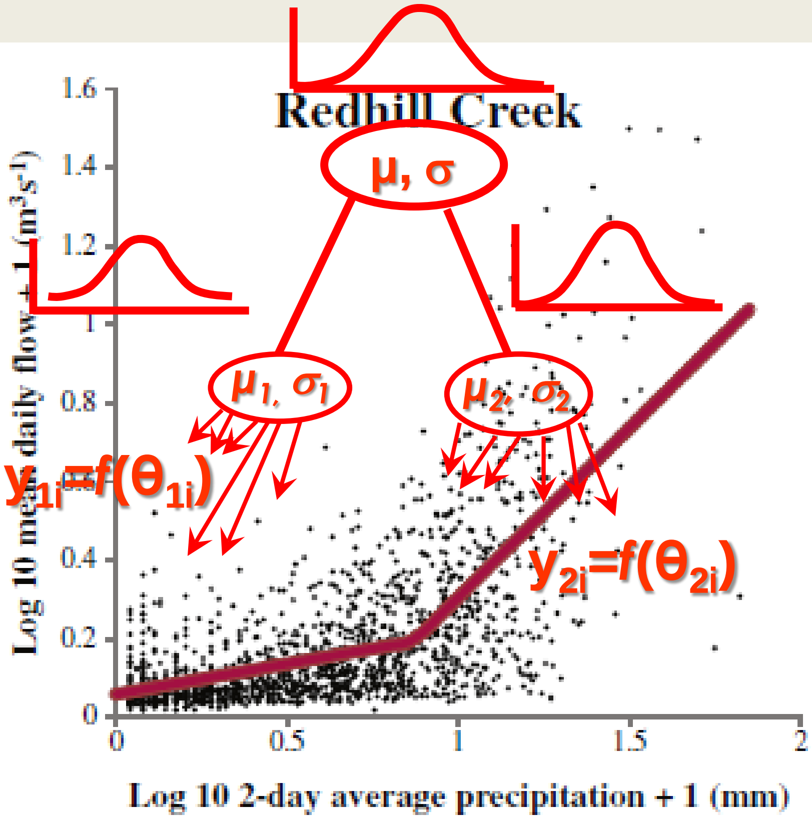



A:NPZD Model
No of MCMC Samples
Total Phosphorus (µg. L-1)
3%
12%
25%
27%
19%
9%
3%
1%
B:Complex Model
1%
5%
11%
19%
22%
20%
13%
6%
3%
1%
C: Averaged Prediction
Old Threshold
New Threshold

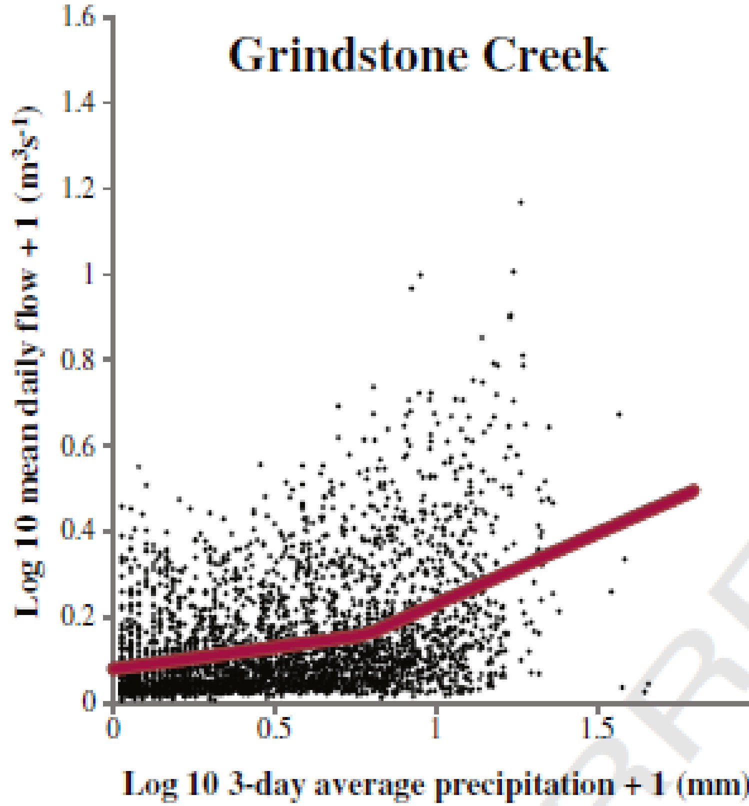
Threshold behaviour



Including Thresholds in Calibration

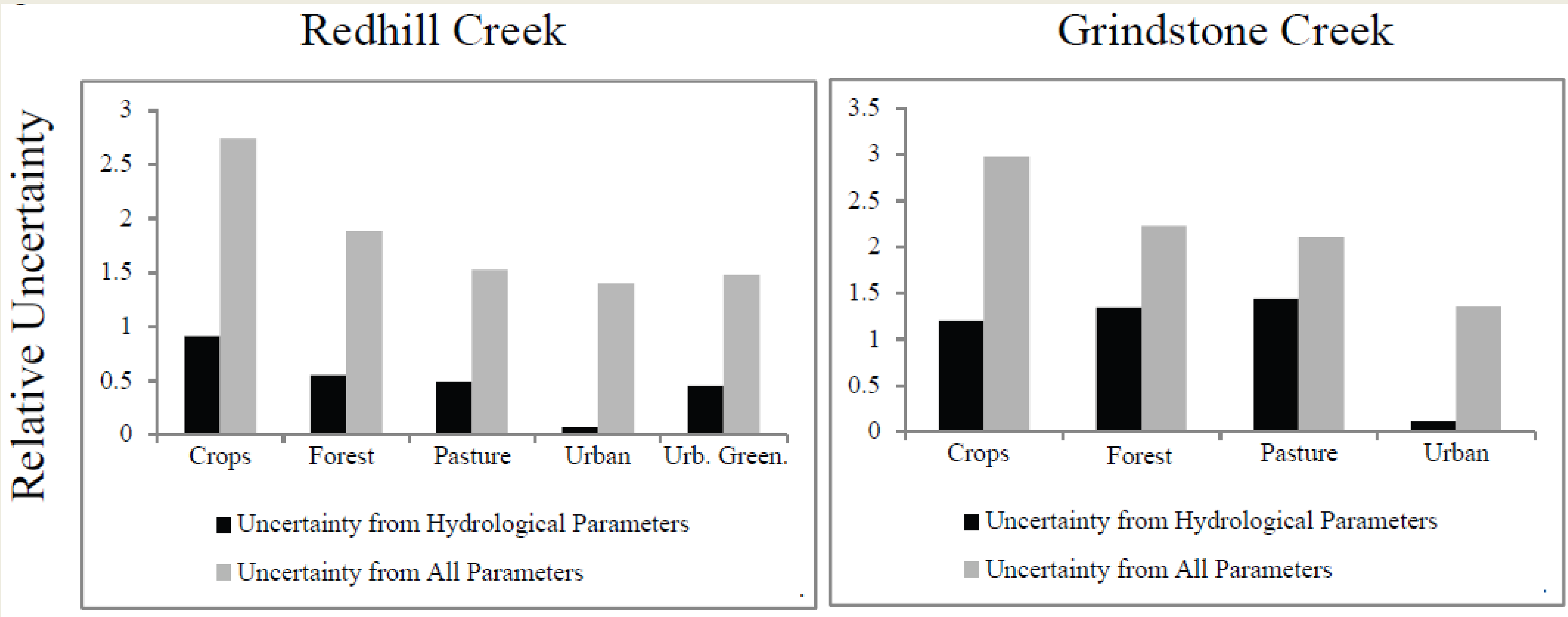


Lower Slope = 0.174 (0.02)
Upper Slope = 1.031 (0.06)
Lower Intercept = 0.20 (0.01)
Changepoint = 0.94 (0.03) = 7.7 (0.6) mm

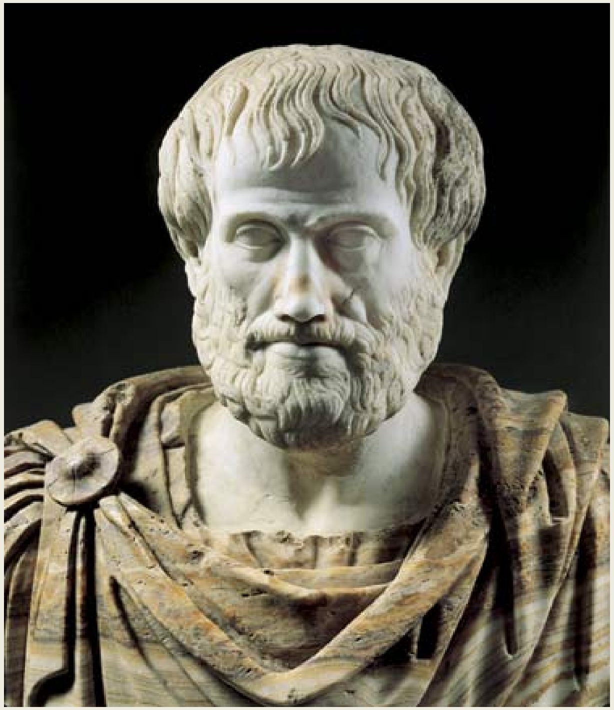


Lower Slope = 0.10 (0.01)
Upper Slope = 0.33 (0.03)
Lower Intercept = 0.16 (0.01)
Changepoint = 0.78 (0.05) = 5.0 (0.6) mm

Where do we go from here?
Improved Uncertainty Characterization



How to Make Environmental Management Decisions in Face of Uncertainty



"The mark of an educated mind is to rest satisfied with the degree of precision which the nature of the problem permits and not seek an exactness where only an approximation is possible."

-Aristotle
(circa 350 BCE)

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Canada

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Canada

Useless Arithmetic? Lessons Learned From Aquatic Biogeochemical Modelling

George Arhonditsis
Ecological Modelling Laboratory
Department of Physical & Environmental Sciences
University of Toronto

Process-Based Modelling

$$\frac{dPO_4}{dt} = -\frac{PO_4}{e+PO_4} a\sigma_{(t)} PHYT\, P/C_{phyto} + \frac{\beta\lambda\left((PHYT \cdot P/C_{phyto})^2 + \omega DET^2\right)}{\mu^2 + (PHYT \cdot P/C_{phyto})^2 + \omega DET^2} \sigma_{(tz)} ZOOP\, P/C_{zoop}$$

$$+\gamma d\sigma_{(tz)} \frac{ZOOP^3}{pred^2 + ZOOP^2} P/C_{zoo} + \phi\sigma_{(t)} DET + k(1-\sigma_{(t)})(PO_{4(hypo)} - PO_4) + PO_{4exog}$$

$$-outflows \cdot PO_4$$

$$\frac{dPHYT}{dt} = \frac{PO_4}{e+PO_4} a\sigma_{(t)} PHYT - r\sigma_{(t)} PHYT - \frac{\lambda(PHYT \cdot P/C_{phyto})^2}{\mu^2 + (PHYT \cdot P/C_{phyto})^2 + \omega DET^2} \sigma_{(tz)} ZOOP$$

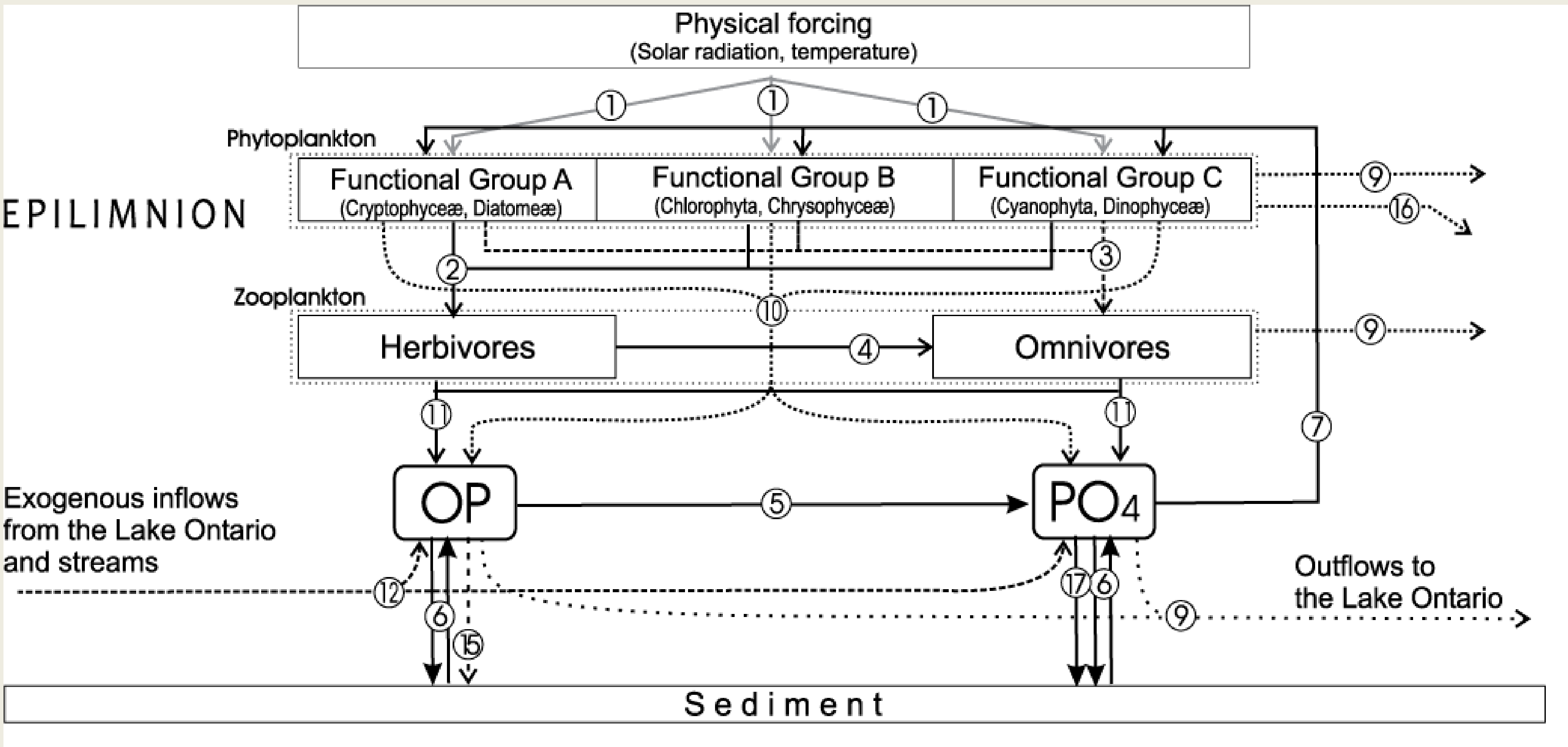
$$-sPHYT - outflows \cdot PHYT$$

$$\frac{dZOOP}{dt} = \frac{\alpha\lambda\left((PHYT \cdot P/C_{phyto})^2 + \omega DET^2\right)}{\mu^2 + (PHYT \cdot P/C_{phyto})^2 + \omega DET^2} \sigma_{(tz)} ZOOP - d\sigma_{(tz)} \frac{ZOOP^3}{pred^2 + ZOOP^2} - outflows \cdot ZOOP$$

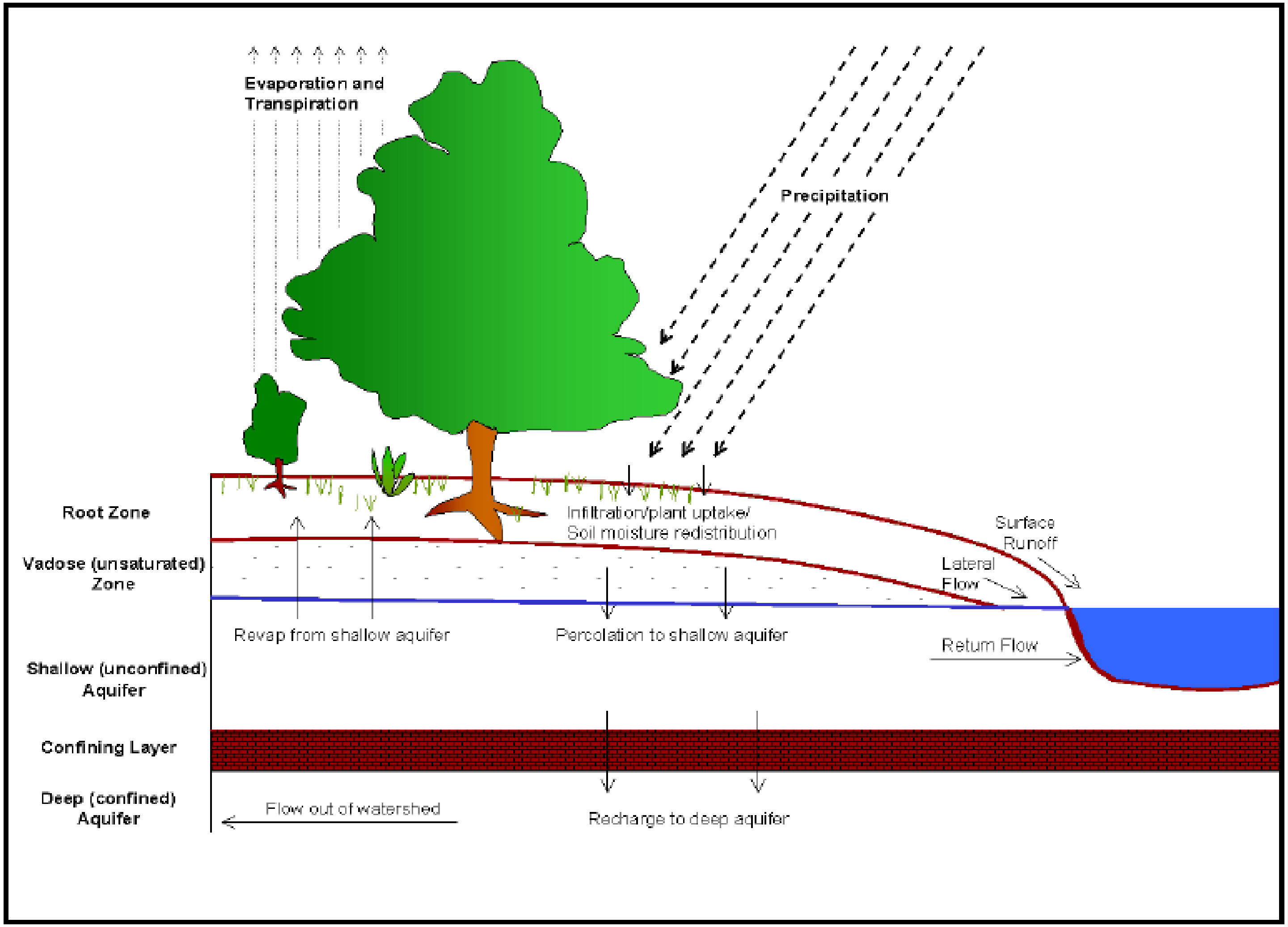
$$\frac{dDET}{dt} = r\sigma_{(t)} PHYT\, P/C_{phyto} + \frac{\left[(1-\alpha-\beta)(PHYT \cdot P/C_{phyto})^2 - (\alpha+\beta)\omega DET^2\right]\lambda}{\mu^2 + (PHYT \cdot P/C_{phyto})^2 + \omega DET^2} \sigma_{(tz)} ZOOP\, P/C_{zoop}$$

$$-\varphi\sigma_{(t)} DET - \psi DET + DET_{exog} - outflows \cdot DET$$

Eutrophication Model



SWAT: A Daily Timescale Model



Models as a Management Tool

ARTICLE

Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences

Naomi Oreskes,* Kristin Shrader-Frechette, Kenneth Belitz

Verification and validation of numerical models of natural systems is impossible. This is because natural systems are never closed and because model results are always non-unique. Models can be confirmed by the demonstration of agreement between observation and prediction, but confirmation is inherently partial. Complete confirmation is logically precluded by the fallacy of affirming the consequent and by incomplete access to natural phenomena. Models can only be evaluated in relative terms, and their predictive value is always open to question. The primary value of models is heuristic.

behavior of the Earth's climate in response to increased CO_2 concentrations; resource estimation models are being used to predict petroleum reserves in ecologically sensitive areas; and hydrological and geochemical models are being used to predict the behavior of toxic and radioactive contaminants in proposed waste disposal sites. Government regulators and agencies may be required by law to establish the trustworthiness of models used to determine policy or to attest to public safety (*1, 2*); scientists may wish to test the veracity of models used in their investigations. As a result, the notion has emerged that numerical models can be "verified" or "validated," and techniques have been developed for this purpose (*1, 3–5*). Claims about verification and validation of model results are now routinely found in

decision-making. However, it is impossible to demonstrate the truth of any proposition, except in a closed system. This conclusion derives directly from the laws of symbolic logic. Given a proposition of the form "p" entails "q," we know that if "p" is true, then "q" is true if and only if the system that this formalism represents is closed.

For example, I say, "If it rains tomorrow, I will stay home and revise this paper." The next day it rains, but you find that I am not home. Your verification has failed. You conclude that my original statement was false. But in fact, it was my intention to stay home and work on my paper. The formulation was a true statement of my intent. Later, you find that I left the house because my mother died, and you realize that my original formulation was not false,

completeness is also introduced when continuum theory is used to represent natural systems. Continuum mechanics necessarily entails a loss of information at the scale lower than the averaging scale. For example, the Darcian velocity of a porous medium is never identical to the velocity structure at the pore scale. Finer scale structure and process are lost from consideration, a loss that is inherent in the continuum mechanics approach.

Another problem arises from the scaling-up of nonadditive properties. The construction of a numerical simulation model of a ground-water flow system involves the specification of input parameters at some chosen scale. Typically, the scale of the model elements is on the order of meters, tens of meters, or kilometers. In contrast,

Models as a Management Tool

Environmental Science & Technology

Critical Review

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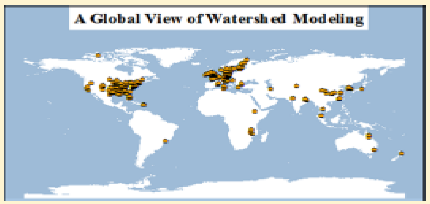
Evaluation of the Current State of Distributed Watershed Nutrient Water Quality Modeling

Christopher Wellen,*[†] Ahmad-Reza Kamran-Disfani, and George B. Arhonditsis

Ecological Modeling Laboratory, Department of Physical & Environmental Sciences, University of Toronto, Toronto, Ontario Canada, M1C 1A4

Supporting Information

ABSTRACT: Watershed models have been widely used for creating the scientific basis for management decisions regarding nonpoint source pollution. In this study, we evaluated the current state of watershed scale, spatially distributed, process-based, water quality modeling of nutrient pollution. Beginning from 1992, the year when Beven and Binley published their seminal paper on uncertainty analysis in hydrological modeling, and ending in 2010, we selected 257 scientific publications which (i) employed spatially distributed modeling approaches at a watershed scale; (ii) provided predictions of flow, nutrient/sediment concentrations or loads; and (iii) reported fit to measured data. Most "best practices" (optimization, validation, sensitivity, and uncertainty analysis) are not consistently employed during model development. There are no statistically significant differences in model performance among land uses. Studies which used more than one point in space to evaluate their distributed models had significantly lower median values of the Nash-Sutcliffe Efficiency (0.70 vs 0.56, $p < 0.005$, nonparametric Mann–Whitney test), and r^2 ($p < 0.005$). This finding suggests that model calibration only to the basin outlet may mask compensation of positive and negative errors of source and transportation processes. We conclude by advocating a number of new directions for distributed watershed modeling, including in-depth uncertainty analysis and the use of additional information, not necessarily related to model end points, to constrain parameter estimation.



1. INTRODUCTION

Watershed models have been extensively used in hydrological science and environmental management research for a number of important tasks, including estimating nonpoint source pollutant inputs to receiving waterbodies and their source areas and predicting the effects of climate and land-use change on water quality.[1] Extensive research has focused on augmenting the mechanistic foundation of these watershed models and making them spatially distributed. Spatially distributed models disaggregate watersheds into multiple discrete units to represent the spatial variability of parameters and inputs.[2] However, the adequacy of earth science models for informing decision making has been questioned.[3,4] Concerns of overparameterization and equifinality have brought to the forefront of modeling efforts the development of methodologies that will obtain "the right answers for the right reasons".[5,6] Distributed, process-based models remain key tools for understanding and managing nonpoint source pollutants and the effects of land use change.[7,8,1,9] Models focused on nutrient pollution have a very long history of development and application for the purposes of management and policy, and form the focus of this paper.[2]

The documented inadequacy of many models to address important societal issues has frequently been attributed to the fact that the field has advanced without the healthy dose of introspection required to obtain good science.[3,4] For example, little work has quantitatively examined the practices of process-based watershed modeling. It is unknown to what extent "best practices" of model application are followed. While there are conventional recommendations of how "accurate" a model should be,[10] there is no sense of how well the existing class of distributed, process-based models performs across a variety of state variables, and how model development affects performance.

In this paper we quantitatively evaluate the state of distributed, process-based watershed models. We assess performance of a number of state variables associated with nutrient pollution and quantify how performance varies with model development. We also assess how often best model development practices are followed. This paper compliments more comparative, review-type approaches,[2,11] and aims to lead to concrete recommendations for the advancement of the field as a whole.

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Review

Phytoplankton functional type modelling: Running before we can walk? A critical evaluation of the current state of knowledge

Yuko Shimoda, George B. Arhonditsis*

Ecological Modelling Laboratory, Department of Physical & Environmental Sciences, University of Toronto, Toronto, Ontario, Canada M1C 1A4

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ABSTRACT

In the context of aquatic biogeochemical modelling, there is an increasing pressure to explicitly treat multiple biogeochemical cycles and to increase the functional diversity of biotic communities. In this study, we evaluate the capacity of 124 aquatic biogeochemical models to reproduce the dynamics of phytoplankton functional groups. Our analysis reinforces earlier findings that aquatic ecosystem modellers do not seem to consistently apply conventional methodological steps during the development of their models. Although there is an improvement relative to earlier critiques, significant portion of published studies did not properly assess model sensitivity to input vectors; aquatic ecosystem modellers are still reluctant to embrace optimization techniques during model calibration; and assess the ability of their models to support predictions in the extrapolation domain. We also found significant variability with respect to the mathematical representation of key physiological processes (e.g., growth strategies, nutrient kinetics, settling velocities) as well as group-specific characterizations typically considered in the pertinent literature. Cyanobacteria blooms are a major concern for water industries as they represent high risk for human health and economic costs for drinking water treatment, and thus one of the outstanding challenges is to offer credible modelling tools that can serve as early warning systems to assist with the operational control of cyanobacteria blooms. Our study suggests that the derivation of distinct functional groups from fairly heterogeneous planktonic assemblages poses challenging problems. Because of the still poorly understood ecology, we do not have robust group-specific parameterizations that can support predictions in a wide array of spatiotemporal domains. In this context, we argue that the most prudent strategies are the gradual incorporation of complexity, where possible and relevant, along with an open dialogue on how we can mathematically depict the interconnections among different phytoplankton subunits or even how we can frame the suitable data collection efforts.

Contents

* Corresponding author. Tel.: +1 416 208 4858; fax: +1 416 287 7279.
E-mail address: georgea@utsc.utoronto.ca (G.B. Arhonditsis).

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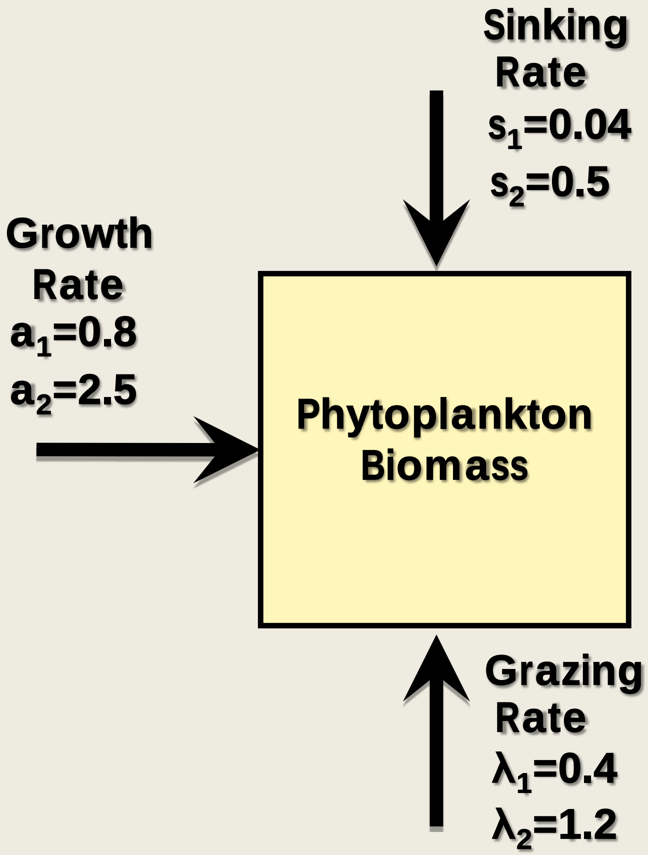
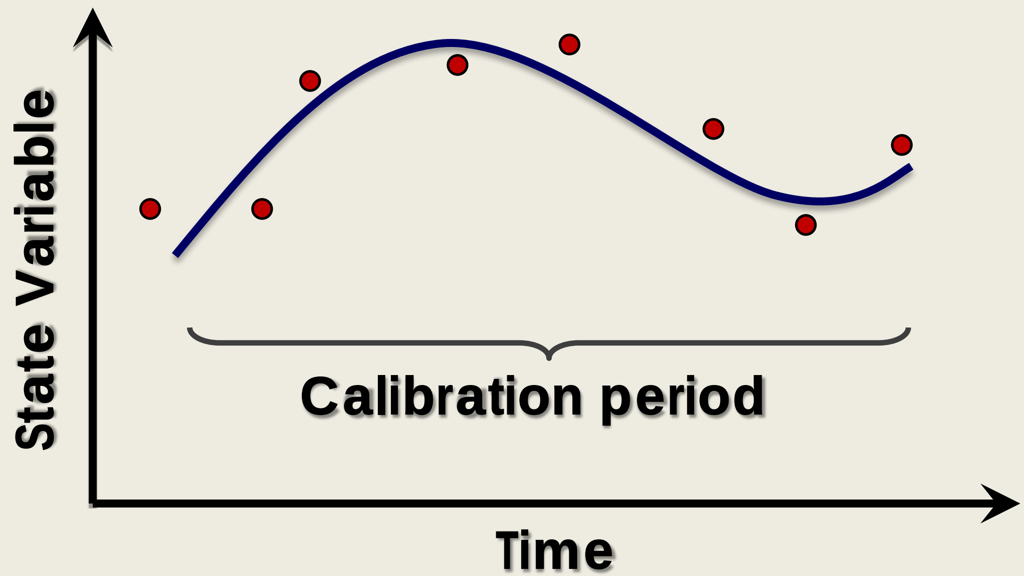
0304-3800/

Criticisms

1. Failure to explicitly account for the uncertainty associated with any modelling exercise!!
2. Failure to recognize that the typically used complex mathematical models are overparameterized!!

“Good results for the wrong reasons”





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