Bayesian Uncertainty Quantification in SPARROW Models

Richard B. Alexander

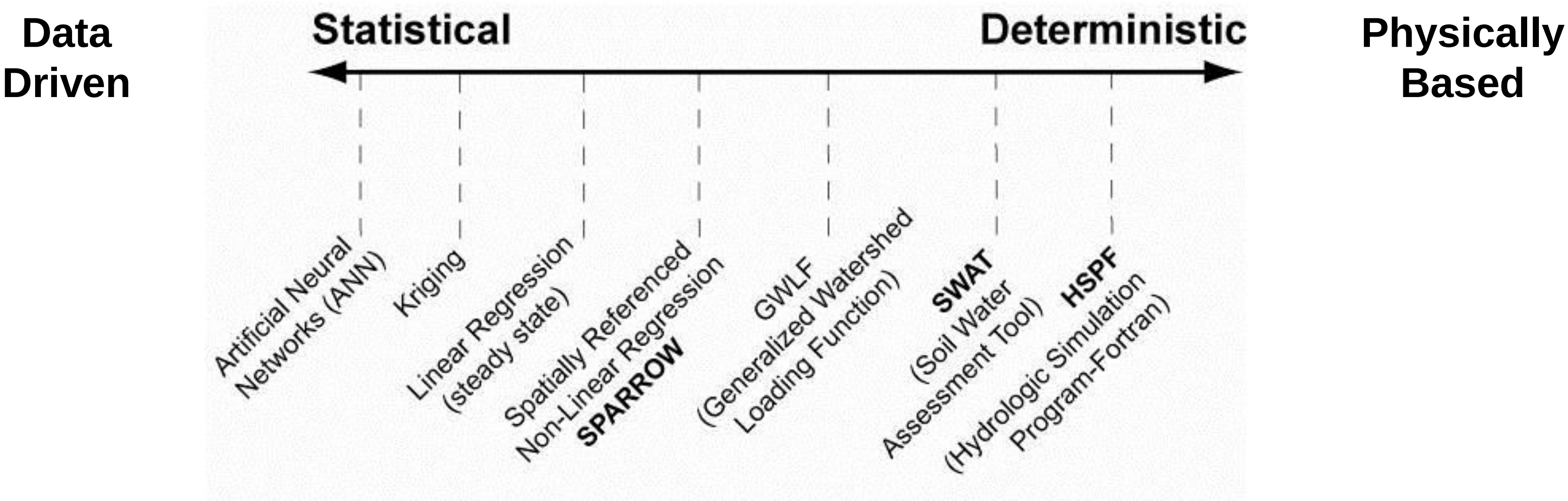
National Water Quality Assessment Project
U.S. Geological Survey
Reston, VA

Chesapeake Bay STAC, Assessing Uncertainty Workshop, February 1-2, 2016

Presentation Topics

- Motivation for investigating uncertainties in watershed models
- Overview of SPARROW modeling: characteristics, capabilities, and uncertainties (statistical, physical)
- Bayesian refinements to SPARROW model estimation and uncertainties:
  - Hierarchical Bayesian methods – a comprehensive tool for uncertainty quantification
  - Summary of key results from national and regional applications
- Concluding remarks

Watershed Modeling Continuum

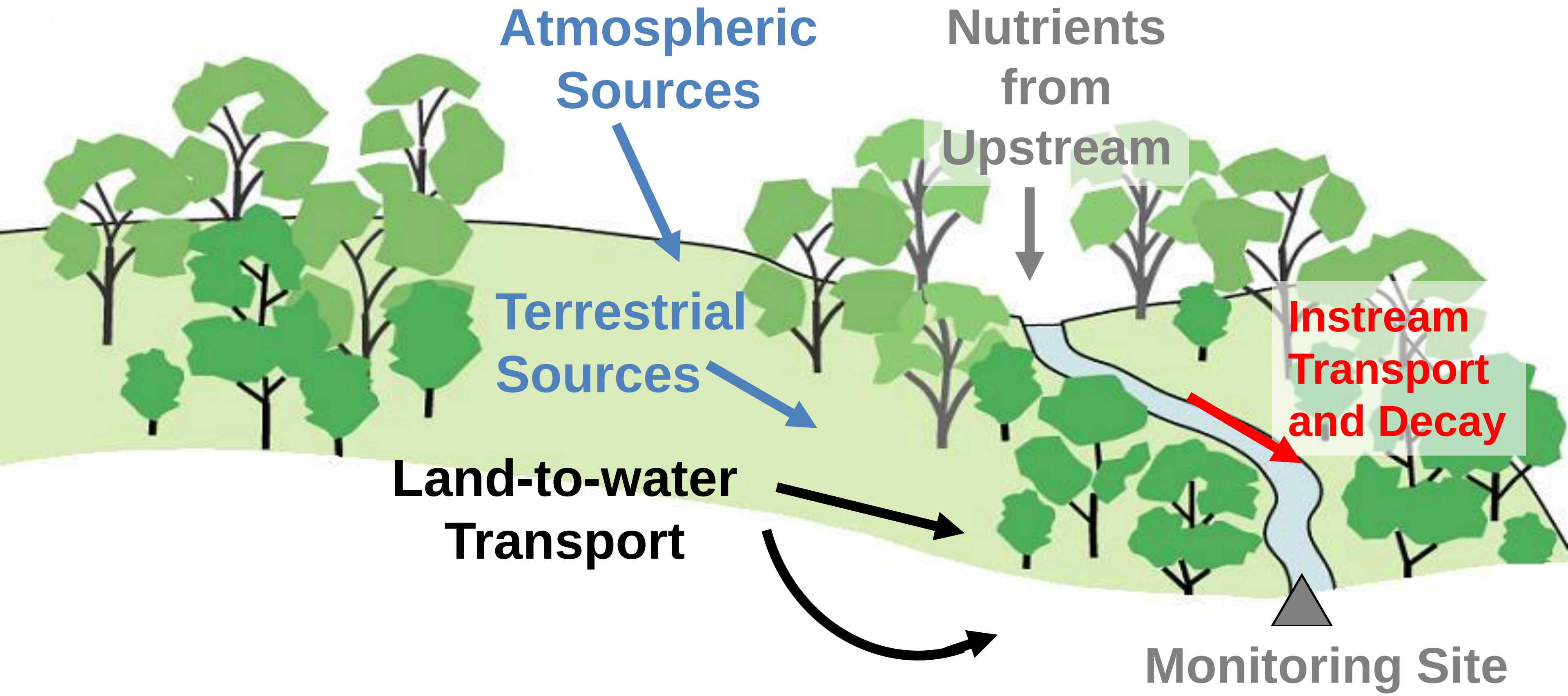


Optimal fit to data, but limited process understanding

Complexity (process interpretability), but possible over-specification and parameter non-uniqueness

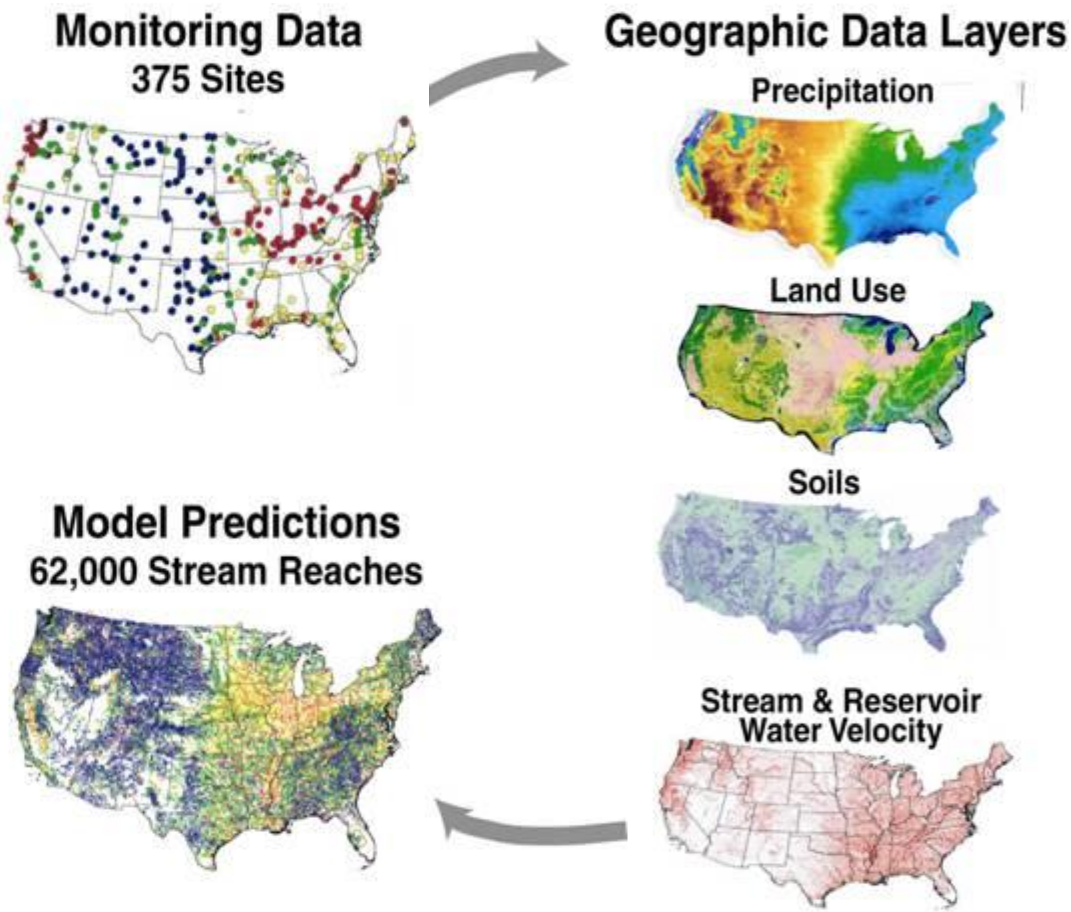
SPARROW uses a hybrid statistical and parsimonious mechanistic based structure with optimization to select the most feasible parameter distributions

SPARROW Conceptual Model



USGS SPARROW Water-Quality Model

SPAtially Referenced Regression on Watershed Attributes (Smith et al., 1997)

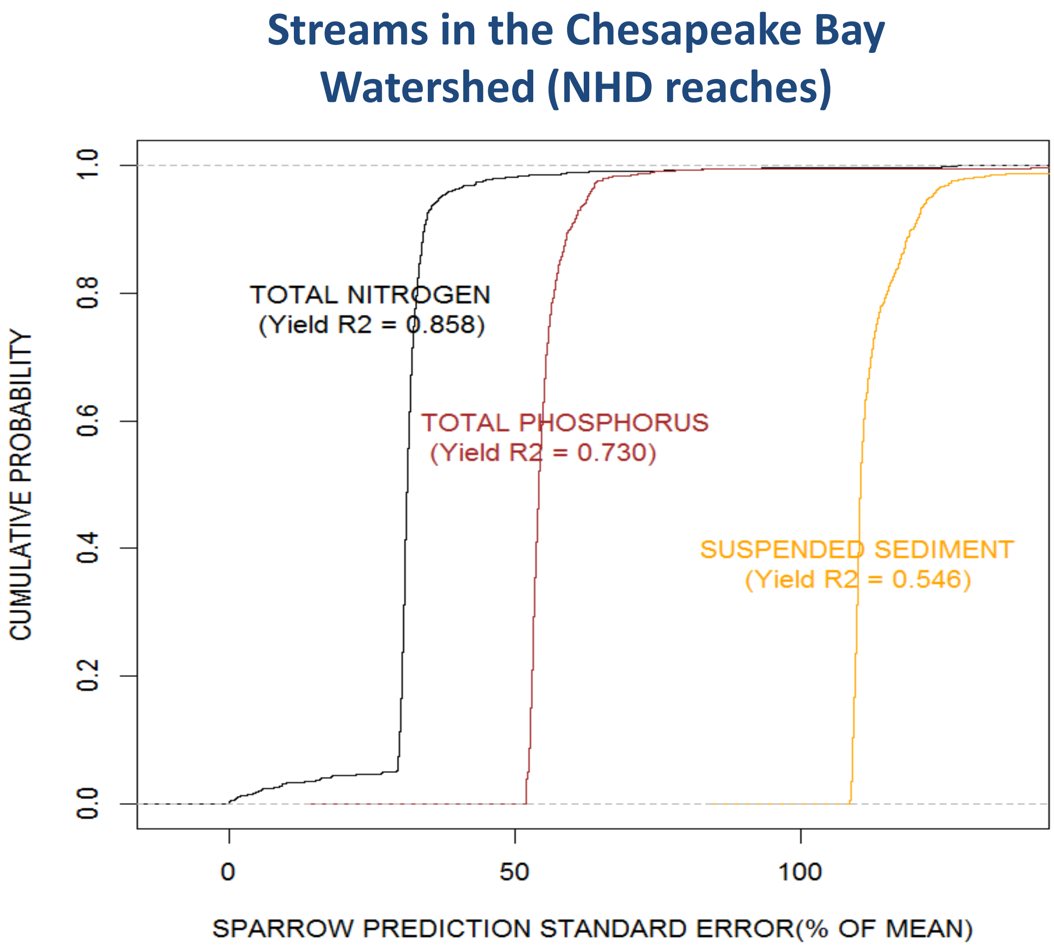


Home page: http://water.usgs.gov/nawqa/sparrow

Mechanistic and statistical features improve model interpretability and prediction accuracy:

- Non-linear structure
- Mass-balance constraints
- Non-conservative transport
- Parameter estimation using least squares optimization
- Steady state; normalization for natural variability (streamflow) and trends in WQ (base year adj.)
- Diagnostics (RMSE, statistical sig., bias/precision, sensitivities, validation)
- Prediction uncertainties:
  - reflect parameter and model errors
  - assumes an accurate model specification and constant model error variance
  - quantified via bootstrapping

SPARROW Load Prediction Uncertainties
Based on Bootstrapping Methods

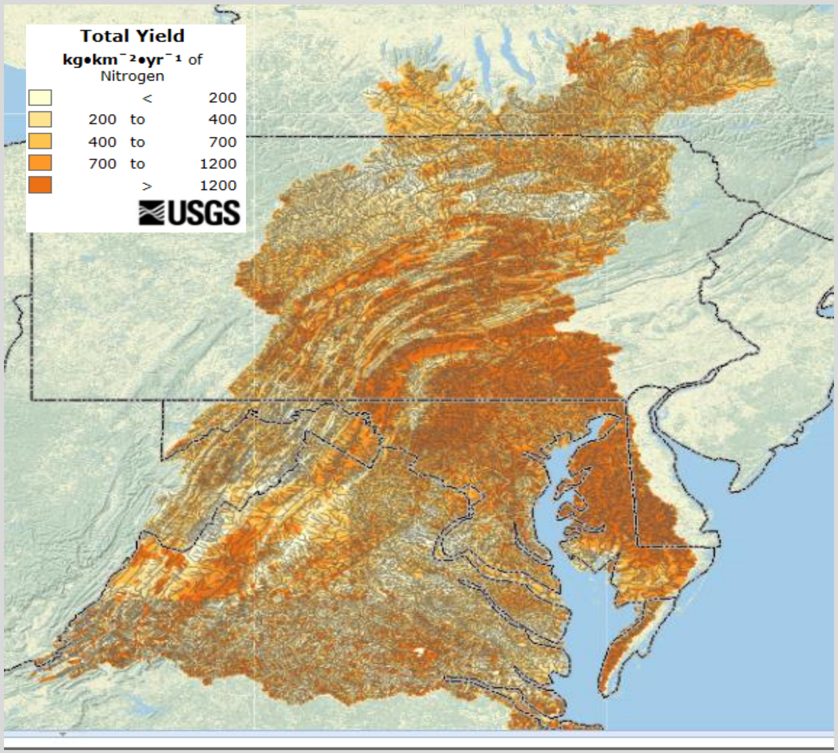


TN: 13 parms.
TP: 11 parms.
Sediment: 7 parms.

Ator et al. 2011 (nitrogen, phosphorus); J. Brakebill, USGS, 2015 (sediment; unpublished model)

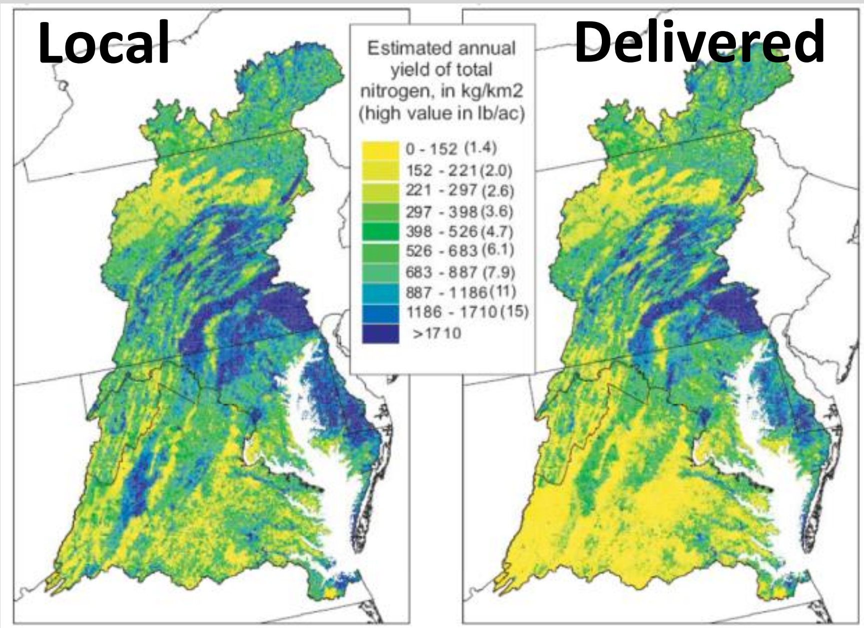
How SPARROW Models Can Inform Nutrient Management Decisions

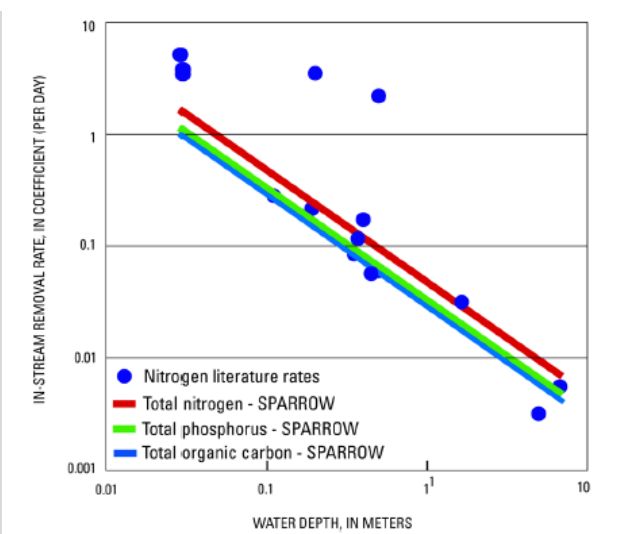
Total Nitrogen



- Predict mean-annual flux, yield and concentration for unmonitored streams
- Predict contaminant flux to downstream receiving waters such as estuaries
- Apportion stream loads to major nutrient sources and upstream watersheds
- Provide a framework for prioritizing areas for management actions; inform mechanistic modeling (e.g., SWAT, CB Phase 6)
- Evaluate the potential effects of landscape change and management scenarios on water quality

How SPARROW Models Can Inform Nutrient Management Decisions

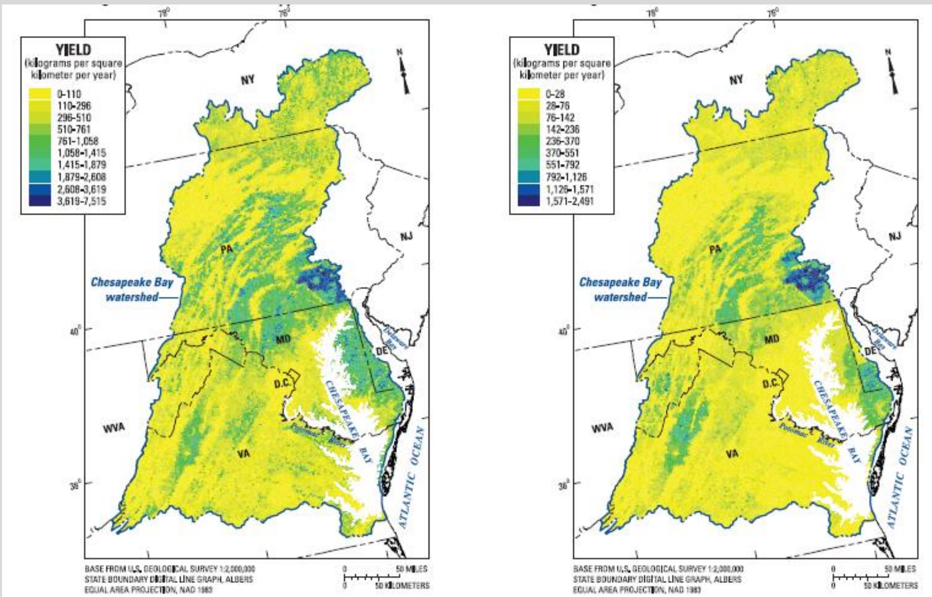


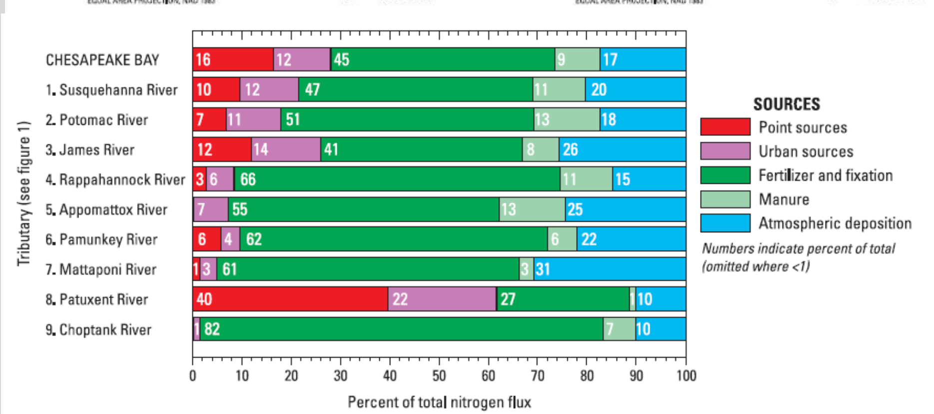


- Predict mean-annual flux, yield and concentration for unmonitored streams
- Predict contaminant flux to downstream receiving waters such as estuaries
- Apportion stream loads to major nutrient sources and upstream watersheds
- Provide a framework for prioritizing areas for management actions; inform mechanistic modeling (e.g., SWAT, CB Phase 6)
- Evaluate the potential effects of landscape change and management scenarios on water quality

How SPARROW Models Can Inform Nutrient Management Decisions

Nitrogen Fertilizer and Fixation | **Manure Nitrogen**

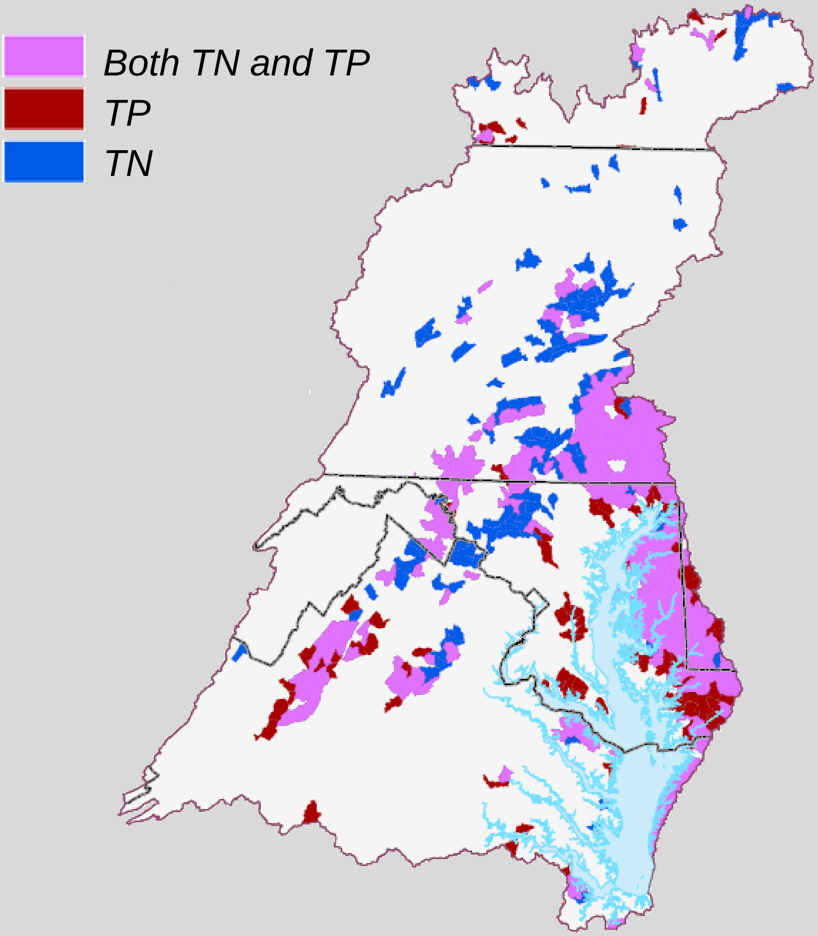




- Predict mean-annual flux, yield and concentration for unmonitored streams
- Predict contaminant flux to downstream receiving waters such as estuaries
- Apportion stream loads to major nutrient sources and upstream watersheds
- Provide a framework for prioritizing areas for management actions; inform mechanistic modeling (e.g., SWAT, CB Phase 6)
- Evaluate the potential effects of landscape change and management scenarios on water quality

How SPARROW Models Can Inform Nutrient Management Decisions

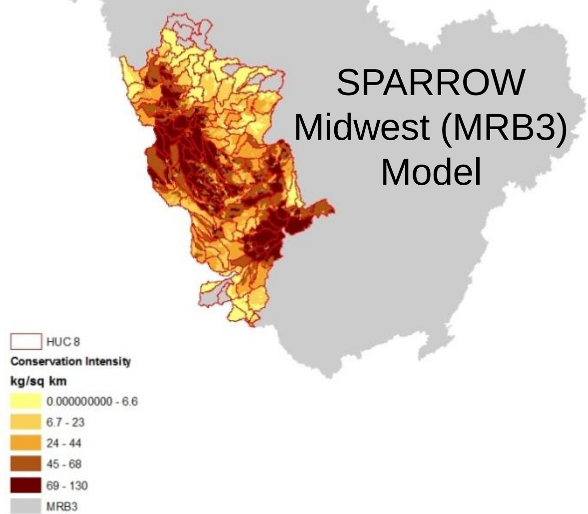
Chesapeake Bay Priority Agricultural Watersheds



- Predict mean-annual flux, yield and concentration for unmonitored streams
- Predict contaminant flux to downstream receiving waters such as estuaries
- Apportion stream loads to major nutrient sources and upstream watersheds
- Provide a framework for prioritizing areas for management actions; inform mechanistic modeling (e.g., SWAT, CB Phase 6)
- Evaluate the potential effects of landscape change and management scenarios on water quality

Uncertainties over Stream Nutrient Response to Agricultural Management

USDA APEX Measure of Conservation Intensity

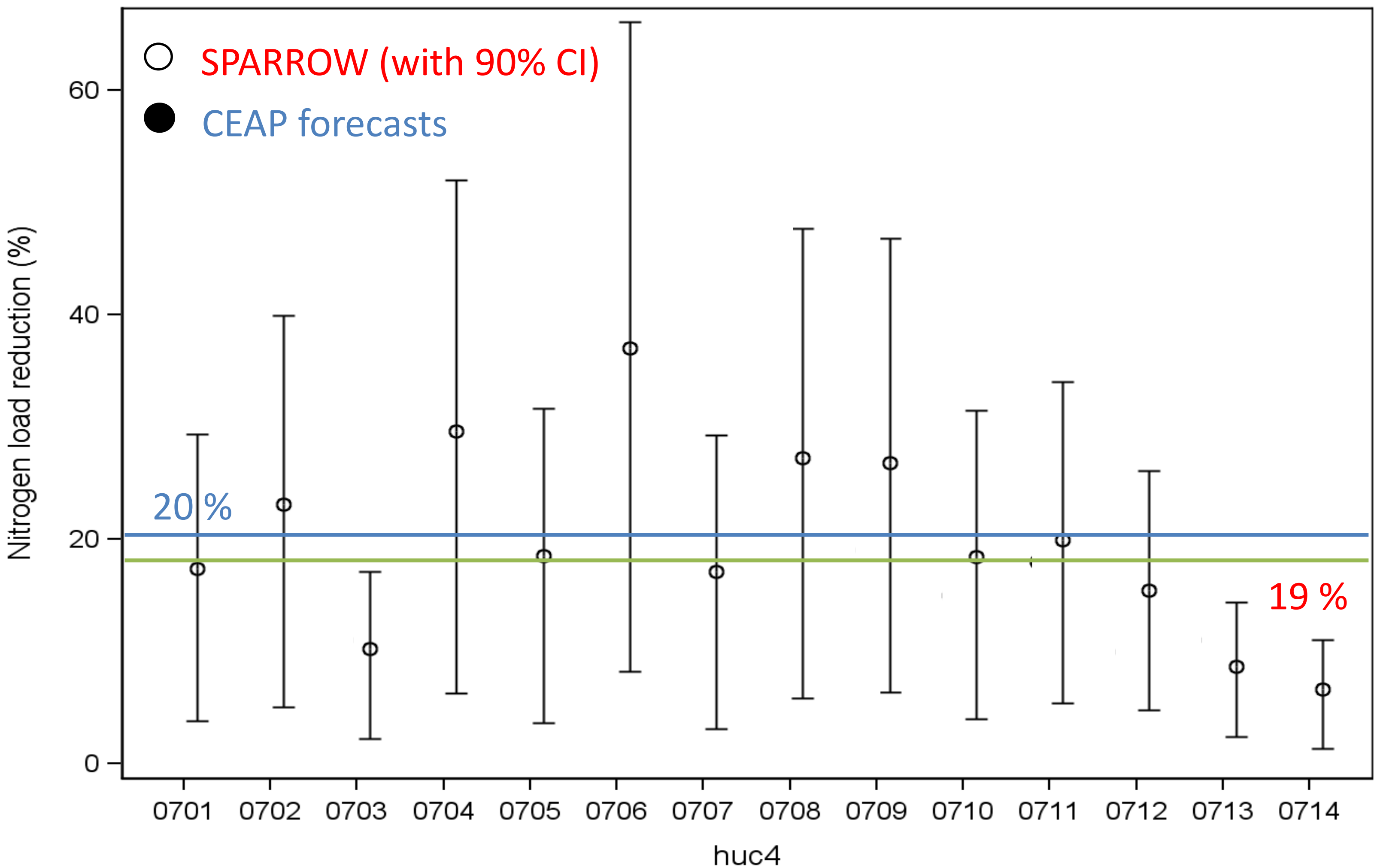


USGS and USDA (ARS, NRCS) collaborative study in the Upper Mississippi basin

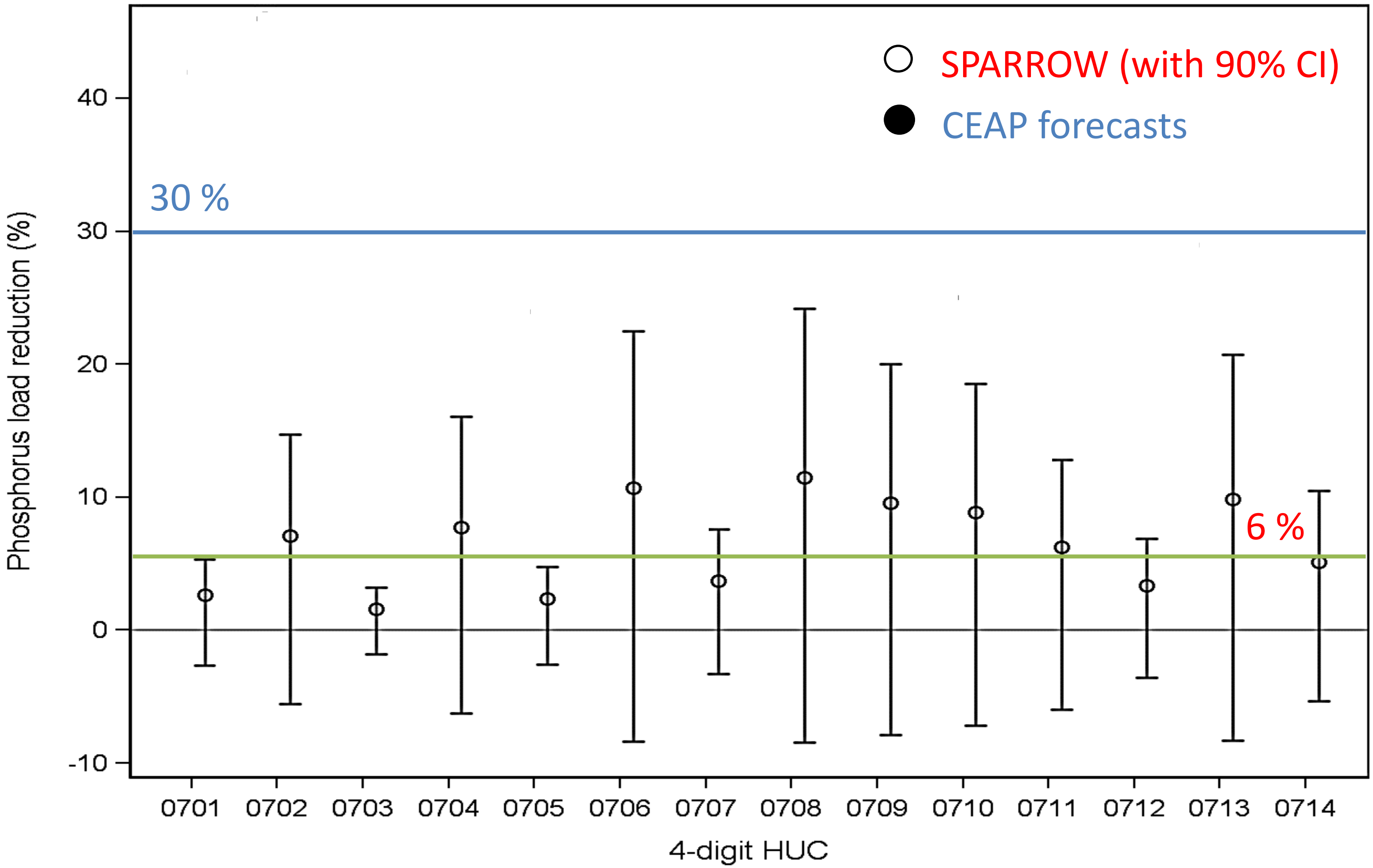
- SPARROW was sequentially coupled with the field-scale APEX model
- APEX predicts "technologically feasible" effects of conservation practices (primarily structural soil/erosion management) on farm runoff
- SPARROW estimates response of stream nutrient loads to spatial variability in conservation intensity (land-to-water factor)
- Study provides an empirical evaluation that employs space for time substitution
- Results are complementary to the USDA simulation (forecasting) measures of conservation effects

Garcia et al. in review

Total Nitrogen reductions associated with conservation: HUC-4 watersheds in Upper Mississippi River Basin



Total Phosphorus reductions associated with conservation: HUC-4 watersheds in Upper Mississippi River Basin



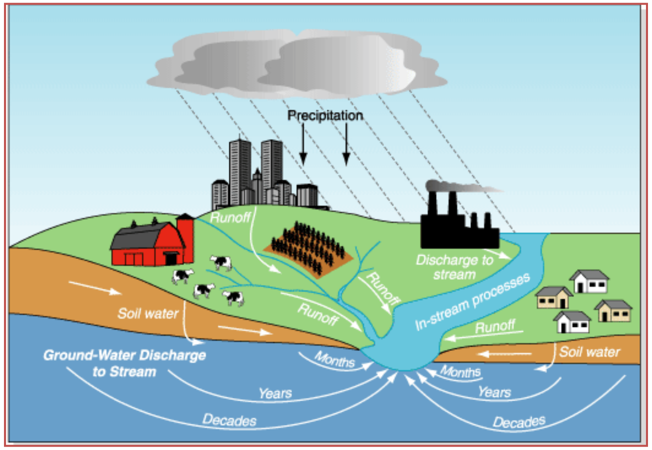
Conclusions – Upper Mississippi Basin APEX-SPARROW Modeling of Conservation Effects

- Physical/chemical contrasts in nutrients serve as key hypotheses
- Nitrogen:
  - Conservation expected to cause greater hydraulic storage, with subsequent higher denitrification (and leaching to groundwater)
  - Greater N mobility: solubility and tile drains accentuate response
- Phosphorus:
  - Results may suggest a slower response (more time required); observed response differs from "technologically feasible" APEX forecasts that simulate immediate and sustained reductions
    - Expected delays in particulate P transport
  - Confounding effects of increased soluble P associated with conservation (growing body of research)
- Study gives limited empirical evidence of regional-scale conservation effects, but with large uncertainties (statistical and physical)
- Application of coupled APEX-SPARROW models needed for other environmental settings (e.g., Chesapeake Bay)

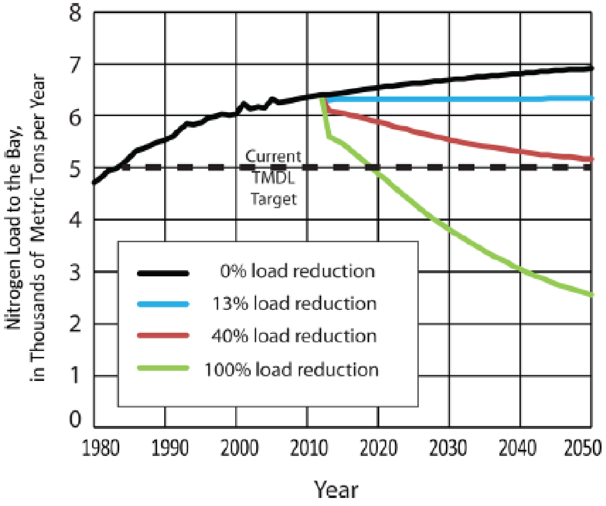
Uncertainties in Nutrient Transport and Stream Response to Management

- What are the effects of ground water residence times on stream response to management?
- Sanford and Pope, 2013: N mass balance regression model coupled with groundwater model and historical source data for Delmarva
- USGS research by Smith and others (Potomac):
  - Groundwater MODFLOW lumped parameter model of water age-distribution and historical sources projects N inputs to dynamic seasonal base-flow SPARROW (obtain GW source attenuation for streams)
  - Contemporaneous sources and predicted base-flow loads input to SPARROW dynamic seasonal model of total loads
  - Potomac lags times are significantly shorter than for Delmarva
  - Lags in mean seasonal stream N response to simulated abrupt cutoff in sources: ~2 years for carbonate-dominated catchments and >7 years for non-carbonate catchments

Chesapeake Bay Watershed Coastal Plain (Sanford and Pope, ES&T, 2013)



Projected Coastal Plain N response to load reductions



Motivation for Bayesian Methods

(1) Improved accuracy of the model parameters and predictions

- **Coefficients and model-error variance** treated as **random variables** that vary over space (time); conventional treatment as fixed quantities over modeled domain
- Consistent with coefficients represented as “effective” conceptual quantities that are not directly measurable

(2) Improved quantification of the sources of uncertainties (parameters, model errors, and observations)

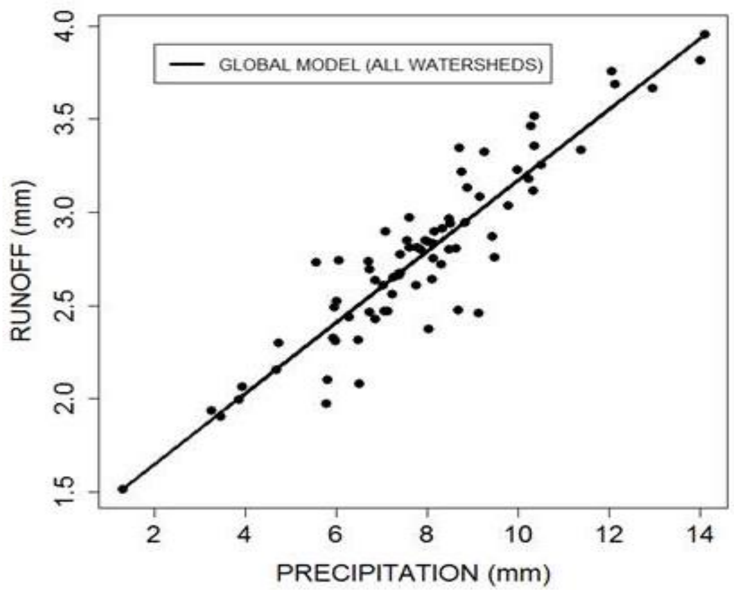
- Allows the latent conditions (model inputs/outputs) to be inferred
- Provides a more precise specification of SPARROW uncertainties

Hierarchical Bayesian *– multi-level structure for the SPARROW equations*

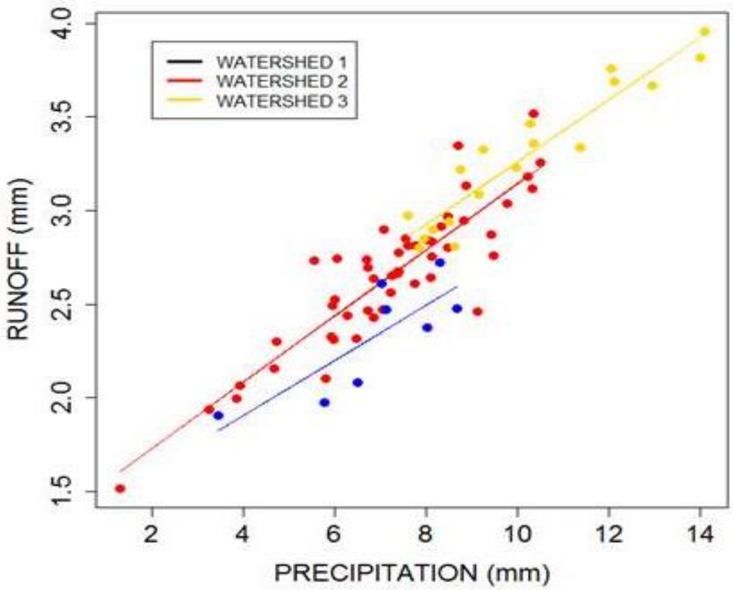
- *Separate model of the parameters (process components) nested within a model of the observations*
- *Multi-level applies to model coefficients and model error variance*

Hierarchical Bayesian: Improved accuracy of model parameters and predictions

Universal multi-watershed model on pooled data



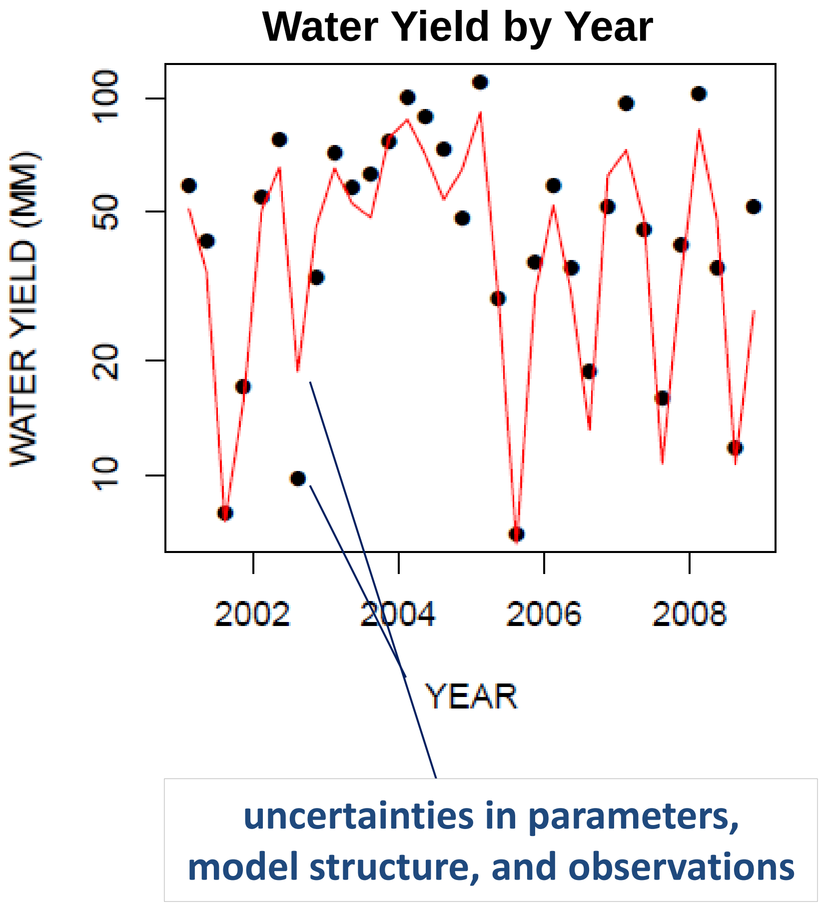
Watershed-specific models on un-pooled data



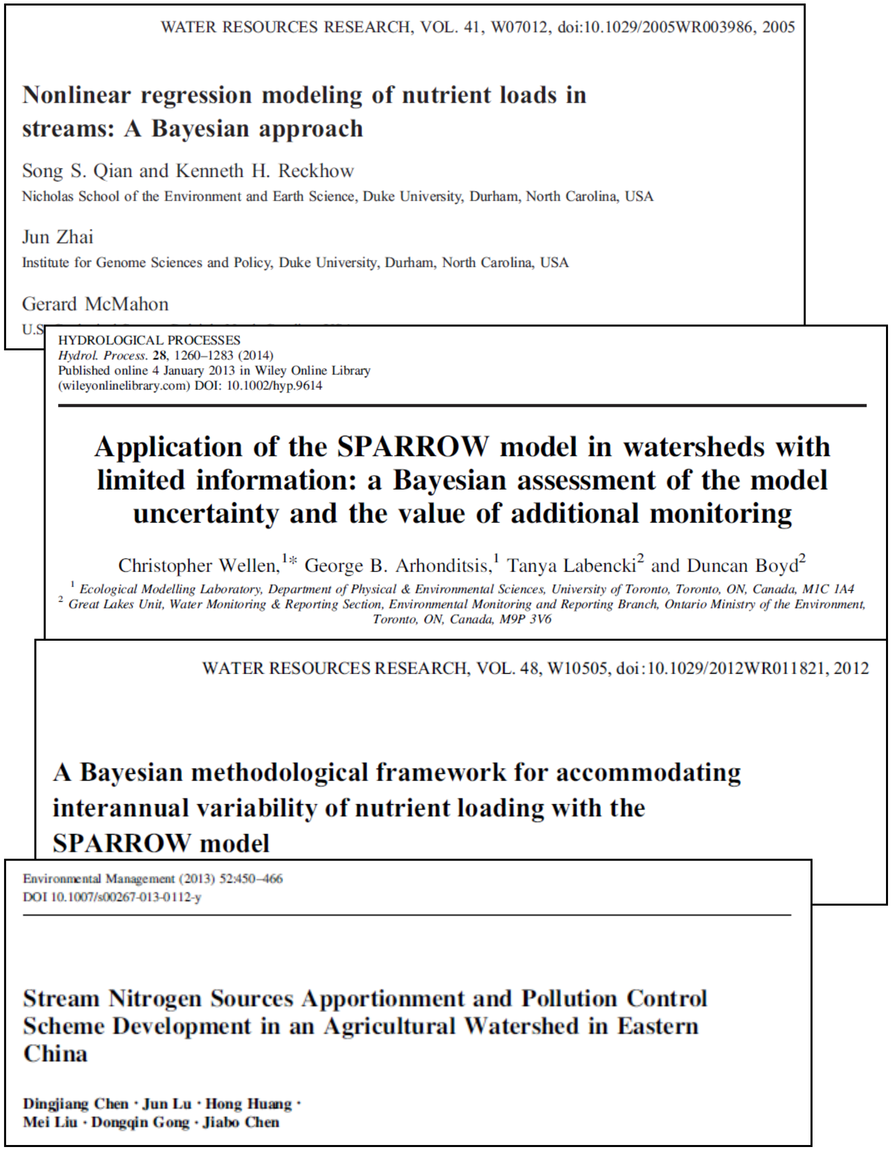
- Methods promote data sharing across watersheds: parameters are weighted combination of two competing models
- Model parameters vary over space (time): **increased sensitivity to "local" process controls and more accurate predictions (less biased, more precise)**

Hierarchical Bayesian: State-space methods unravel uncertainties related to model structure and observations

- Applicable to spatial networks and dynamic systems (recursive structures)
- Quantify latent "true" states (model output) over space and time
- Nested model structure separates model uncertainties by space and time
  - Model of the deterministic structure and residual process variability (incremental reach catchments)
  - Model of the observations and associated measurement errors (e.g., sampling errors)
- Propagate the process variability in the river network (exclude measurement errors)



Hierarchical Bayesian SPARROW Modeling



WATER RESOURCES RESEARCH, VOL. 41, W07012, doi:10.1029/2005WR003986, 2005

Nonlinear regression modeling of nutrient loads in streams: A Bayesian approach

Song S. Qian and Kenneth H. Reckhow
Nicholas School of the Environment and Earth Science, Duke University, Durham, North Carolina, USA

Jun Zhai
Institute for Genome Sciences and Policy, Duke University, Durham, North Carolina, USA

Gerard McMahon

HYDROLOGICAL PROCESSES
Hydrol. Process. **28**, 1260–1283 (2014)
Published online 4 January 2013 in Wiley Online Library
(wileyonlinelibrary.com) DOI: 10.1002/hyp.9614

Application of the SPARROW model in watersheds with limited information: a Bayesian assessment of the model uncertainty and the value of additional monitoring

Christopher Wellen,[1*] George B. Arhonditsis,[1] Tanya Labencki[2] and Duncan Boyd[2]
[1] *Ecological Modelling Laboratory, Department of Physical & Environmental Sciences, University of Toronto, Toronto, ON, Canada, M1C 1A4*
[2] *Great Lakes Unit, Water Monitoring & Reporting Section, Environmental Monitoring and Reporting Branch, Ontario Ministry of the Environment, Toronto, ON, Canada, M9P 3V6*

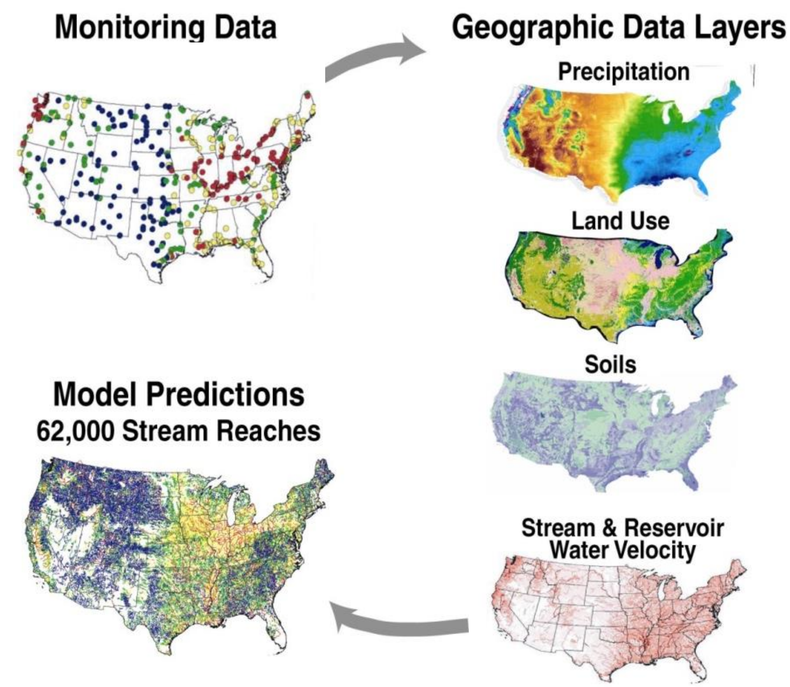
WATER RESOURCES RESEARCH, VOL. 48, W10505, doi:10.1029/2012WR011821, 2012

A Bayesian methodological framework for accommodating interannual variability of nutrient loading with the SPARROW model

Environmental Management (2013) 52:450–466
DOI 10.1007/s00267-013-0112-y

Stream Nitrogen Sources Apportionment and Pollution Control Scheme Development in an Agricultural Watershed in Eastern China

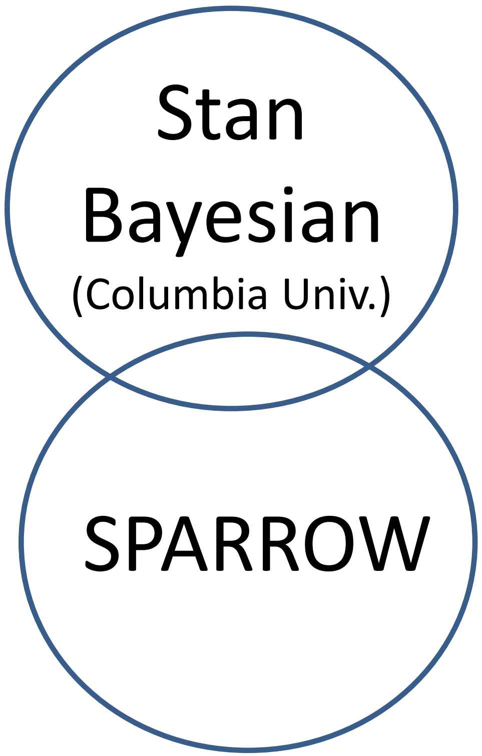
Dingjiang Chen · Jun Lu · Hong Huang ·
Mei Liu · Dongqin Gong · Jiabo Chen



Limitations of Bayesian studies:

- Small catchments with little diversity; few systematic comparisons of all hierarchical structures
- Used an earlier generation of Bayesian methods

A New-Generation Bayesian Method

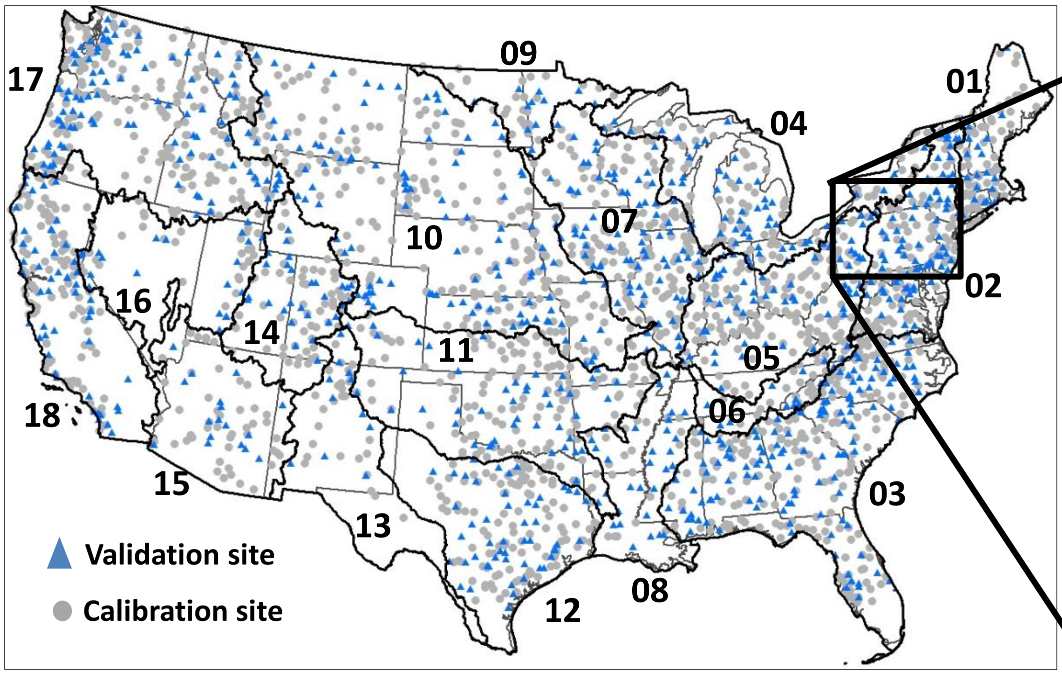


- Stan ~10x faster than previous generation
- Hamiltonian Monte Carlo (HMC) – more efficient and robust; improved sampling of parameter distributions
- C++ imperative language (order matters) well suited for coding hydrological process features (and existing code)
- Automated version developed for SPARROW (SPARROW-R)

SPARROW Hierachical Bayesian Streamflow Models

Mean Annual Streamflow (1997-2007)

1:500,000 RF1 streams (18 HUC-2 regions)

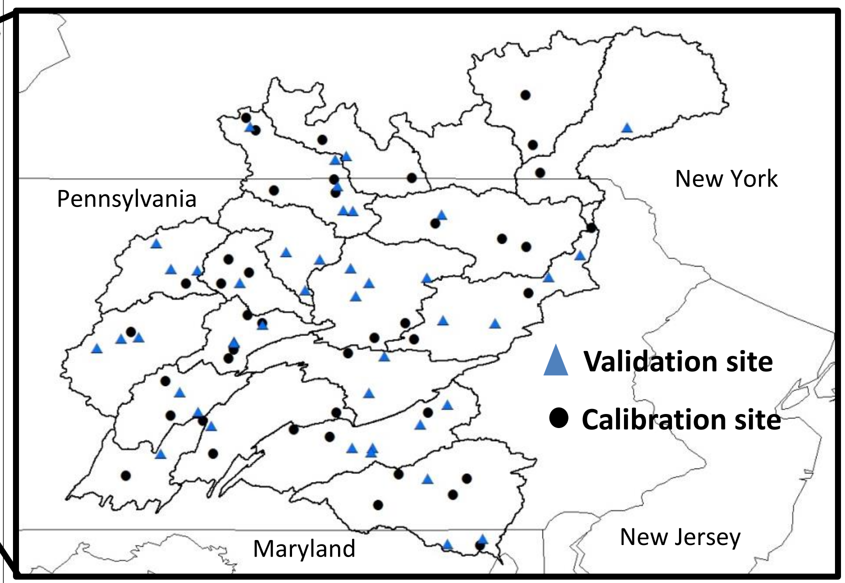


Susquehanna River Basin

Mean Seasonal Streamflow, 2001-08

1:100,000 NHD streams

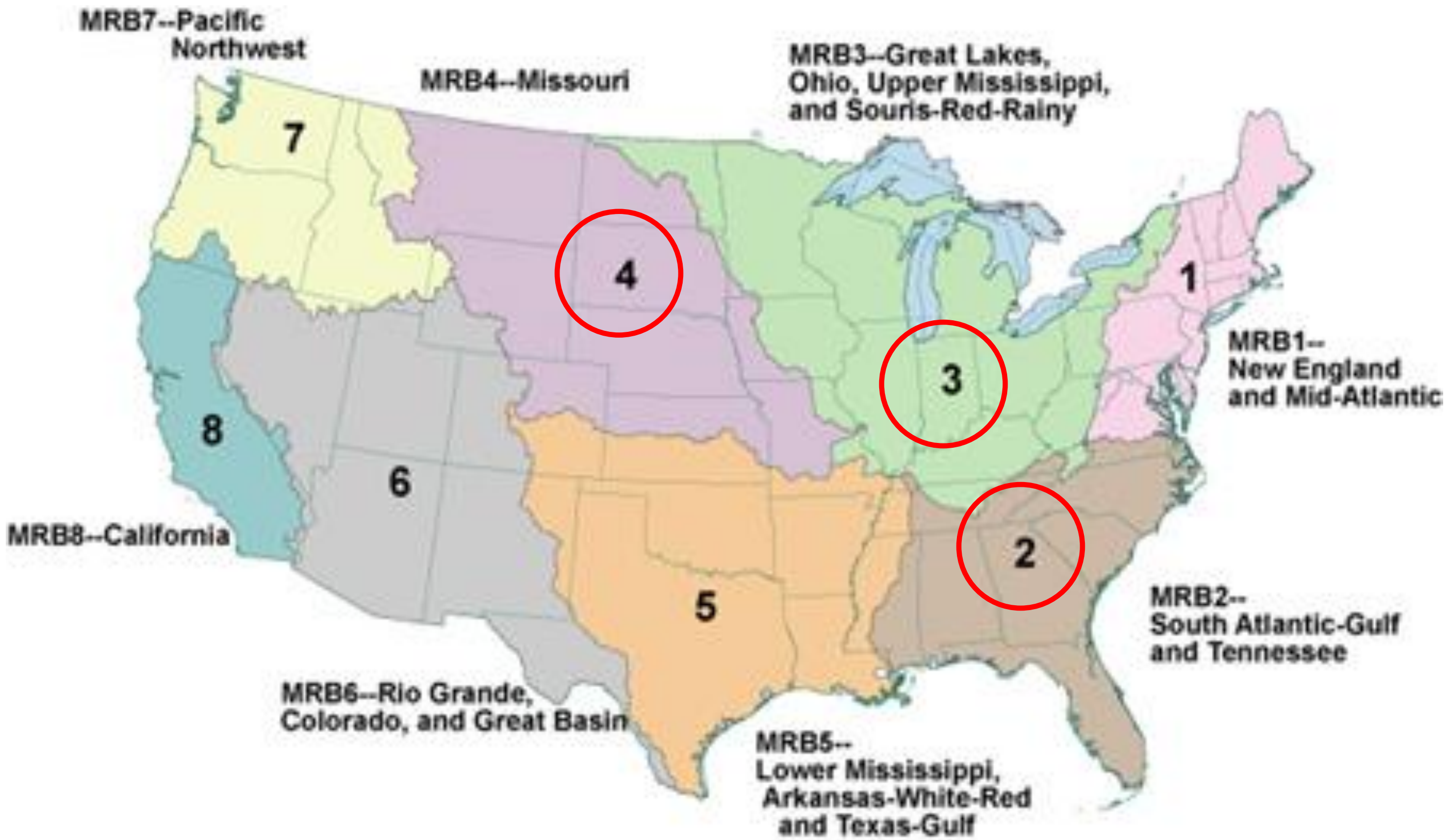
(19 HUC-8 watersheds)



Studies also compared the use of simple SPARROW models with sequentially coupled reach-level water-balance and SPARROW models

Preliminary Evaluations of Bayesian SPARROW Regional Nutrient Models

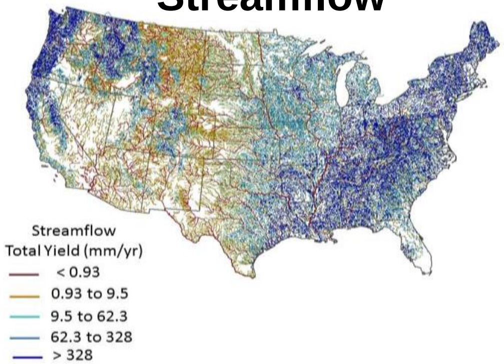
Mean Annual Total Nitrogen*



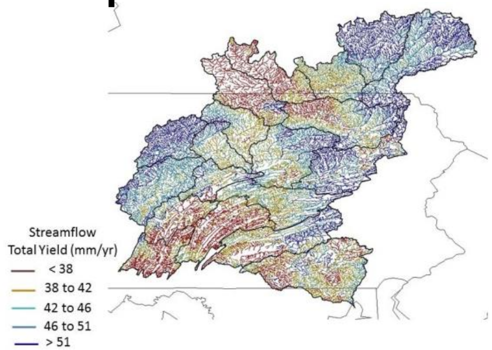
** SPARROW Regional nutrient models published in JAWRA, 2011, Featured Collection*

Bayesian SPARROW Evaluations
Summary of Key Findings

Mean Annual Streamflow



Mean Seasonal Streamflow Susquehanna River Basin



Mean Annual Total Nitrogen

- NLLS informs initial complexity and parm. prior ranges
- Improved "local" spatial and temporal specificity (coefficients, model error variance), with improved interpretability
- Increased accuracy (reduced bias, increased precision)
- Improved uncertainty quantification via state-space estimation of latent variables:
  - Very modest effect on model coefficients
  - Process uncertainties >> measurement errors
  - Process uncertainties >> H and conventional non-H SPARROW model errors (~5 to 25% TN)
  - Spatial covariance in process uncertainties can inform improved model structure and updated model predictions; space/time scale-dependence
  - Evaluate errors in cumulative (decay) processes
- Model input uncertainties dependent on informed prior information (e.g., Kavetski et al. 2006); testing of alternative input error models

Conclusions: SPARROW and Hierarchical Bayesian Modeling

- Desirable to use a diverse set of models to address different questions and benefit from model averaging ("wisdom of the crowd" effects)
- Data-informed, spatially explicit modeling offers flexible structure to explore and quantify major sources and biophysical controls and uncertainties:
  - Identifies the level of complexity that's consistent with observations
  - Increasing use of coupled mechanistic model predictions (e.g., water balance, ground water, field-scale agricultural; CMAQ deposition); evaluations needed to track error propagation
- Bayesian methods provide an enhanced structure that:
  - Improves the specificity of process effects and uncertainties over space and time
  - Quantifies sources of uncertainties related to parameters, model errors, and observations
- Parsimonious, lower-dimensional models well suited for use with hierarchical Bayesian methods; key computational constraints exist (related to reach segments, time steps, calibration sites, iterations)

USGS science for a changing world