

Eutrophication control in lakes and reservoirs using simultaneous dynamic optimization approaches

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Outline

- ✓ Motivation
- ✓ Objective
- ✓ Biological and biochemical determinations
- ✓ Global sensitivity analysis
- ✓ Dynamic parameter estimation problem
- ✓ Optimal control problem
- ✓ Simultaneous approach for dynamic optimization
- ✓ Discussion of results
- ✓ Conclusions

Motivation

- ✓ Eutrophication as natural process of aging of water body
- ✓ Water bodies increasingly eutrophic due to anthropogenic inputs of nutrients
- ✓ Application of restoration strategies requires systematic study, modeling and optimization of eutrophication processes

Cultural Eutrophication

- ✓ Main anthropogenic source of nutrients: Agricultural activities (fertilization)
- ✓ Main point source: discharge of agricultural, industrial and urban wastewater
- ✓ Over enrichment of nutrients (mainly P and N)
- ✓ Increase in the production levels and biomass
- ✓ Very strong development of phytoplankton community
- ✓ Decrease in water depth caused by sediment accumulation



Objective

- ✓ Development of ecological water quality (eutrophication) model
- ✓ Analysis of the trophic state of a water body through its composition and abundance of plankton
- ✓ Global sensitivity analysis and determination of sensitivity indices
- ✓ Parameter estimation based on available data:
- ✓ Model validation
- ✓ Study of the effect of nutrients concentration and environmental parameters on plankton population dynamics
- ✓ Determination of optimal bio-restoration policies

Trophic classification of water bodies

Oligotrophic

< [nutrients]
< Productivity

Mesotrophic

Eutrophic

> [nutrients]
> Productivity

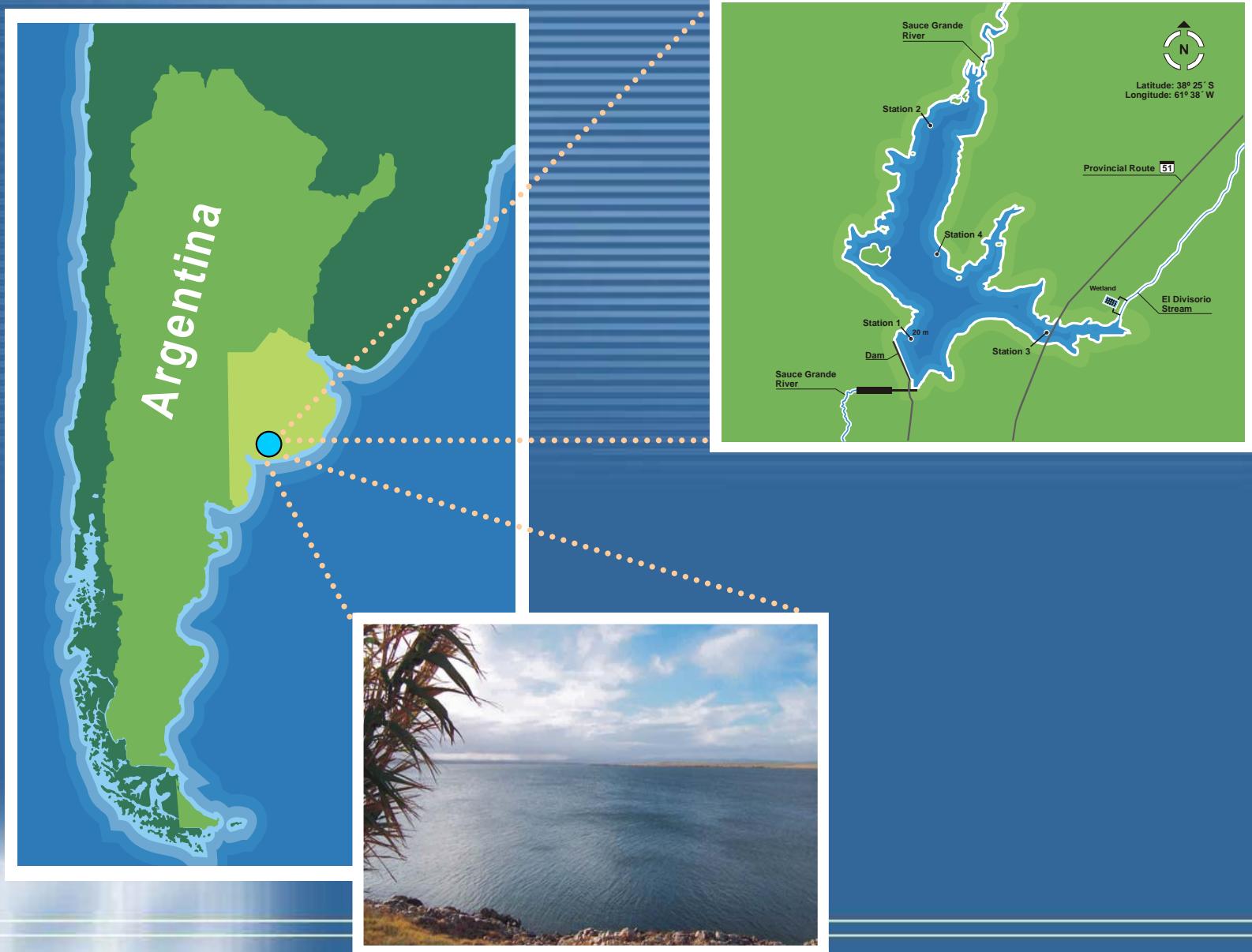
Hipereutrophic



Trophic classification of water bodies

	OLIGOTROPHIC	MESOTROPHIC	EUTROPHIC	HYPEREUTROPHIC
Inorganic phosphorus (μgl^{-1})	1-10	10-20	20-100	>100
Inorganic nitrogen (μgl^{-1})	<150	150-300	>300	
Phytoplankton (cellml^{-1})	2000	2000-5000	>5000	
Superficial chlorophyll a (μgl^{-1})	1-2	2-5	5-50	>50
Depth of Secchi disk (m)	5-10	3-5	1-3	<1

Paso de las Piedras Reservoir

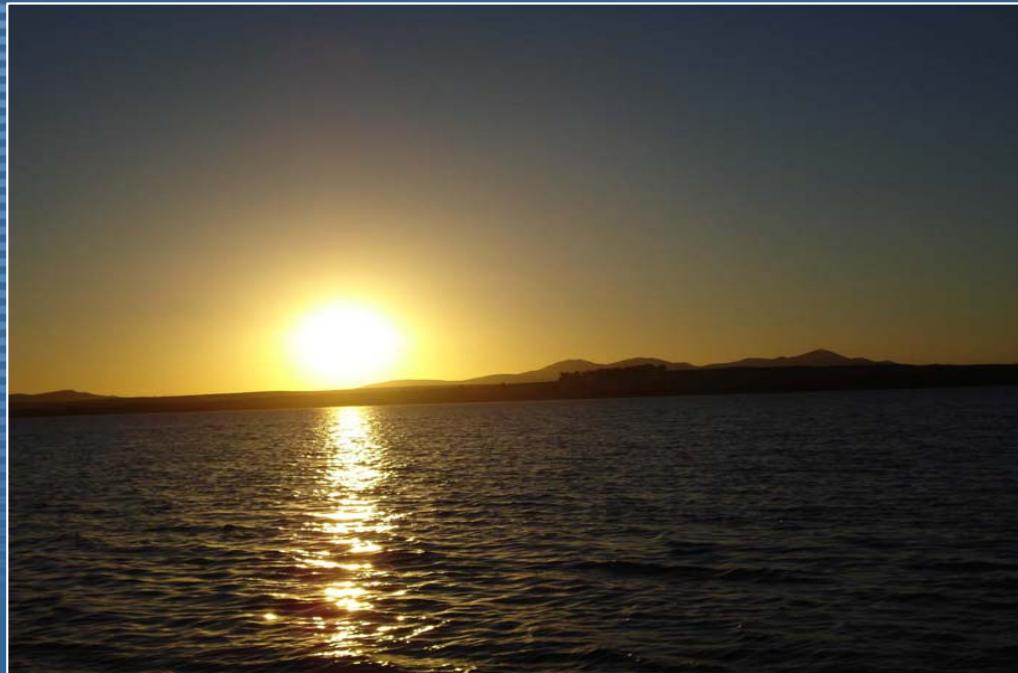


Paso de las Piedras Reservoir



Provides drinking water to more than 450.000 inhabitants
from Bahía Blanca, Punta Alta and to a petrochemical complex

Lake Characteristics

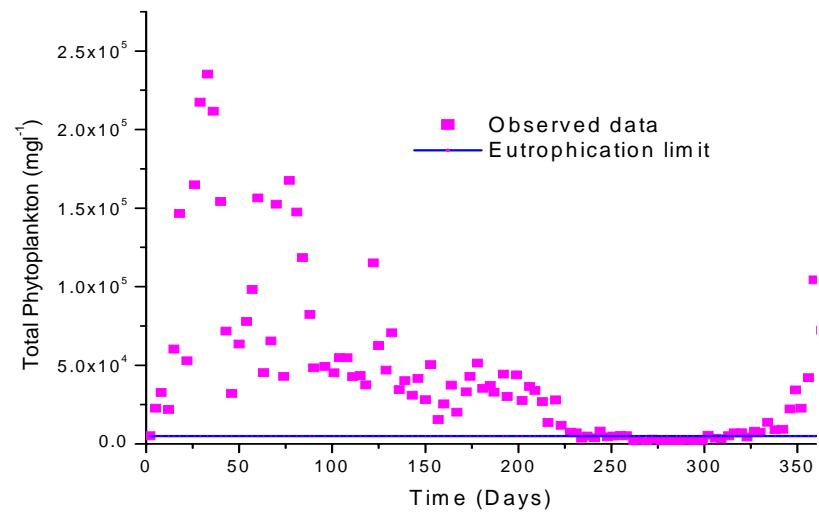
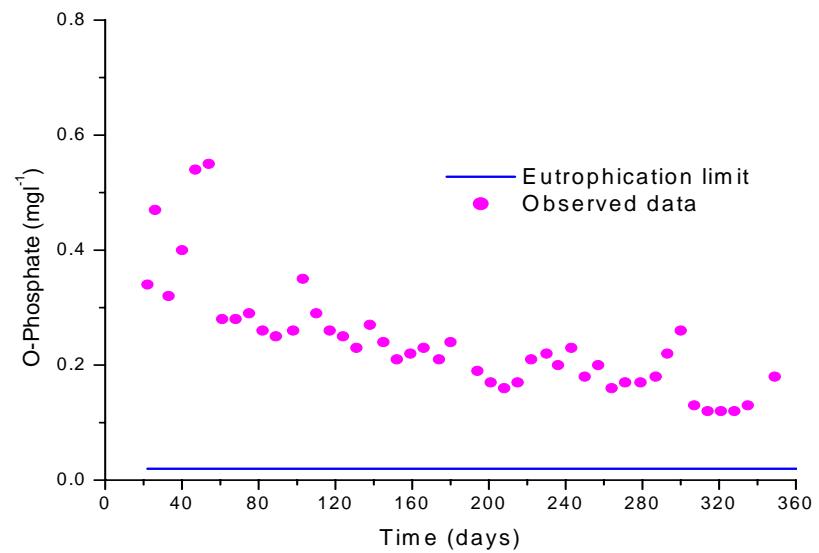


Area of drainage basin	1620 km ²	Maximum depth	28 m
Perimeter of coastline	60 km	Maximum volume	328 Hm ³
Surface	36 km ²	Retention time	4 years
Mean depth	8.2 m		

Paso de las Piedras Reservoir

i

- ✓ Eutrophic
- ✓ Main source of nutrients: agricultural activities
- ✓ High phytoplankton concentration during spring and summer: surface water blooms



Surface water blooms

- ✓ Natural phenomena caused by phytoplankton.
- ✓ Phytoplankton: microscopic floating algae (first link of the trophic chain).
- ✓ In favorable environmental conditions they are multiplied and concentrated in the surface,
➡ fast increase in algal biomass.



Photosynthesis



Solar radiation



algae

Problems caused by water blooms

For man

- ✓ Blockage of water-filters
- ✓ Unpleasant odor and taste
- ✓ Aesthetics
- ✓ Presence of potentially toxic algae

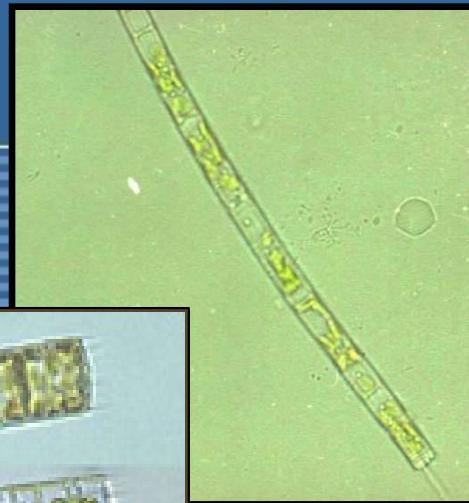
For ecosystem

- ✓ Reduction of biodiversity
- ✓ Anoxic conditions
- ✓ Shade
- ✓ Blockage of fish gills

Blockage of water-filters

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Aulacoseira spp.



Closterium spp.



Staurastrum spp.

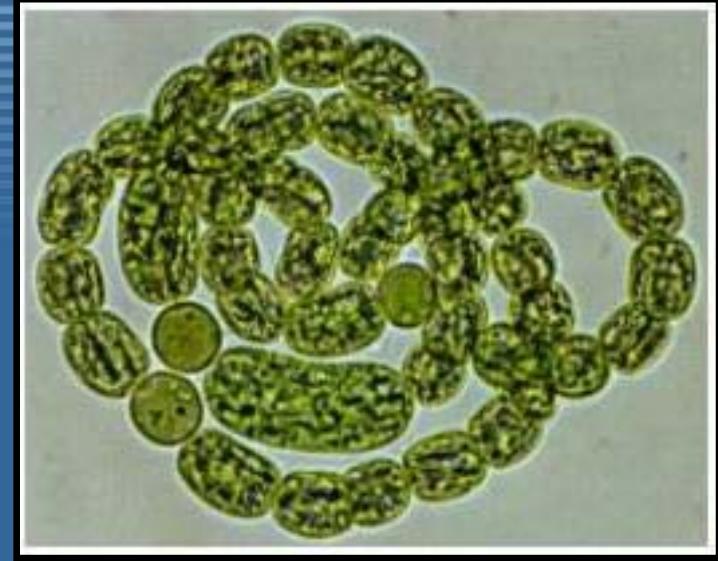


Unpleasant odor and taste

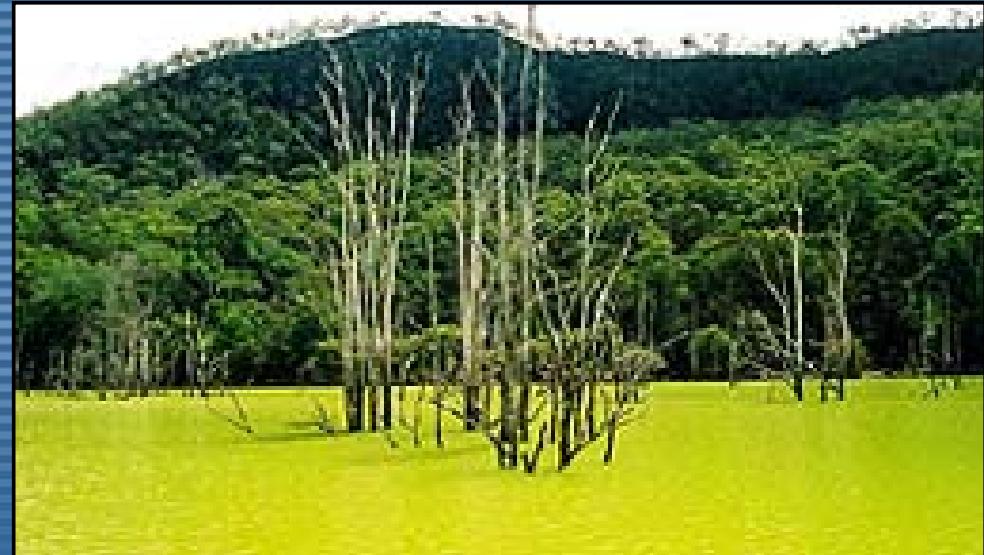
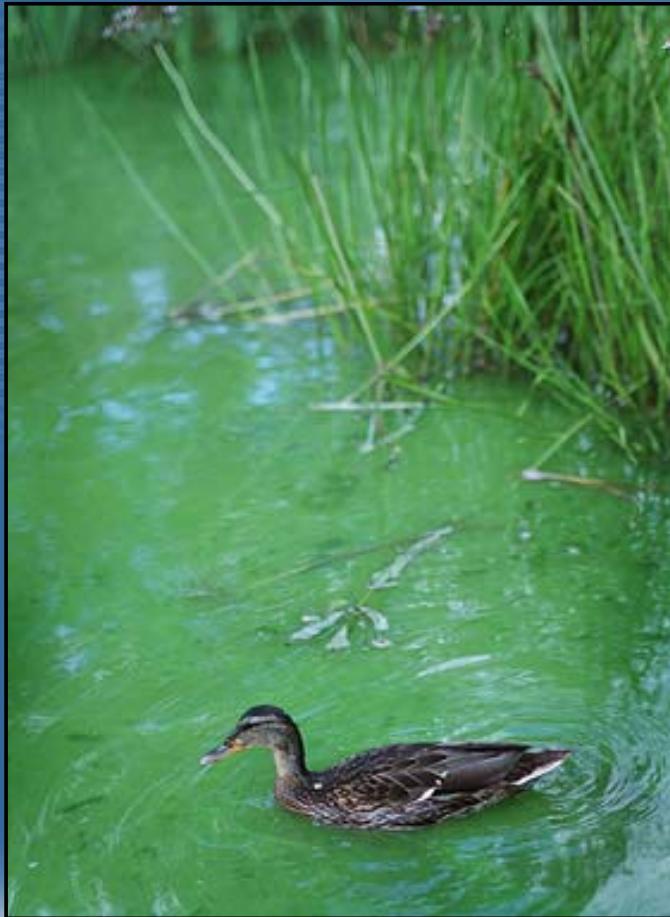
Ceratium hirundinella



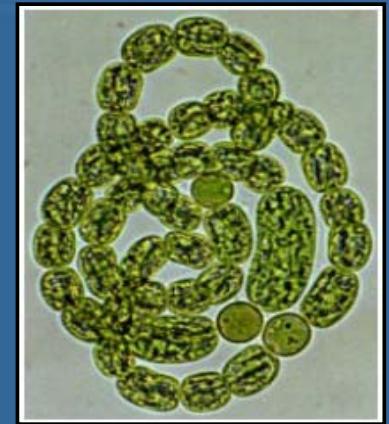
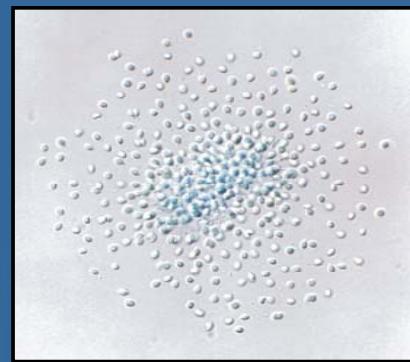
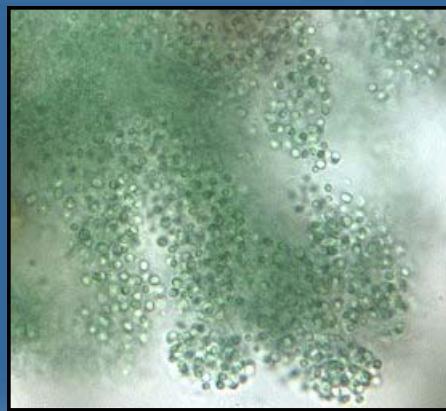
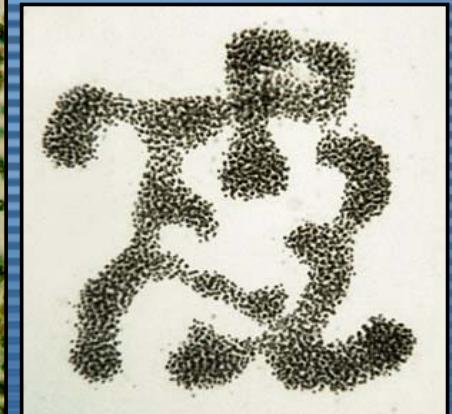
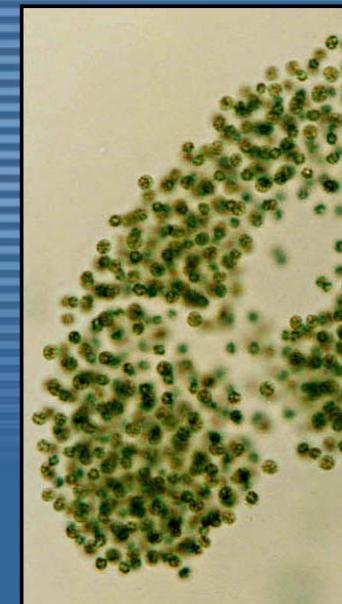
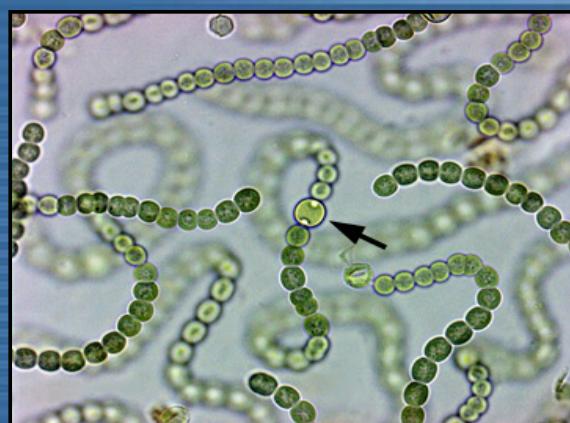
Anabaena circinalis



Aesthetics



Toxic Cyanobacteria



Biological determinations

Qualitative analysis

- ✓ Plankton net (30 µm)
- ✓ Observation to the optical microscope of the alive and fixed samples (formol 4%)
- ✓ Determination based on keys



Quantitative analysis

- ✓ Rutner water sampler
- ✓ *In situ* fixation with Lugol's solution
- ✓ Phytoplankton enumeration in inverted microscope by Utermöhl method (1958)
- ✓ Phytoplankton biovolume
- ✓ Calculation of mgC.



- ✓ Cyanobacteria
- ✓ Diatoms
- ✓ Chlorophytes

Physico-chemical determinations

- ✓ Nitrates
- ✓ Nitrites
- ✓ Ammonium
- ✓ Organic Nitrogen
- ✓ Phosphates
- ✓ Organic Phosphorus
- ✓ Silice



- ✓ Water temperature
- ✓ Solar radiation
- ✓ pH
- ✓ Dissolved Oxygen
- ✓ Biochemical Demand of Oxygen
- ✓ Depth of Secchi disk

Ecological Water Quality Model

Dynamic mass balances for nutrients and phytoplankton



Concentration gradients along water column height



Partial Differential Equations System



Spatially Discretization: Horizontal layers



Differential Algebraic System (DAE)

Assumptions

- ✓ Horizontally averaged concentration
- ✓ Phosphorus limiting nutrient (for algae growth)
- ✓ Constant density
- ✓ Constant transversal area in lake

Mass balance for horizontal layers

$\left[\frac{\text{mg}}{\text{day}} \right]$

$$\frac{d(C_{ij}V_i)}{dt} = \sum_{k=1}^{NIN} Q_{INi,k} C_{INijk} - \sum_{m=1}^{NOUT} Q_{OUTim} C_{INij} + r_{ij} V_i - \frac{kdA}{\Delta h_i} (C_{ij} - C_{i+1,j}) - \frac{kdA}{\Delta h_{i-1}} (C_{ij} - C_{i-1,j})$$

$$\frac{dC_{ij}}{dt} = \sum_{k=1}^{NIN} \frac{Q_{INi,k}}{V_i} C_{INijk} - \sum_{m=1}^{NOUT} \frac{Q_{OUTim}}{V_i} C_{INij} + r_{ij} - \frac{kdA}{\Delta h_i h_i} (C_{ij} - C_{i+1,j}) - \frac{kdA}{\Delta h_{i-1} h_{i-1}} (C_{ij} - C_{i-1,j}) - \frac{C_{ij}}{h_i} \frac{dh_i}{dt}$$

i = horizontal layer

k = Tributary inflows: El Divisorio, Sauce Grande

m = Withdrawals: drinking water+complex, Sauce Grande

j = Cyanobacteria, Diatoms, Chlorophyta, $\text{NO}_3, \text{NH}_4, \text{ON}, \text{PO}_4, \text{OP}, \text{BDO}, \text{DO}$



Mass balance for horizontal layers

Upper Layer

$$\frac{dC_{Uj}}{dt} = \sum_{k=1}^{NIN} \frac{QIN_{U,k}}{V_U} C_{IN_{Ujk}} - \sum_{m=1}^{NOOUT} \frac{QOUT_U}{V_U} C_{Uj} + r_{Uj} - \frac{kdA}{\Delta h_U h_U} (C_{Uj} - C_{Lj}) - \frac{C_{Uj}}{h_U} \frac{dh_U}{dt}$$

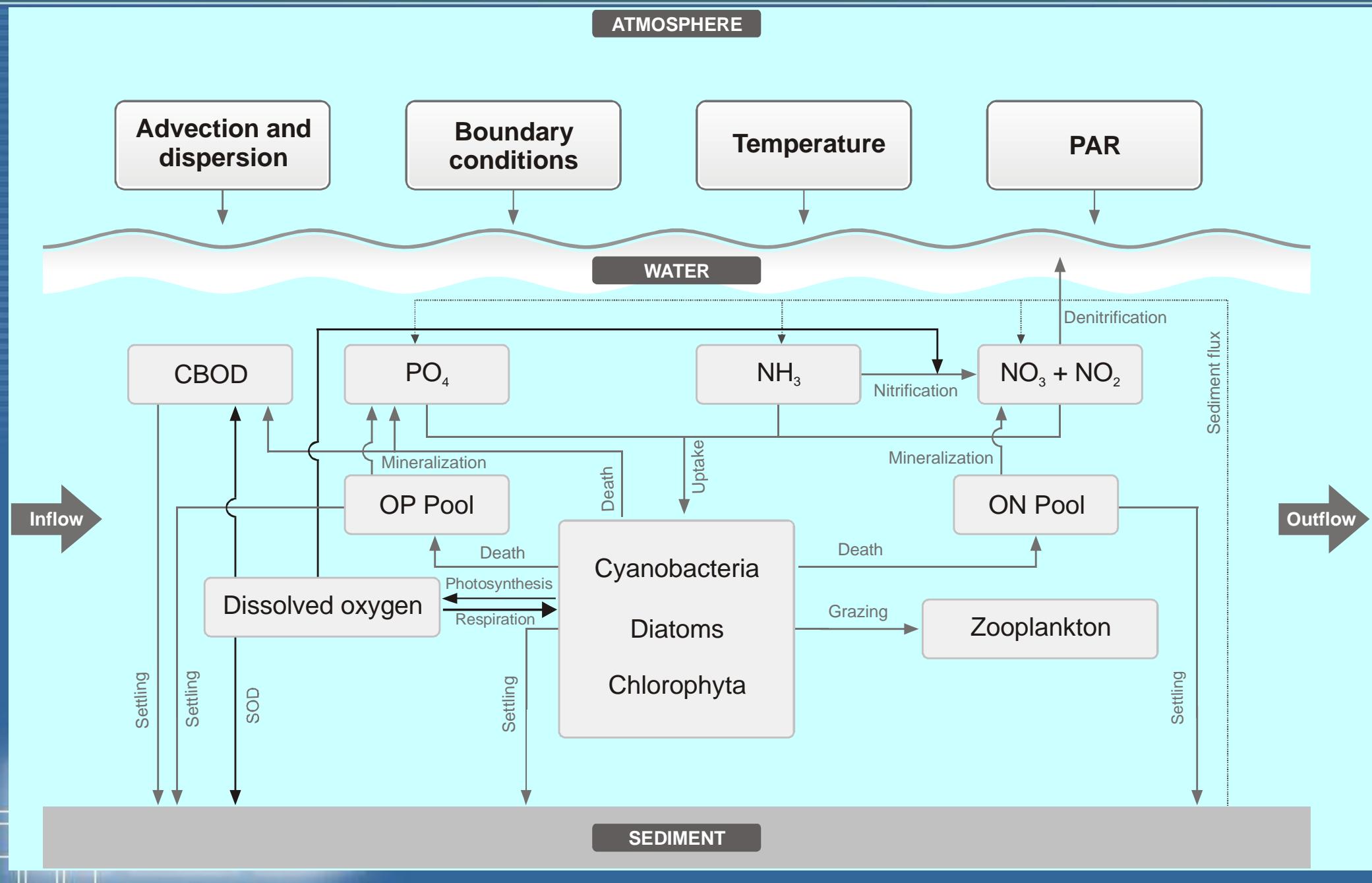
$i = U$

Lower Layer

$$\frac{dC_{Lj}}{dt} = \sum_{m=1}^{NOOUT} \frac{QOUT_L}{V_L} C_{Lj} + r_{Lj} + \frac{kdA}{\Delta h_L h_L} (C_{Lj} - C_{U,j}) - \frac{C_{Lj}}{h_L} \frac{dh_L}{dt}$$

$i = L$

State variables and biogeochemical processes



Rate equations (r_{ij})

$$r_{ij} = R_{ij,growth} - R_{ij,resp} - R_{ij,death} - R_{ij,settling} - R_{ij,graz}$$

Growth

$$R_{ij,growth} = k_{j,growth} * f(T) * f(I) * f(N) * C_{ij}$$

$$f(T)_{ij} = -\frac{(T_j - T_{opt_i})^2}{T_{opt_i}^2}$$

$$f(I) = \frac{I}{I_j} \exp(1 - \frac{I_i}{I_j})$$

$$f(N) = \frac{C_{iPO4}}{C_{iPO4} + kpj}$$

Respiration

$$R_{ij,resp} = k_{i,resp} \theta_r^{(T-20)} C_{ij}$$

Death

$$R_{ij,death} = k_{i,death} \theta_m^{(T-20)} C_{ij}$$

Settling

$$R_{ij,settling} = k_{j,settling} * \frac{1}{h_i} * C_{ij}$$

Grazing

$$R_{ij,graz} = k_{j,graz} \frac{C_{ij}}{C_{ij} + K_{graz}} C_{Zoo_j}$$

i = upper and lower layers

j = Cyanobacteria, Diatoms,

Chlorophytes

Rate equations (r_{ij})

$$r_{ij} = R_{ij,death} - R_{ij,miner} - R_{ij,sedim}$$

Death

$$R_{ij,death} = \sum_{m=1}^3 (a_{jc} * k_{m,death} * f_j * C_{im})$$

Mineralization

$$R_{ij,miner} = k_{miner} * \theta_{miner} * \exp(Temp - 20) * \frac{\sum_{m=1}^3 C_{im} * C_{ij}}{k_{mj} + \sum_{m=1}^3 C_{im}}$$

Settling

$$R_{ij,sedim} = \frac{k_{j,sedim} * (1 - fDj)}{Di} * C_{ij}$$

i = upper and lower layers

j = ON, OP

Rate equations (r_{ij})

$$r_{ij} = R_{ij,death} + R_{ij,miner} - R_{ij,uptake}$$

Death

$$R_{ij,death} = \sum_{m=1}^3 (apc * k_{m,death} * (1 - f_{po}) * C_{im})$$

Mineralization

$$R_{ij,miner} = k_{miner} * \theta_{miner} * \exp(Temp - 20) * \frac{\sum_{m=1}^3 C_{im} * C_{iOP}}{k_{mineralization} + \sum_{j=1}^3 C_{im}}$$

Uptake

$$R_{ij,uptake} = \sum_{m=1}^3 (R_{im,growth} * a_{pc} * C_{im})$$

i = upper and lower layers

j = PO₄

Rate equations (r_{ij})

$$r_{ij} = R_{ij,nitri} - R_{ij,uptake} - R_{ij,denitr}$$

Nitrification

$$R_{ij,nitri} = k_{nitri} * \theta_{nitri} * \exp(Temp - 20) * \frac{C_{iNH4} * C_{iDO}}{k_{nio} + C_{iDO}}$$

Uptake

$$R_{ij,uptake} = \sum_{m=1}^3 (a_{nc} * R_{im,growth} * (1 - PNH4) * C_{im})$$

Denitrification

$$R_{ij,denitr} = k_{denitr} * \theta_{denitr} * \exp(Temp - 20) * \frac{C_{iNO3} * k_{no3}}{k_{no3} + C_{iDO}}$$

i = upper and lower layers

j = NO₃

Rate equations (r_{ij})

$$r_{ij} = R_{ij,death} + R_{ij,miner} - R_{ij,uptake}$$

Death

$$R_{ij,death} = \sum_{m=1}^3 (anc * k_{m,death} * (1 - f_{ON}) * C_{im})$$

Mineralization

$$R_{ij,miner} = k_{miner} * \theta_{miner} * \exp(Temp - 20) * \frac{\sum_{m=1}^3 C_{im} * C_{iON}}{kmpc + \sum_{m=1}^3 C_{im}}$$

Uptake

$$R_{ij,uptake} = \sum_{m=1}^3 (a_{nc} * R_{im,growth} * PNH4 * C_{im})$$

i = upper and lower layers

j = NH₄

Global sensitivity analysis

- ✓ Local vs. Global Sensitivity Analysis
- ✓ Quantitative variance-based Global Sensitivity Analysis
 - ❖ Model independent
 - ❖ Incorporate the effect of range of input variation and its pdf
 - ❖ Allow multidimensional averaging
 - ❖ Allow parameter grouping

Global sensitivity analysis

Given model output $Y=f(\mathbf{x})$, \mathbf{x} vector of input factors

Output variance

$$V(Y) = E(V(Y|x_i)) + V(E(Y|x_i))$$

$E(V(Y|x_i))$ mean output variance that remains if x_i fixed (known)

$V(E(Y|x_i))$ expected reduction in output variance if x_i fixed

Sensitivity index

input x_i

$$S_i = \frac{V(E(Y|x_i))}{V(Y)}$$

Global sensitivity analysis

Decompose model output $Y=f(\mathbf{x})$, as the sum of terms of increasing dimensionality

$$f(x_1, \dots, x_k) = f_0 + \sum_{i=1}^k f_i(x_i) + \sum_{1 \leq i < j \leq k} f_{ij}(x_i, x_j) + \dots + f_{1,2,\dots,k}(x_1, \dots, x_k)$$

If input parameters are mutually independent ($\int_0^1 f_{i_1, \dots, i_s} dx_k = 0$)
unique decomposition of f such that the summands are orthogonal.

$$V = \sum_{i=1}^k V_i + \sum_{1 \leq i < j \leq k} V_{ij} + \dots + V_{1,2,\dots,k}$$

$V_i, V_{ij}, V_{1,2,\dots,k}$: Variance of $f_i, f_{ij}, f_{1,2,\dots,k}$

Global sensitivity analysis

$$1 = \sum_{i=1}^k \frac{V_i}{V} + \sum_{1 \leq i < j \leq k} \frac{V_{ij}}{V} + \dots + \frac{V_{1,2,\dots,k}}{V}$$

$$1 = \sum_{i=1}^k S_i + \sum_{1 \leq i < j \leq k} S_{ij} + \dots + S_{1,2,\dots,k}$$

Sobol' sensitivity indices

Higher orders indices calculation: computationally expensive

Total sensitivity index

$$S_i^T = \frac{E(V(Y|x_{-i}))}{V(Y)}$$

Global sensitivity analysis

Calculation of Sobol' sensitivity indices (Monte Carlo)

- ✓ Generate two independent random sets ξ and ξ' ,
let $\xi = (\eta, \zeta)$; $\xi' = (\eta', \zeta')$
- ✓ Evaluate
 - ❖ $f(\eta, \zeta)$
 - ❖ $f(\eta, \zeta')$
 - ❖ $f(\eta', \zeta)$

Global sensitivity analysis

✓ Calculate

$$\frac{1}{N} \sum_{i=1}^N f(\xi_i) \xrightarrow{p} E(Y)$$

$$\frac{1}{N} \sum_{i=1}^N f^2(\xi_i) \xrightarrow{p} V(Y) + E^2(Y)$$

$$\frac{1}{N} \sum_{i=1}^N f(\xi_i) f(\eta_i, \zeta_i) \xrightarrow{p} V_y + E^2(Y)$$

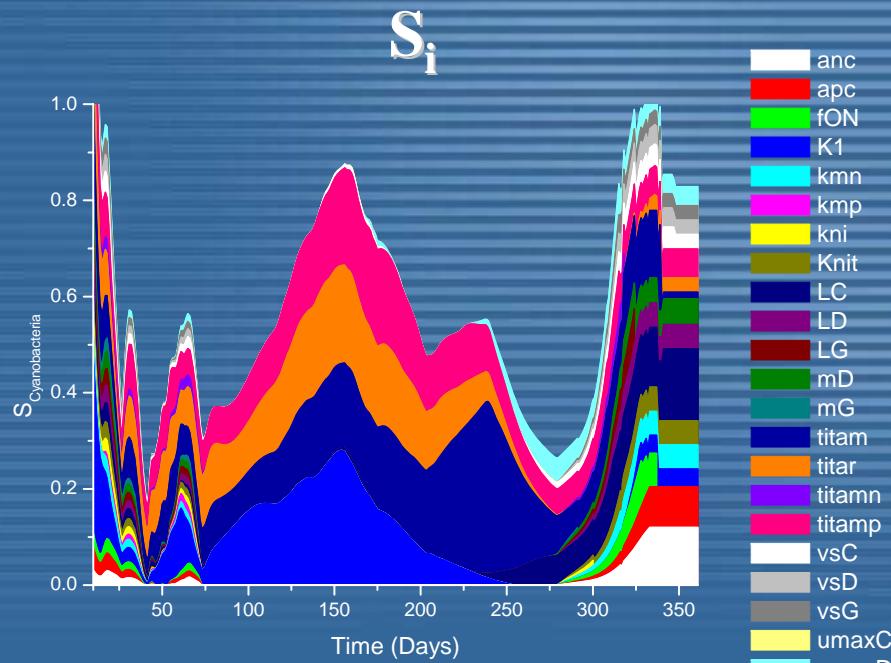
$$\frac{1}{N} \sum_{i=1}^N f(\xi_i) f(\eta_i, \zeta_i) \xrightarrow{p} V_y^T + E^2(Y)$$

Sobol' indices

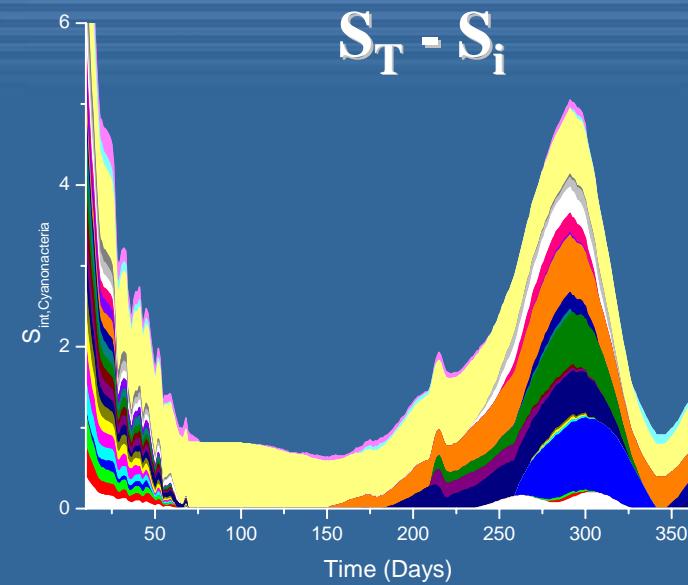
$$S_i = \frac{V_y}{V(Y)}$$

$$S_i^T = 1 - \frac{y}{V(Y)}$$

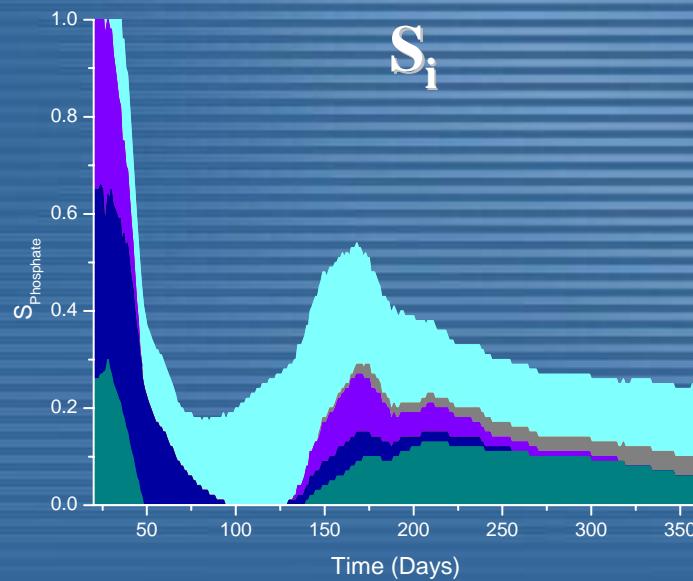
Sensitivity Indices: S_i



Cyanobacteria

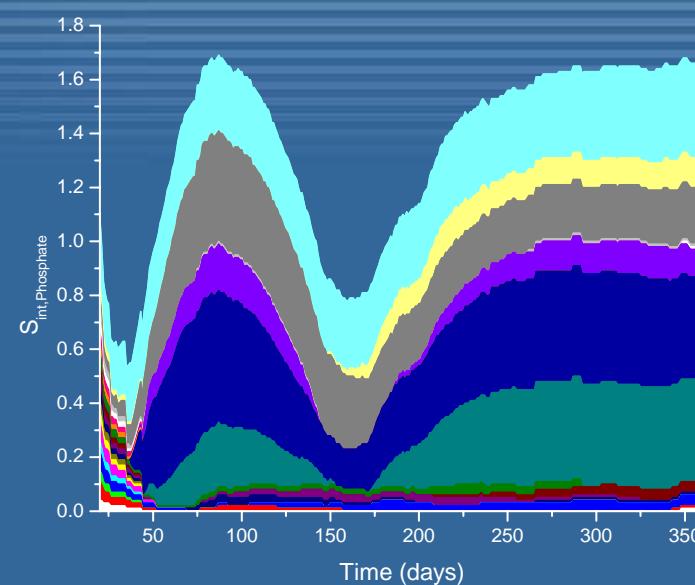


Sensitivity Indices: S_i



Phosphate

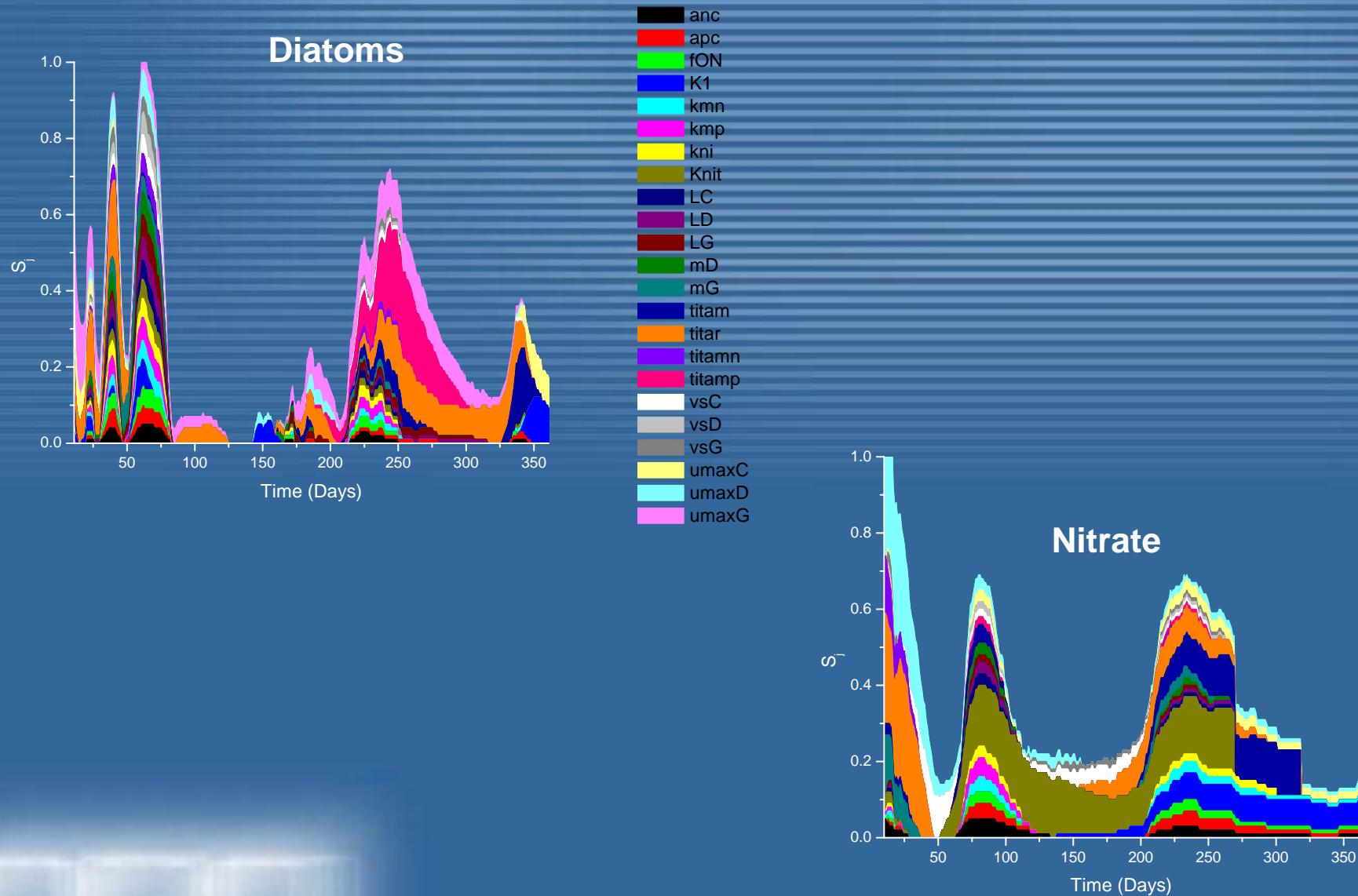
$S_T - S_i$



- anc
- apc
- fON
- K1
- knn
- kmp
- kni
- Knit
- LC
- LD
- mD
- mG
- titam
- titar
- titamn
- titamp
- vsC
- vsD
- vsG
- umaxC
- umaxD
- umaxG



Sensitivity Indices: S_i



Dynamic Parameter Estimation Model



Parameter Estimation Problem

Process Model

$$f(\dot{x}, x, y, u, p, t) = 0$$

$$g(x, y, u, p, t) = 0$$



Variable Bounds

$$x_L \leq x \leq x_U, y_L \leq y \leq y_U$$

$$u_L \leq u \leq u_U, p_L \leq p \leq p_U$$

Initial Conditions

$$x(t_0) = x_0$$

Objective Function

$$\min \phi = \frac{1}{2} \sum_{i=1}^{NINV} \sum_{j=1}^{NL} \sum_{k=1}^{NV} (x_{ij}^M - x_{ij})^T V^{-1} (x_{ij}^M - x_{ij}),$$

$$V = \text{diag}\{\sigma^2\}$$

Simultaneous Approach for Dynamic Optimization

Dynamic Parameter Estimation Problem

Process Model

$$f(\dot{x}, x, y, u, p, t) = 0$$
$$g(x, y, u, p, t) = 0$$

Variable Bounds

$$x_L \leq x \leq x_U, y_L \leq y \leq y_U$$
$$u_L \leq u \leq u_U, p_L \leq p \leq p_U$$

Initial Conditions

$$x(t_0) = x_0$$

Objective Function

$$\min \phi = \frac{1}{2} \sum_{i=1}^{NINV} \sum_{j=1}^{NL} \sum_{k=1}^{NV} (x_{ij}^M - x_{ij})^T V^{-1} (x_{ij}^M - x_{ij}),$$
$$V = \text{diag}\{\sigma^2\}$$

Nonlinear DAE optimization problem

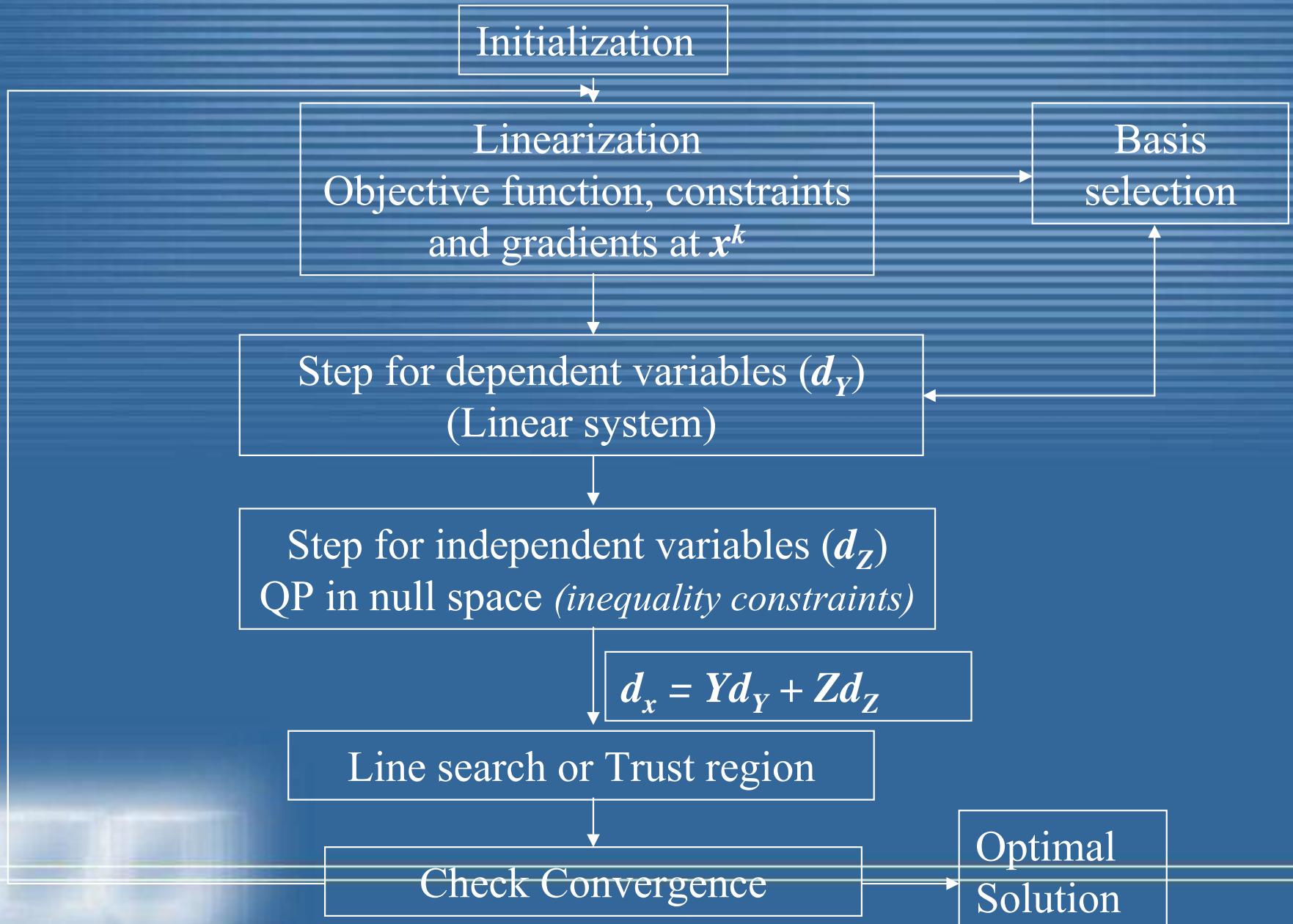
Discretization of Control and State variables
Collocation on finite elements

Large-Scale Nonlinear Programming Problem
Interior Point Method (Biegler et al., 2002)



rSQP Algorithm

(Biegler et al., 2002)



Nonlinear Programming Problem

Application of Barrier method

$$\min f(x)$$

$$\text{s.t } c(x) = 0$$

$$x \geq 0$$



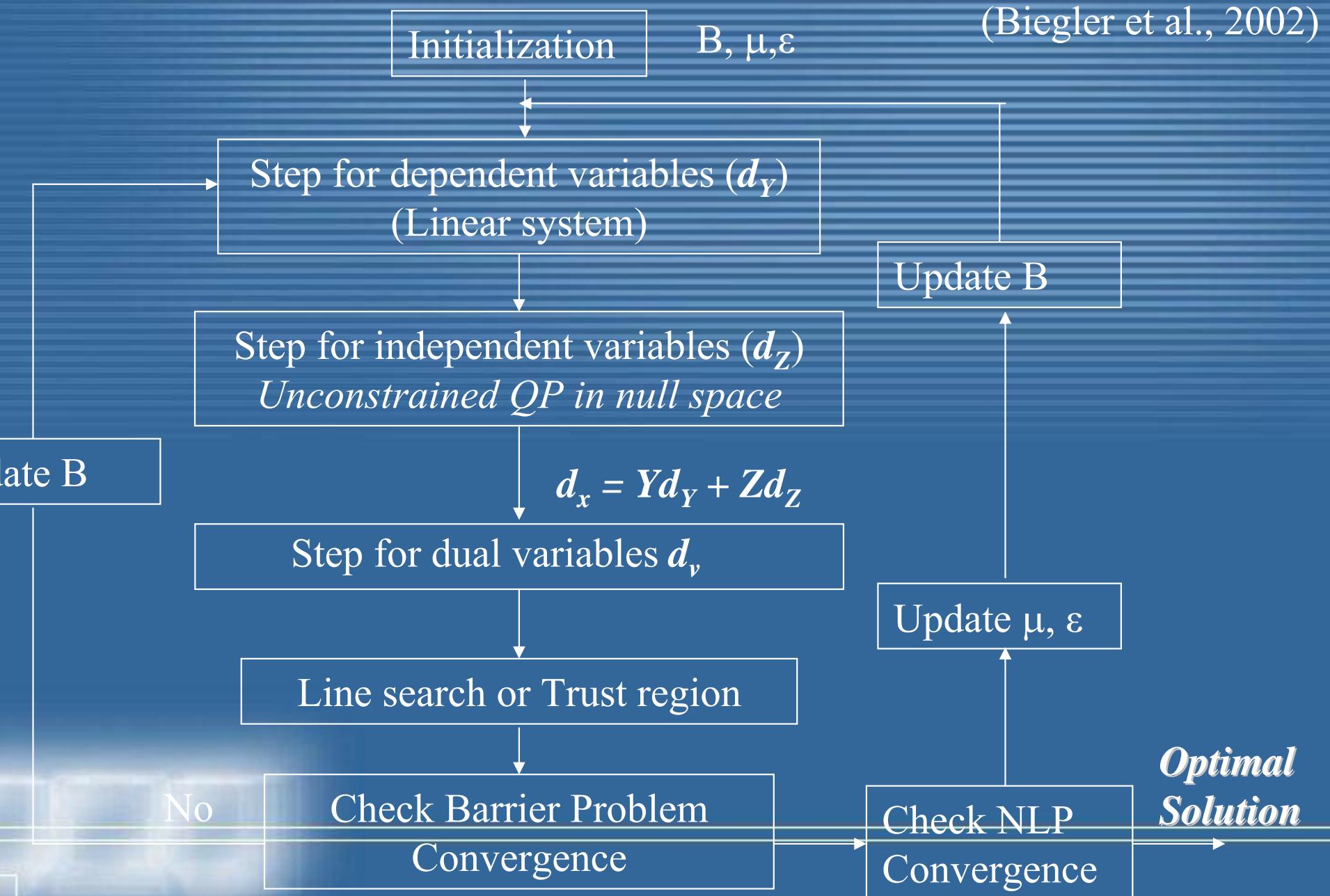
$$\min f(x) - \mu \sum_{j=1}^n \ln x_j$$

$$\text{s.t } c(x) = 0$$

As $\mu \rightarrow 0$, $x^*(\mu) \rightarrow x^*$

Sequence of barrier problems for decreasing μ values

Barrier Method Algorithm: Primal-Dual Approach



Parameter Estimation Problem

Input data

- ✓ Descriptive data for lake
- ✓ Temperature, solar radiation, lake depth time profiles
- ✓ Inflows and outflows time profiles
- ✓ Nutrients concentration profiles in inflows
- ✓ Initial conditions
- ✓ State variables profiles for upper and lower layer (measured)

Numerical Results

(Estrada et al., 2008a,b)

Symbol	Parameter	Estimated
$k_{cyanob,growth}$ (d ⁻¹)	Max growth of cyanobacteria	0.210
I_c (ly/d)	Optimal growth radiation cyano	109.9
$k_{diatom,growth}$ (d-1)	Max growth of diatoms	0.405
I_d (ly/d)	Optimal growth radiation of diatoms	24.52
$k_{cyanoph,growth}$ (d ⁻¹)	Max growth of chlorophytes	0.654
I_g (ly/d)	Optimal growth radiation chlorophytes	89.74
$k_{ON,miner}$ (d-1)	Rate coeff. mineralization ON	0.092
$k_{OP,miner}$ (d-1)	Rate coeff. mineralization OP	0.015
K_{nio} (mg/l)	Half-sat. conc. for oxygen lim. of nitrification	0.343

Time horizon: 365 days – Data frequency: twice a week

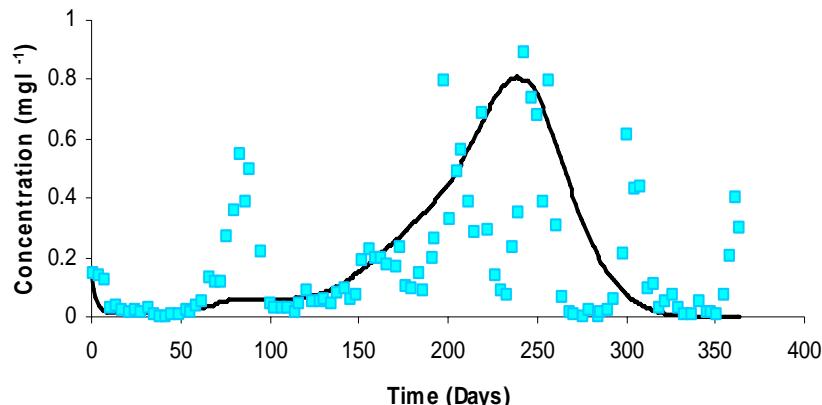
DAE: 20 differential equations, 60 algebraic equations, NE =40 NC=3

NLP: 10432 nonlinear equations, 52 Iterations, 4 barrier problems

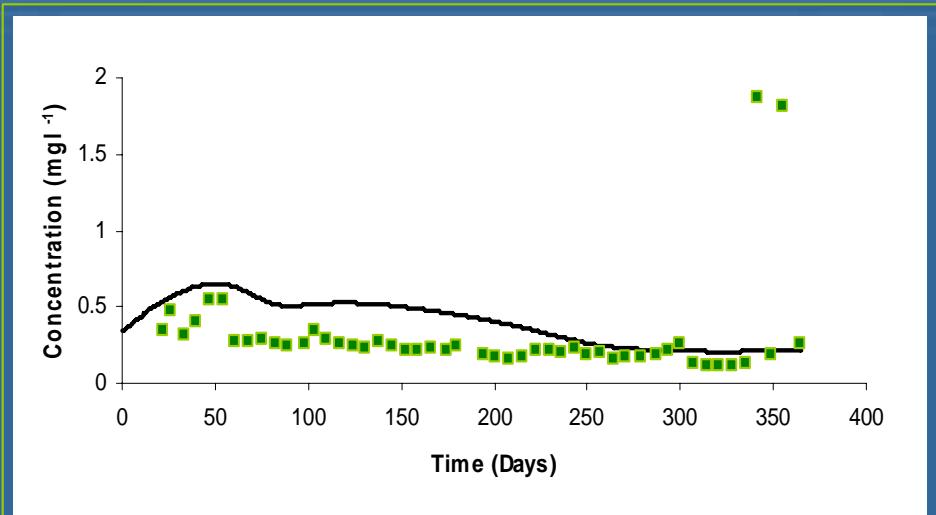


Numerical Results

Diatoms

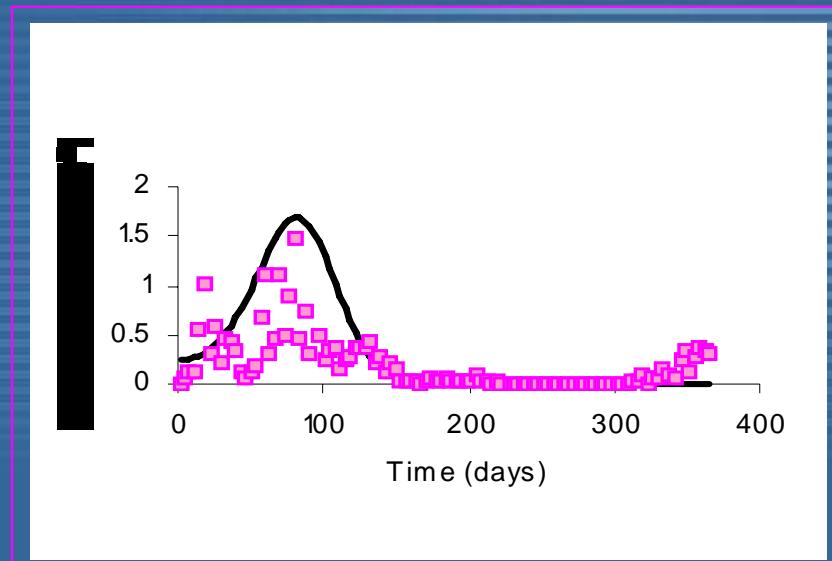


Phosphate

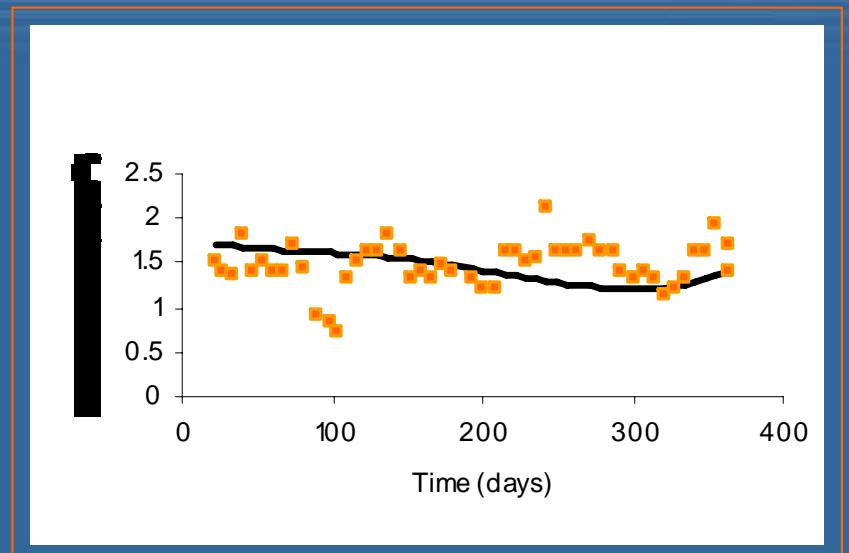


Numerical Results

Cyanobacteria



Nitrate



Bio-restoration policies

- ✓ Excessive nutrients that promote algal growth were identified as the most important problem in 44% of all U.S. lakes surveyed in 1998 (U.S. EPA 2000)
- ✓ Nutrient management:
 - How much do nutrients have to be reduced to eliminate algal blooms?
 - How long will it take for lake water quality to improve once controls are in place?
 - How successful will restoration be, based on water quality management goals?
 - Are proposed lake management goals realistic and cost effective?

Bio-restoration policies

Artificial wetland

- ✓ Built for nitrogen and phosphorus removal
(Lopez et al., 2007)
- ✓ Next to El Divisorio Stream
- ✓ Global retention: 64%
(phosphate)
- ✓ Derivation of tributary inflows through wetland



Optimal control problem: Tributary inflows derivation

- ✓ Case 1: Control variable: Tributary inflows profiles derivation to wetland for bio-remediation

$$\min \int_0^{tf} \left(\sum_{j=phyto} C_j(t) - 0.25 \right)^2 dt$$

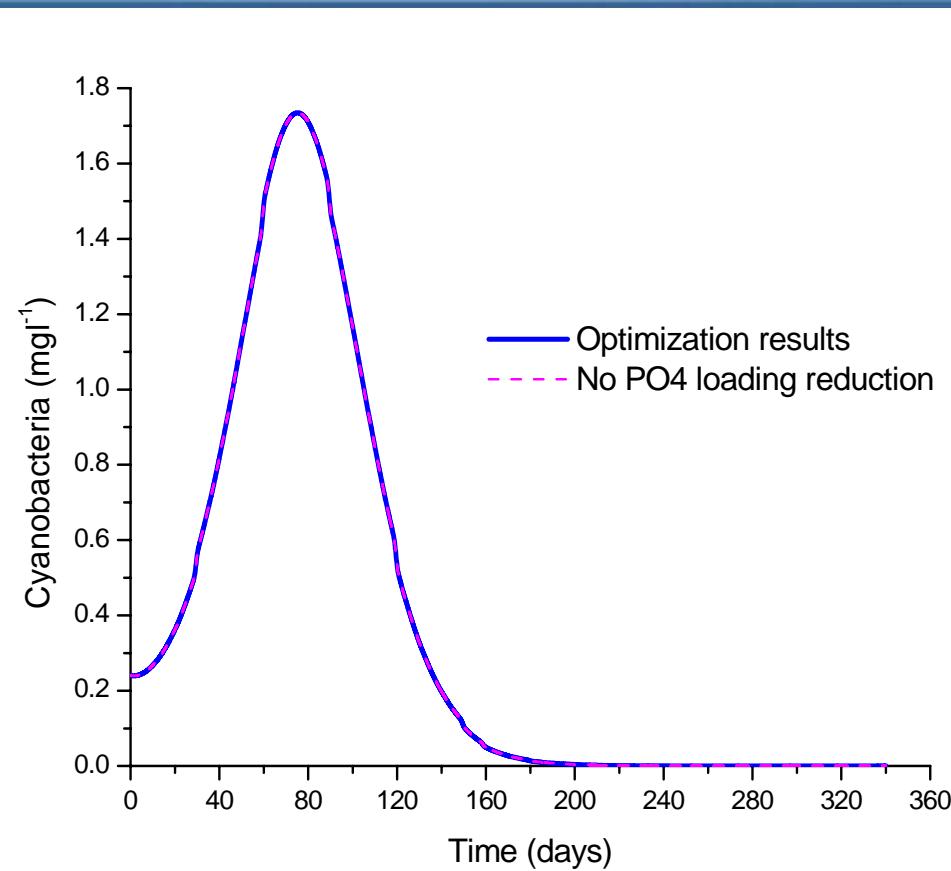
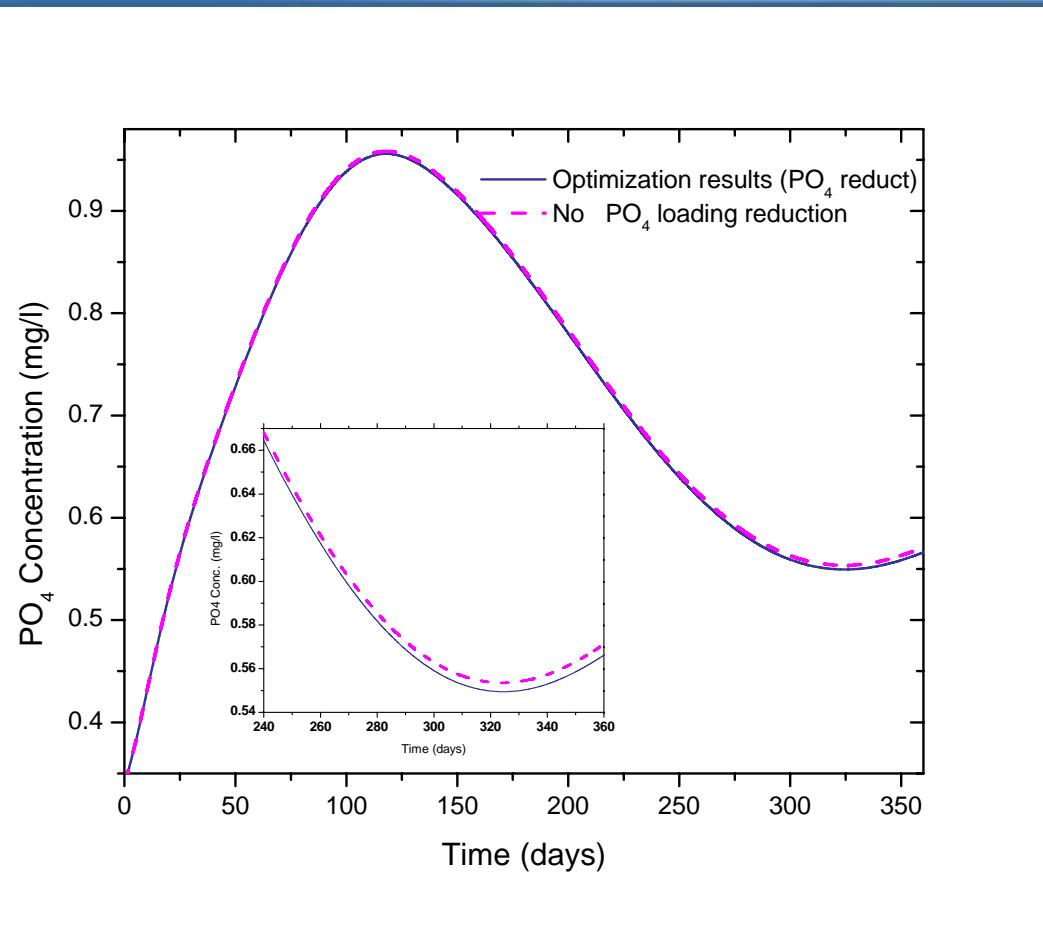
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DAE Eutrophication model

$$0 \leq F_{WETLAND} \leq 0.5F_{DIVISORIO}(l/d)$$

Case 1: Numerical results

(Estrada et al., 2008d)



NE = 40, NC = 3

NLP: 10581 nonlinear equations



Optimal control problem: Inlake bio-restoration

- ✓ Case 2: Control variables: Tributary inflows profiles derivation to wetland for bio-remediation and Zooplankton concentration profiles (Removal of zoo-planktivorous fish)

$$\min \int_0^{tf} \left(\sum_{j=phyto} C_j(t) - 0.25 \right)^2 dt$$

st

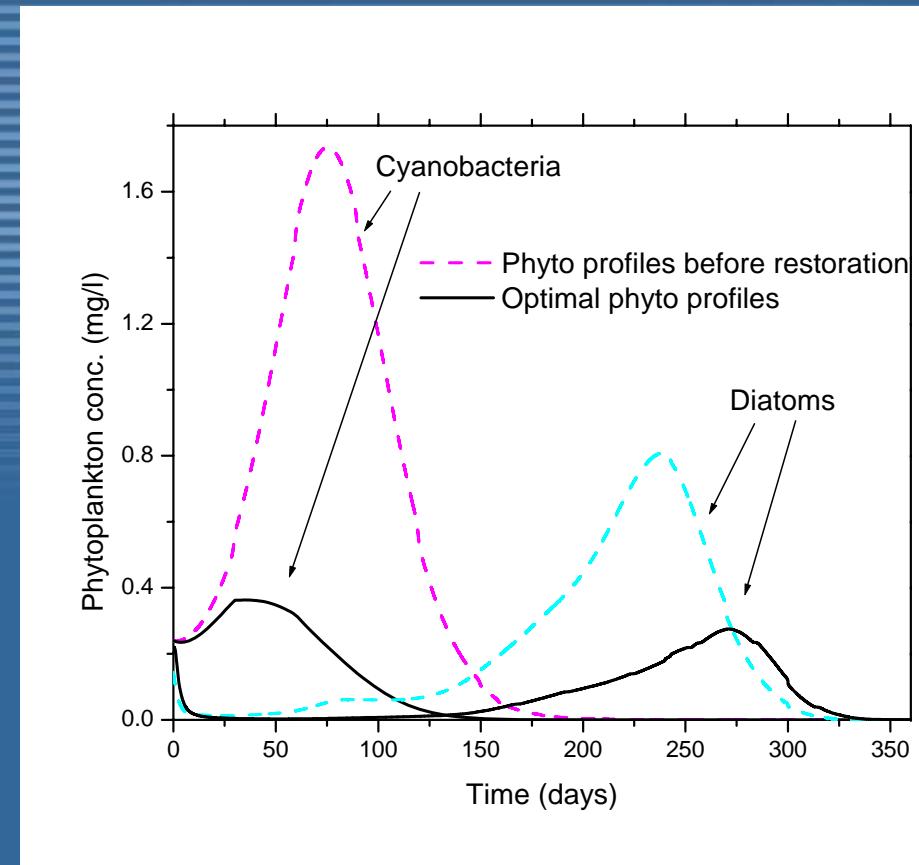
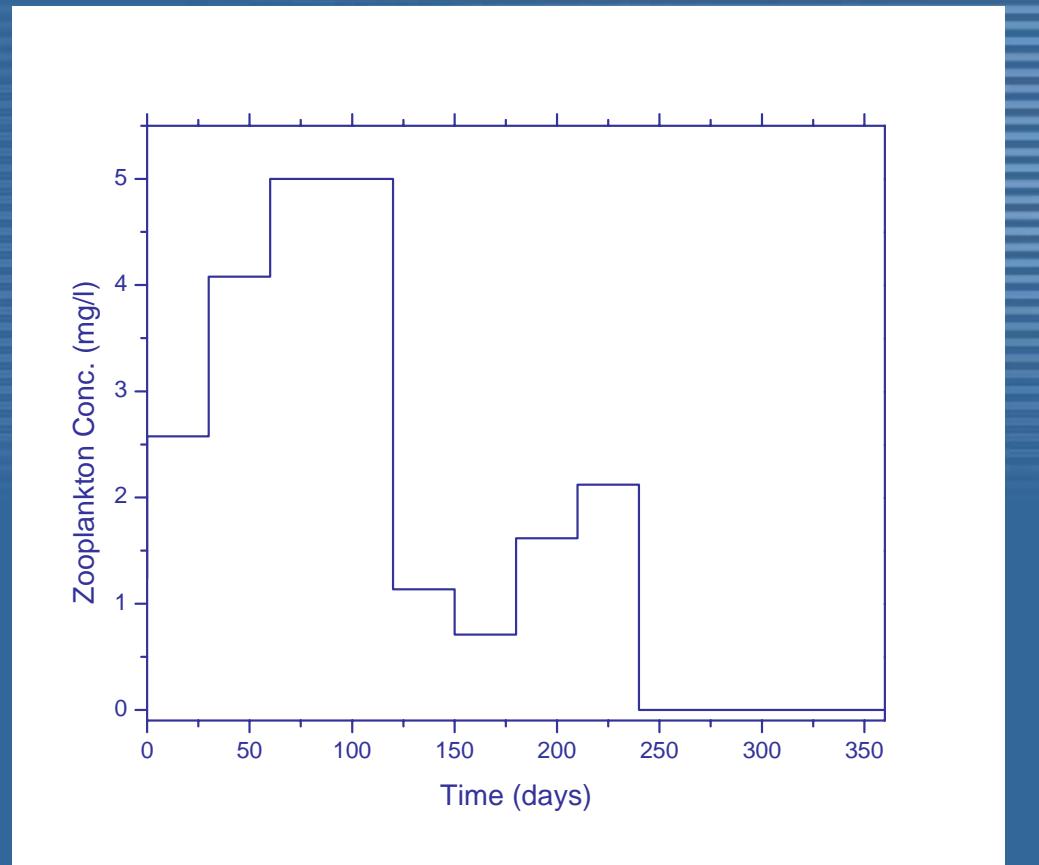
DAE Eutrophication model

$$0 \leq F_{WETLAND} \leq 0.5 F_{DIVISORIO}^{(l/d)}$$

$$0.01 \leq C_{zoo} \leq 5(mg/l)$$

Case 2: Control and state variables profiles

(Estrada et al., 2008d)



NE = 40, NC = 3

NLP: 10741 nonlinear equations



Conclusions

- ✓ Biological and physico chemical determinations at two depth level in Paso de las Piedras Reservoir. Current data collection at eight levels.
- ✓ Development of rigorous eutrophication model
- ✓ Global sensitivity analysis: ranking of input parameters
- ✓ Formulation of parameter estimation problem subject to DAE system
- ✓ Parameter estimation problem solved with advanced dynamic optimization techniques: simultaneous approach
- ✓ Resolution of optimal control problem: bio-restoration policies

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