

Linking hydraulic circulation and biogeochemical models: example from the Curonian lagoon



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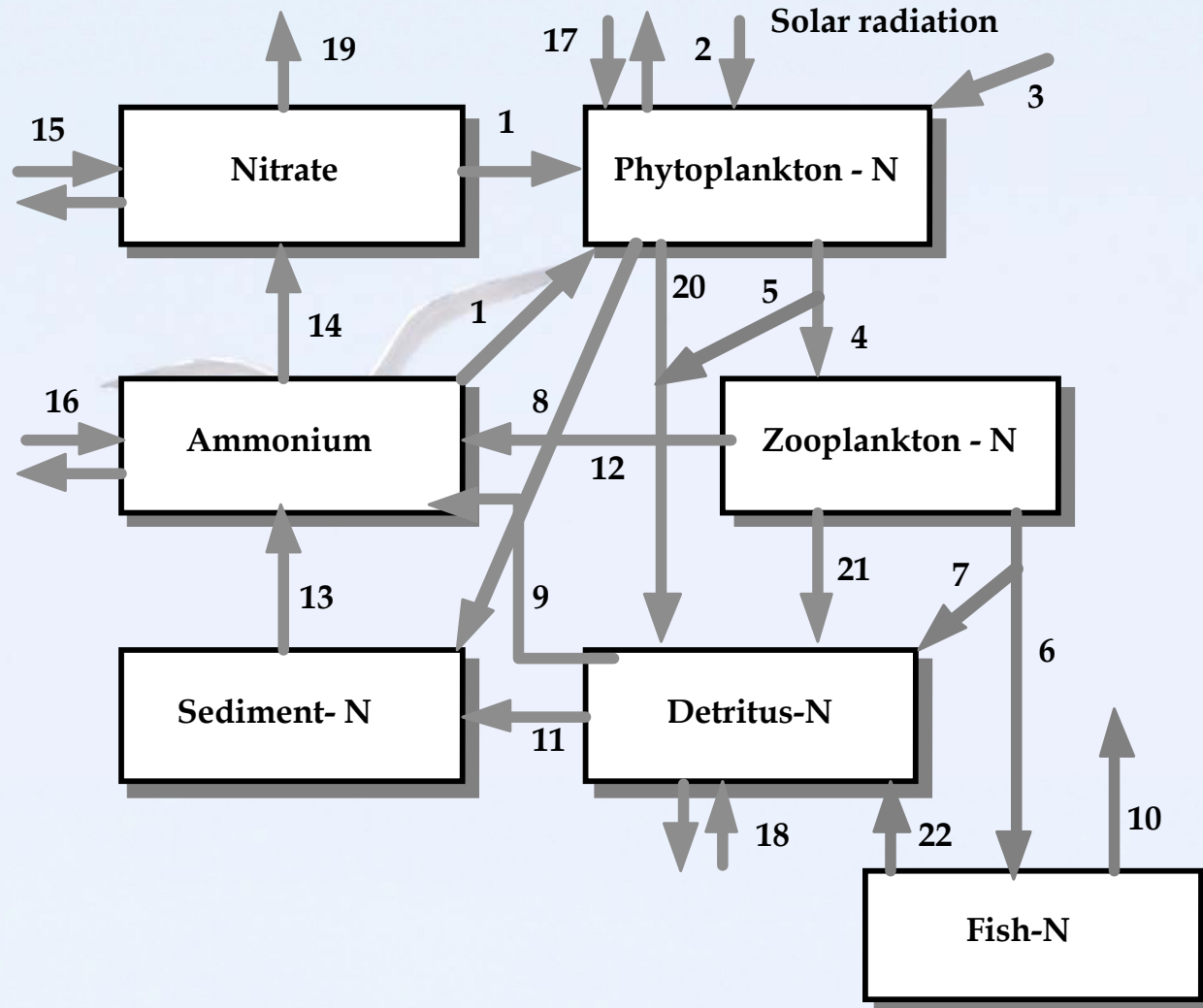
About models

- Models are simplified picture of reality (systems).
- In case of mathematical models this picture is “painted” using mathematical tools (variables, equations, computers, etc.)
- “All Models Are Wrong But Some Are Useful” - George Box.
- The main task of modellers is to develop useful models.

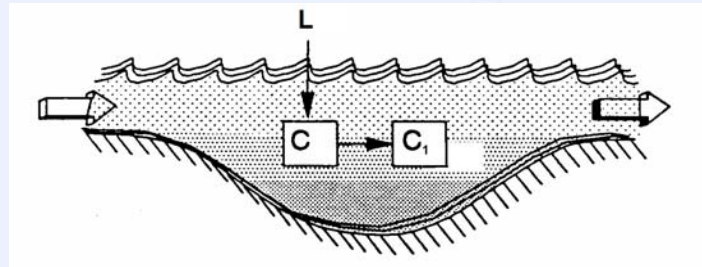


Continuous stirring case

- The main goal of biogeochemical models is to describe the cycles of chemicals (dynamics and spatial distribution of concentrations)



- The easiest way to do it is for so called continuous stirred reactors, i.e. for water bodies when concentration of chemicals is spatially uniform.

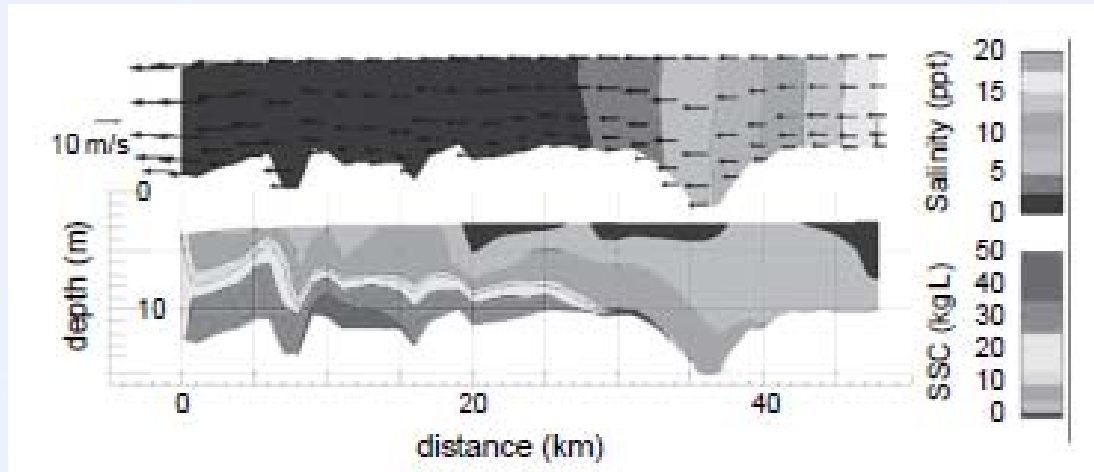


0-D model – set of ordinary differential equations derived from mass balance equation:

$$Accumulation = INFLOW - OUTFLOW \pm \sum \text{reaction_rates}$$

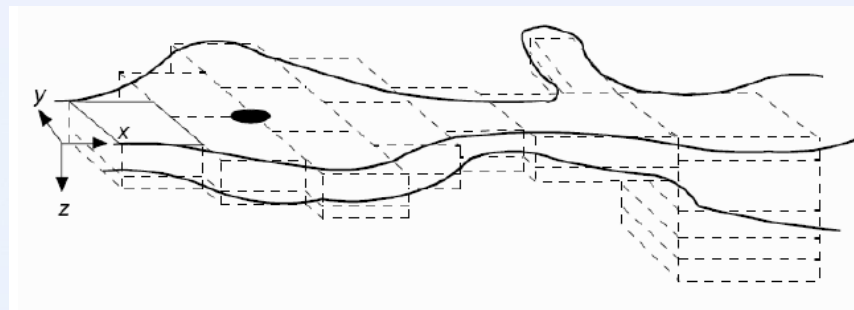
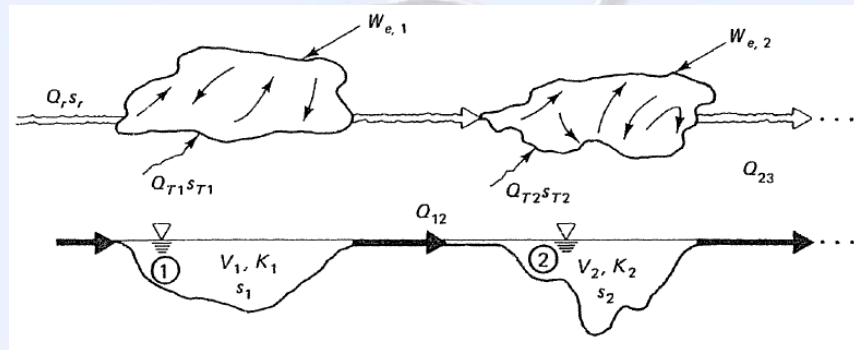


- Continuous stirred reactor assumption may be not valid for water bodies with a big area or high enough depth.
- More detailed description of hydrodynamics is necessary.



How to account for heterogeneity

- **Box model approach. Box models** are simplified versions of complex systems, reducing them to boxes (or reservoirs) linked by fluxes. The boxes are assumed to be mixed homogeneously.



Advantages and disadvantages of box models

- Box model – set of ordinary differential equations that can be solved fast on ordinary computer.
- Not good in case of strong gradients of concentrations.



Spatially continuous model approach

- Together with hydrodynamic equations

$$\frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + \nabla \cdot (\vec{v}\vec{v}) = \vec{g} - \frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{v} - 2\vec{\Omega} \times \vec{v} + \vec{F}_{fr}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

→

$$\vec{v} = (u, v, w)$$

→

g - gravitational force

→

Ω - angular velocity of the Earth

→

F_r - external forces



- Advection-diffusion equation should be solved for each constituent:

$$\frac{\partial C}{\partial t} = \underbrace{-\frac{\partial uC}{\partial x} - \frac{\partial vC}{\partial y} - \frac{\partial wC}{\partial z}}_{\text{advection}} + \underbrace{\frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right)}_{\text{diffusion}} + \frac{\partial C}{\partial t} \Big|_{\text{reactions}} + S_L + S_B$$

where:

C - concentration of the water quality constituent, mg/L or g/m³

t - time, days

u, v, w - longitudinal, lateral, and vertical advective velocities, m/day

D_x, D_y, D_z - longitudinal, lateral, and vertical diffusion coefficients, m²/day

S_L - direct and diffuse loading rate, g/m³ per day

S_B - boundary loading rate (including upstream, downstream, benthic, and atmospheric), g/m³ per day

$\frac{\partial C}{\partial t} \Big|_{\text{reactions}}$ - total kinetic transformation rate (reactions); g/m³ per day



Levels of coupling

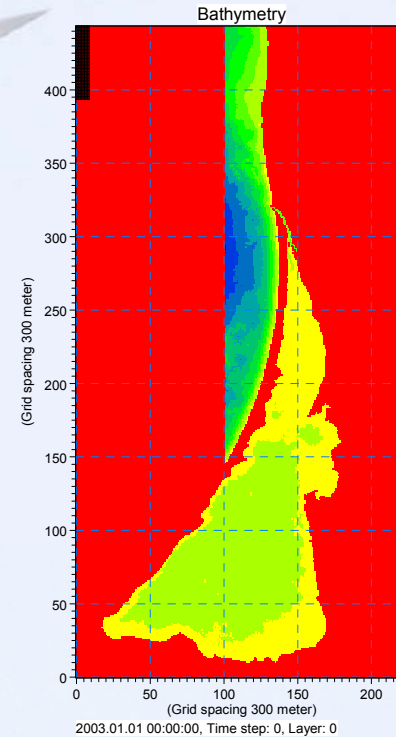
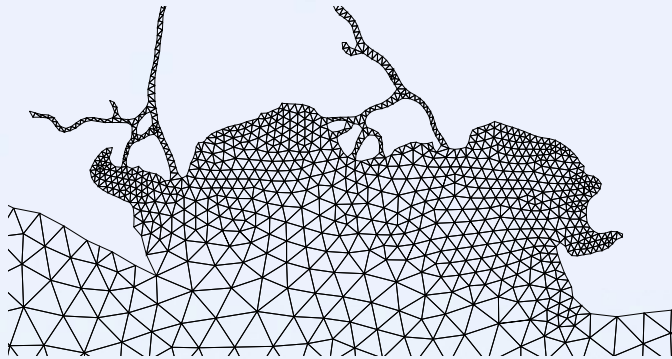
- Coupling on the source code level : one computer program.
- Coupling on the data level : standalone programs for hydrodynamics and biogeochemistry (solves kinetic equations together with advection diffusion equations).
 - Exchange of hydrodynamic data through files.
 - Spatial and time resolution may be different for hydrodynamics and biogeochemistry.



Numerical solution methods:

Finite difference method

Finite element method



Computer time consumption

- Solution of partial differential equations is rather computer time consumptive.
- Coupling hydrodynamics with biogeochemistry makes it even more complicated because of advection-diffusion equation should be solved for each state variable of biochemical model.
- The parallel computing and high performance computers are welcomed in order to get results in a reasonable time.



Parallel Computing Models

- **Computer Architecture Shared memory (SMP):** one computer, many processors.

Programming Standard: **OpenMP**. Implemented into compiler. Directives – comments in source code

- **Computer Architecture Distributed Memory:**
Computer clusters or SMP

Programming Standard: **MPI** (Message Passing Interface). Library of functions called using statement CALL.



Example of OpenMP FORTRAN program

```
PROGRAM HELLO

  INTEGER NTHREADS, TID, OMP_GET_NUM_THREADS,
+   OMP_GET_THREAD_NUM

C   Fork a team of threads giving them their own copies of variables
!$OMP PARALLEL PRIVATE(NTHREADS, TID)

C   Obtain and print thread id
TID = OMP_GET_THREAD_NUM()
PRINT *, 'Hello World from thread = ', TID

C   Only master thread does this
IF (TID .EQ. 0) THEN
  NTHREADS = OMP_GET_NUM_THREADS()
  PRINT *, 'Number of threads = ', NTHREADS
END IF

C   All threads join master thread and disband
!$OMP END PARALLEL

END
```



Example of MPI FORTRAN program

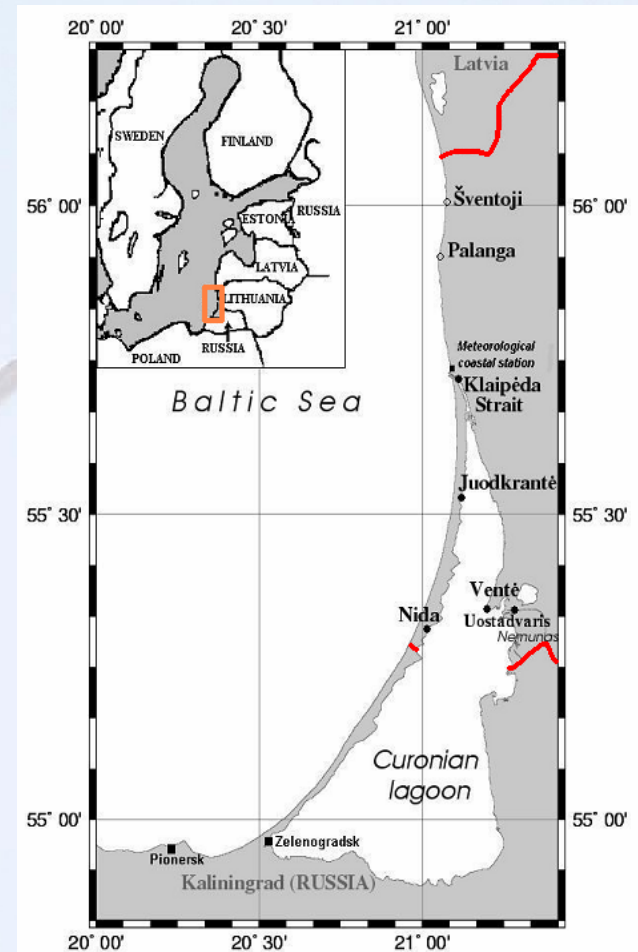
```
program main
include 'mpif.h'
integer ierr, rank, size

call MPI_INIT( ierr )
call MPI_COMM_RANK( MPI_COMM_WORLD, rank,
  ierr )
call MPI_COMM_SIZE( MPI_COMM_WORLD, size,
  ierr )
print *, 'I am ', rank, ' of ', size
call MPI_FINALIZE( ierr )
end
```

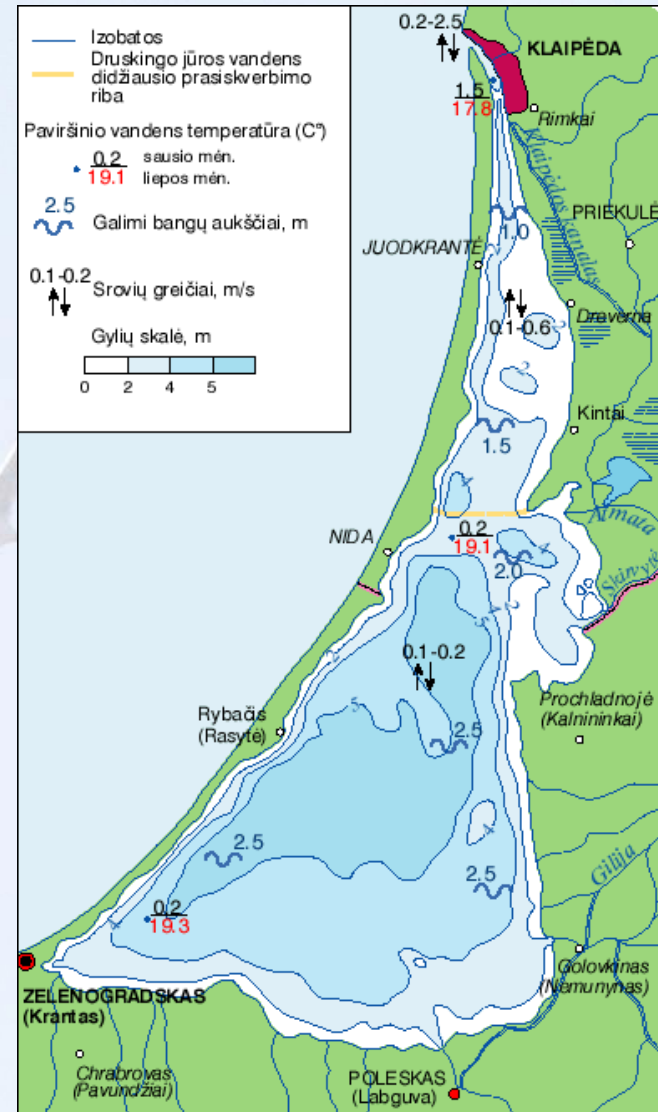


Curonian lagoon

- Total area 1600km²
- Total volume 6.2km³



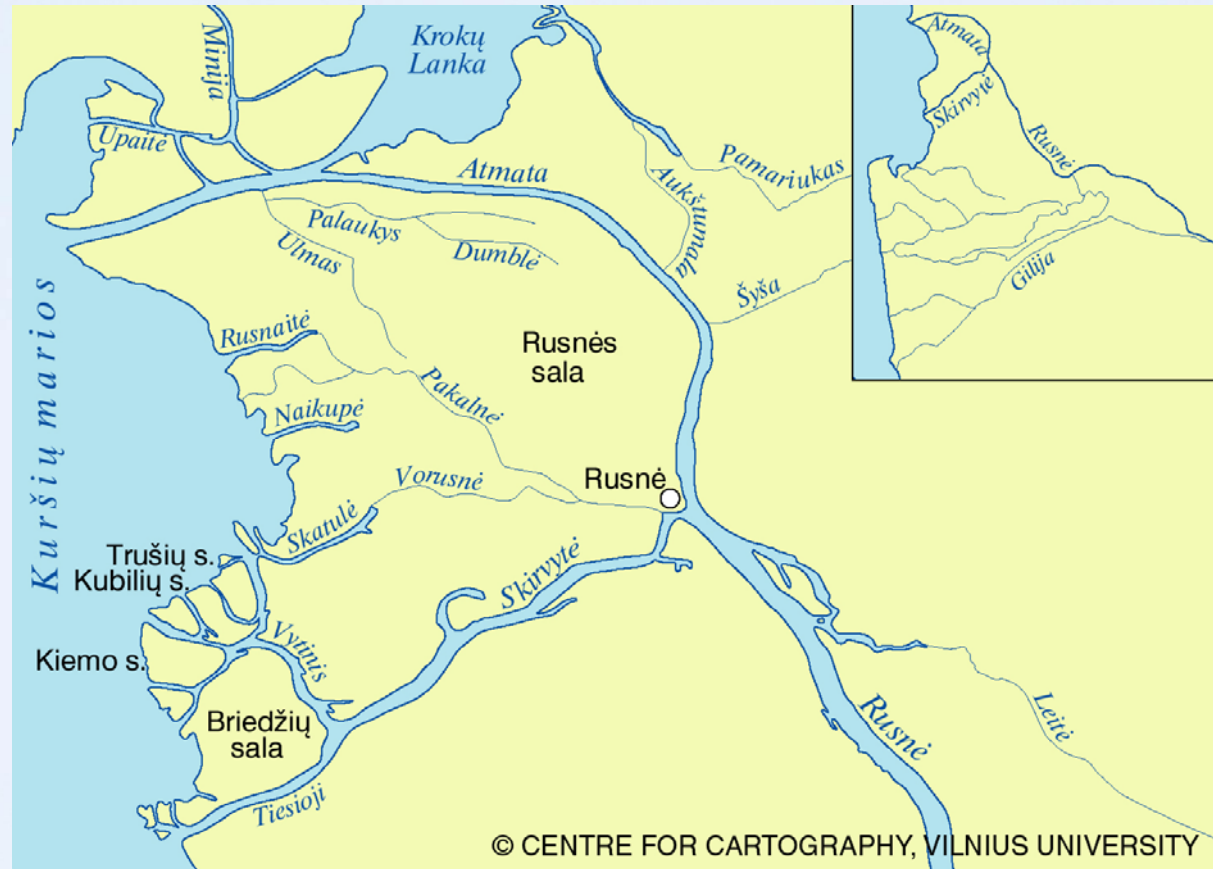
- Average depth 3.8m
- Southern part max depth ~5m.
- Klaipeda strait max depth 16m
- Klaipeda strait width ~ 300m



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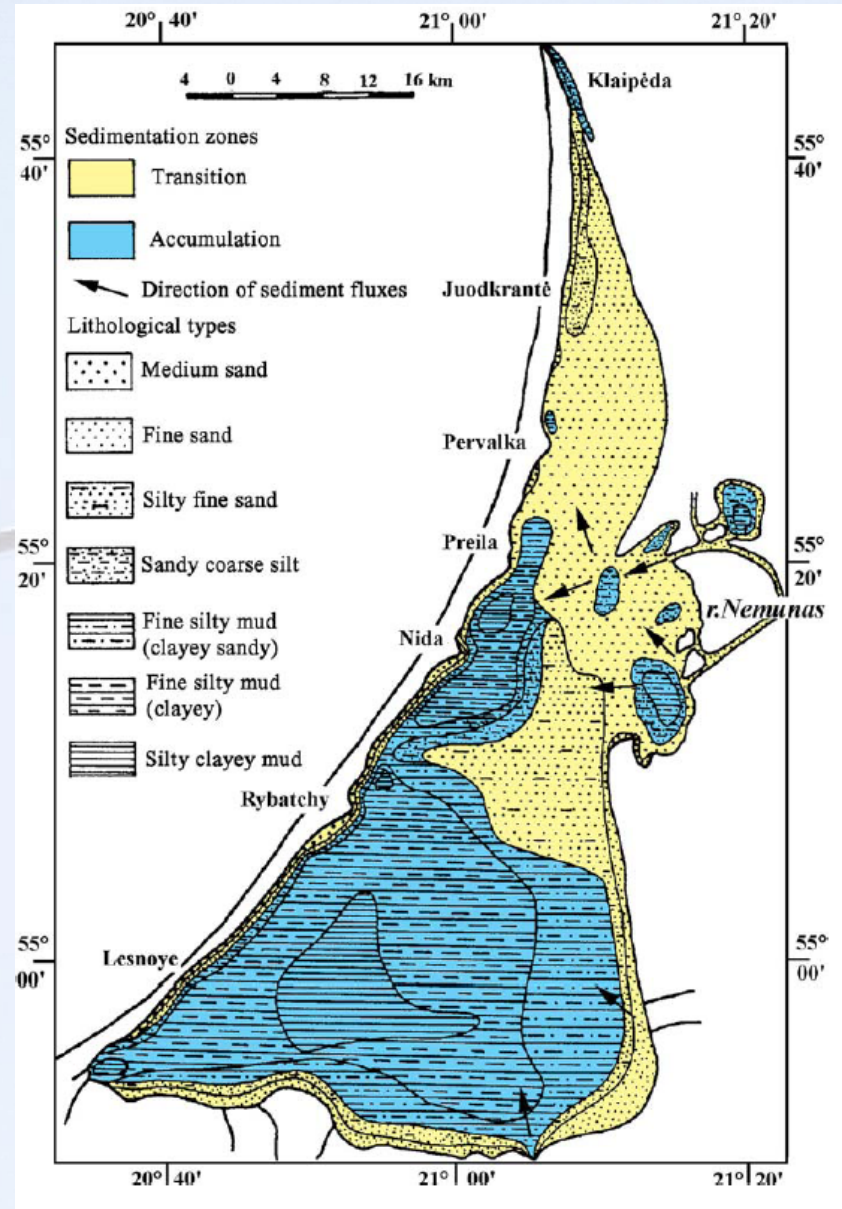
- Fresh water runoff is dominated by Nemunas river ($22\text{km}^3/\text{y}$)
- Nemunas mouth is rather complicated



- Complicated network of small rivers and channels in Kaliningrad region. Discharge data are not available.



- Bottom sediment map and transition accumulation areas (Gulbinskas, 1995).



Model applications

- Finite difference 2D models (mainly for circulation investigation).
 - Chubarenko & Chubarenko (1995)
 - Raudsepp & Kõuts (2002)
 - Davulienė et al. (2002)



- Application of finite element model (SHYFEM,2D) in 2003-2004 (Ferrarin et al. 2008).



- Much useful information was obtained.



- Circulation patterns

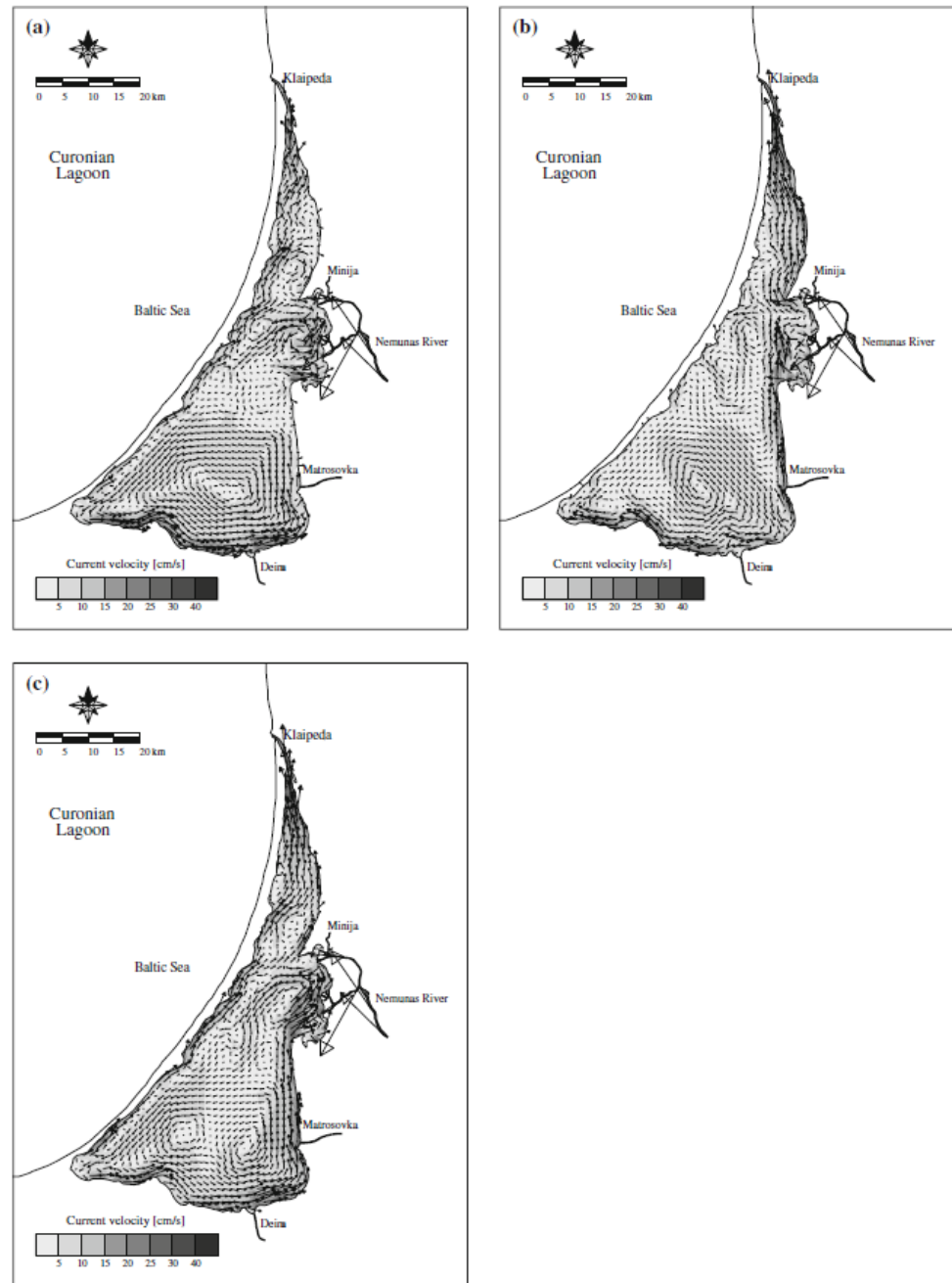
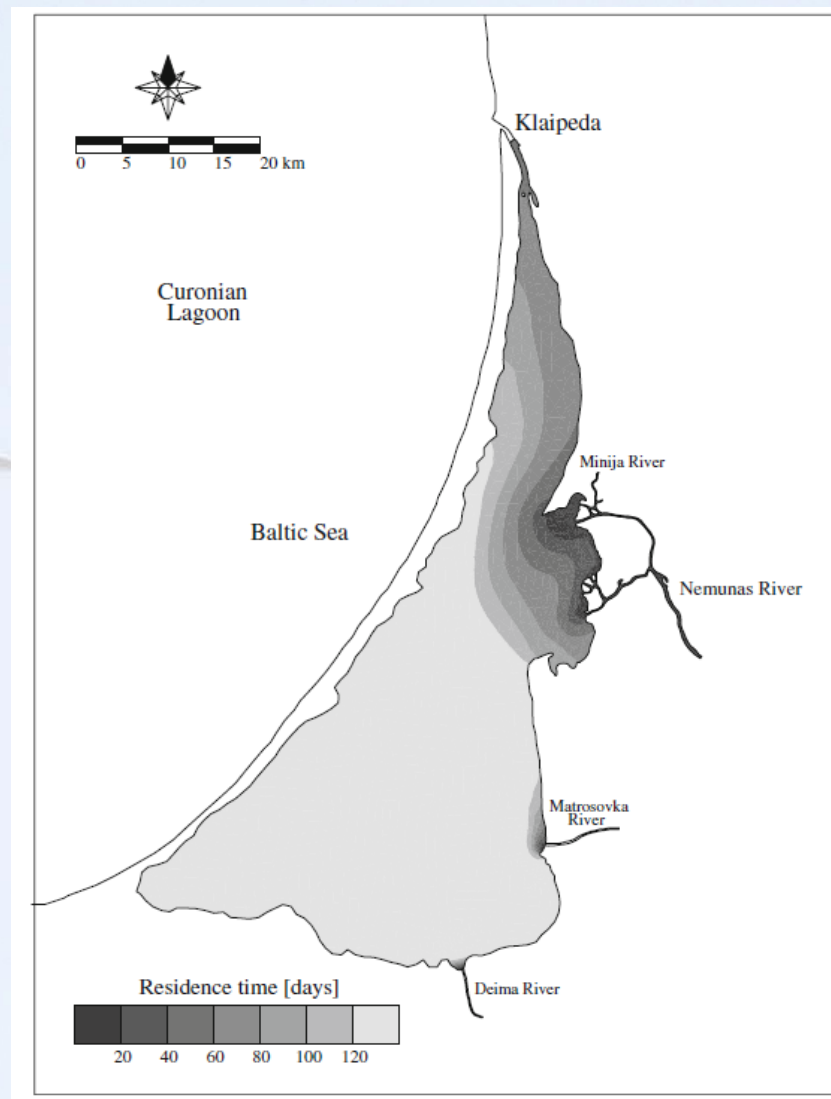


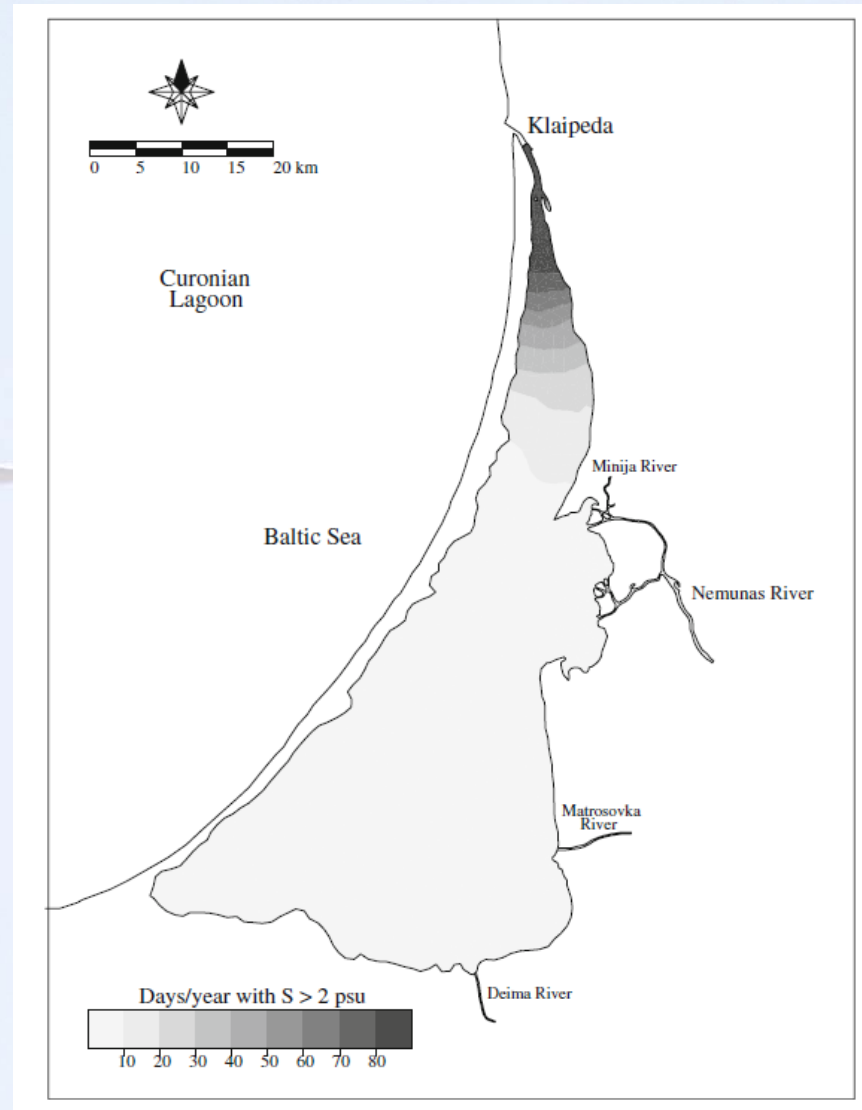
Fig. 2 Simulated water circulation imposing idealized wind forcing. (a) West wind; (b) South-East wind; (c) South-West wind



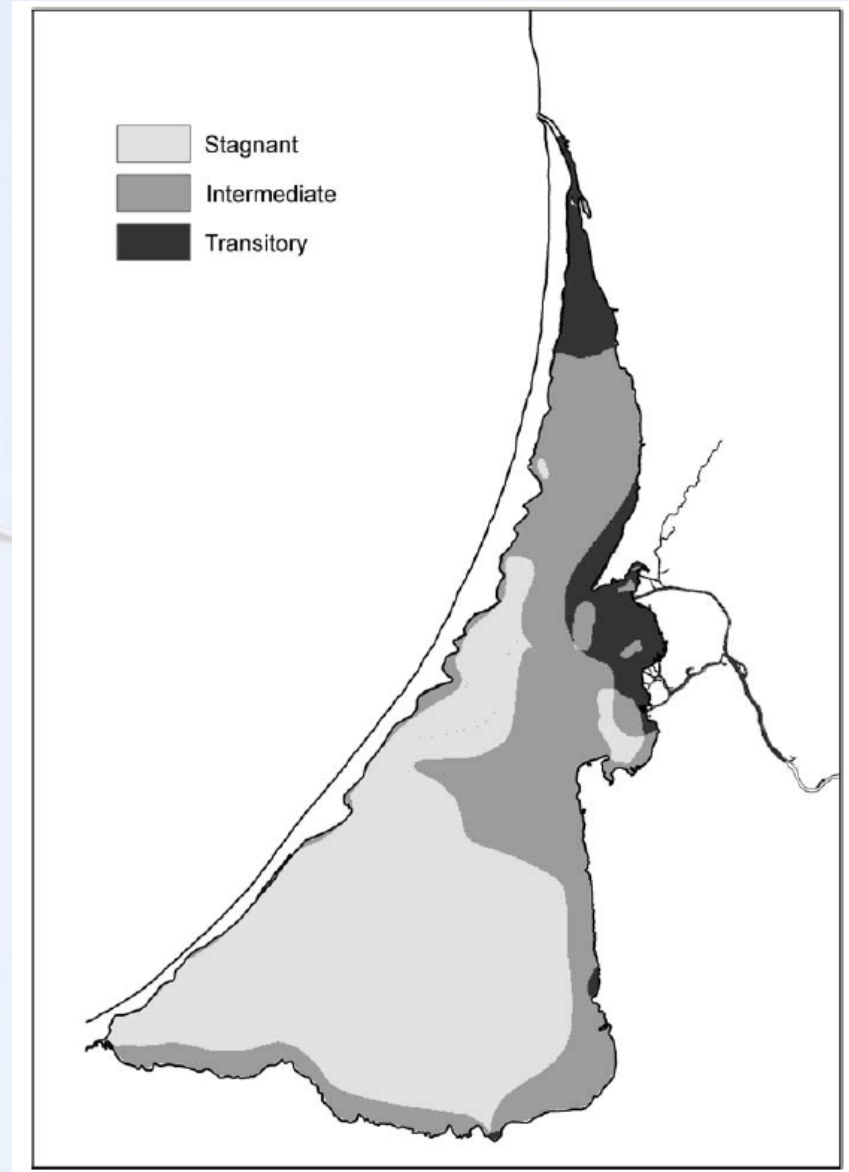
- Average residence time



- Salinity:
 - Days per year with salinity higher than 2 psu



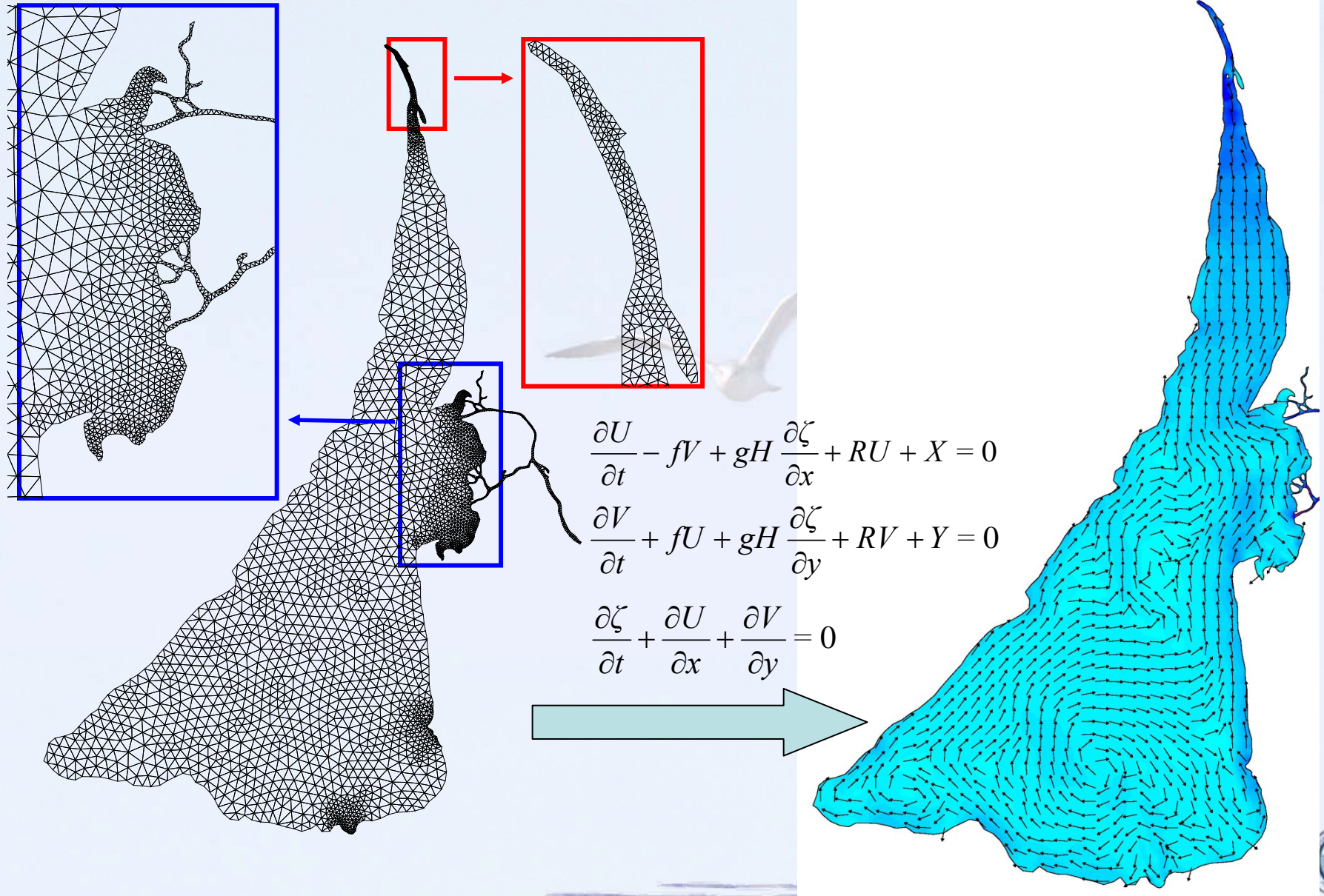
- Hydraulic regime based zonation scheme of the Curonian Lagoon derived by combining the simulated hydrodynamic results and the sediment classification



***SHYFEM* advantages**

- Flexible mesh enables to resolve complex spatial features.





- Multidimensionality. Possibility to create 2D and 3D models.
- Interface for coupling of hydrodynamics with ecological models (code level).



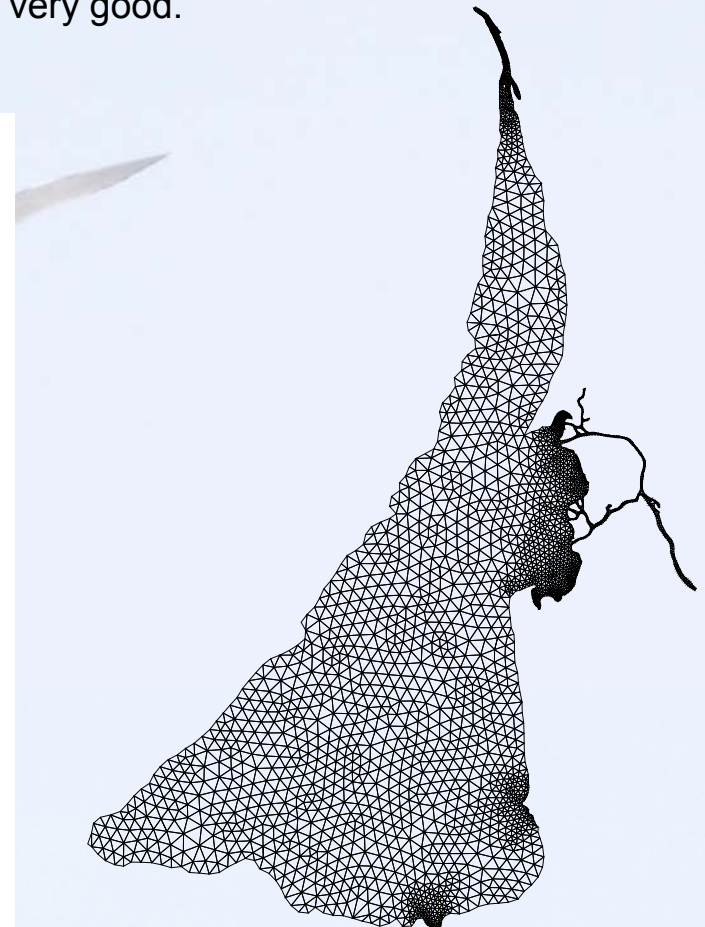
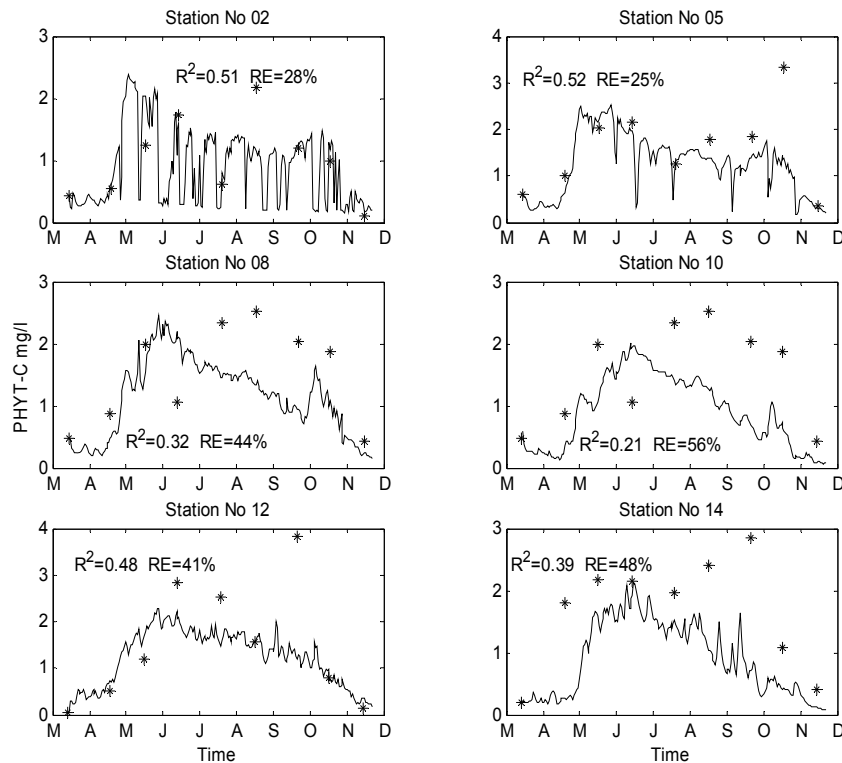
Coupling with biochemical models

- First SHYFEM version coupled (code level) with biogeochemical model EUTRO (WASP) was developed by G.Umgiesser in 2000.
- First application of SHYFEM/WASP for Curonian lagoon by A. Erturk and P.Zemlys in 2004 (P.Zemlys et al. 2008).



SHYFEM/EUTRO for Curonian lagoon

- Main features
 - 9 WQ state variables.
 - One phytoplankton group.
 - Pelagic part only.
 - Reproduction of phytoplankton dynamics was not very good.



Model SHYFEM/AQUABC (2D)

- Development supported by EU and Norway fund.
- Work was done in collaboration with Venice Marine Institute and Istanbul Technical University as a part of the project:
 - **A system for the sustainable management of Lithuanian marine resources using novel surveillance, modeling tools and ecosystem approach.**
- AMBER
- Beside of development of water quality model 3D finite element hydrodynamic model was applied first to the Curonian lagoon.



- **AQUABC** was started to be developed as biochemical model coupled with SHYFEM, later as the water column part of box model ESTAS under name ALUKAS by A.Erturk and finally was ported to SHYFEM again as water column module of biochemical model AQUABC.
- AQUABC consists of two modules: 1) Water column module (ALUKAS); 2) Bottom sediment module (under development)



- Main features of the water column module:
 - 22 WQ state variables.
 - 3 phytoplankton groups (diatoms, cyanobacteria, greens). Simulation of nitrogen fixation.
 - One zooplankton group.
 - Nutrients: Nitrogen, phosphorus, silica

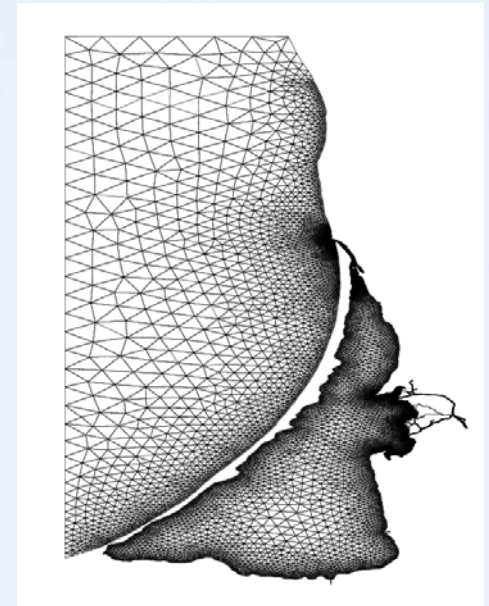
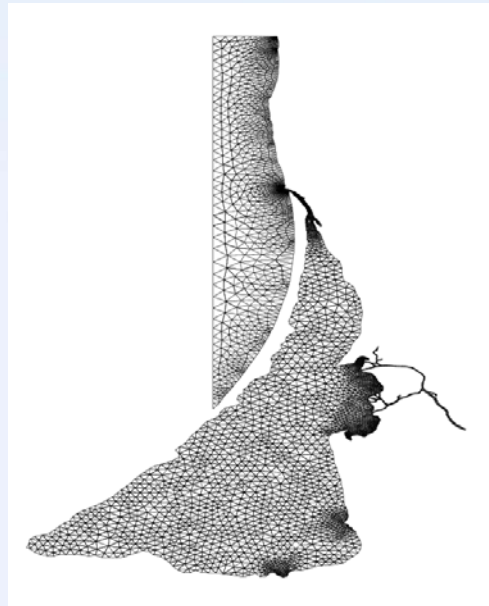
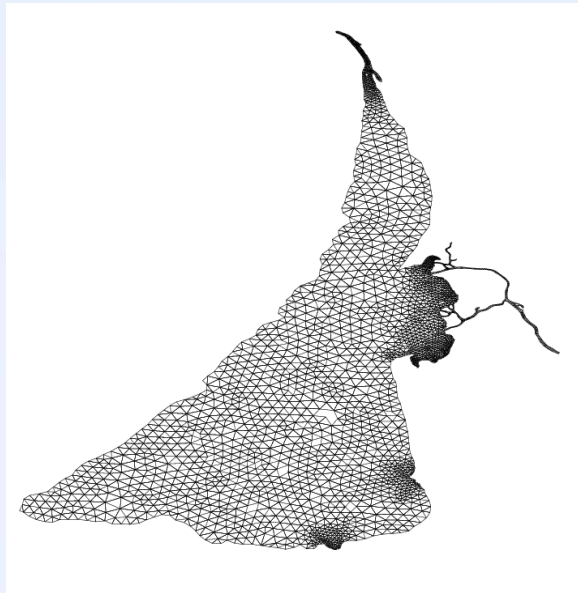


Water column state variables

- 1. AMMONIUM NITROGEN
- 2. NITRATE NITROGEN
- 3. ORTHOPHOSPHATE PHOSPHORUS
- 4. PHYTOPLANKTON CARBON FOR GREENS
- 5. EXTERNAL LABILE DISSOLVED DETRITUS CARBON
- 6. DISSOLVED OXYGEN
- 7. EXTERNAL LABILE PARTICULATE DETRITUS CARBON
- 8. EXT. REFRACTORY DISS. DETRITUS CARBON
- 9. ZOOPLANKTON CARBON
- 10. NONBIOGENIC SILICA
- 11. EXTERNAL REFRACTORY PARTICULATE DETRITUS CARBON
- 12. PHYTOPLANKTON CARBON FOR DIATOMS
- 13. PHYTOPLANKTON CARBON FOR CYANOBACTERIA
- 14. INORGANIC CARBON
- 15. GREENS DISSOLVED DETRITUS CARBON
- 16. GREENS PARTICULATE DETRITUS CARBON
- 17. DIATOM DISSOLVED DETRITUS CARBON
- 18. DIATOM PARTICULATE DETRITUS CARBON
- 19. CYANOBACTERIA DISSOLVED DETRITUS CARBON
- 20. CYANOBACTERIA PARTICULATE DETRITUS CARBON
- 21. ZOOPLANKTON DISSOLVED DETRITUS CARBON
- 22. ZOOPLANKTON PARTICULATE DETRITUS CARBON



Modelling grids



Open sea boundary condition

- Operational hydrodynamic model HIROMB (1 nautical mile horizontal resolution).
- Lithuania coastal area HIROMB (300m horizontal resolution).
- Monitoring data for water quality and phytoplankton.



Parallelisation

- OpenMP
- No traditional domain decomposition.
- Implementation of parallelism:
 - Kinetic equations solution loop on nodes.
 - Advection-diffusion equations solution loop on kinetic state variables.

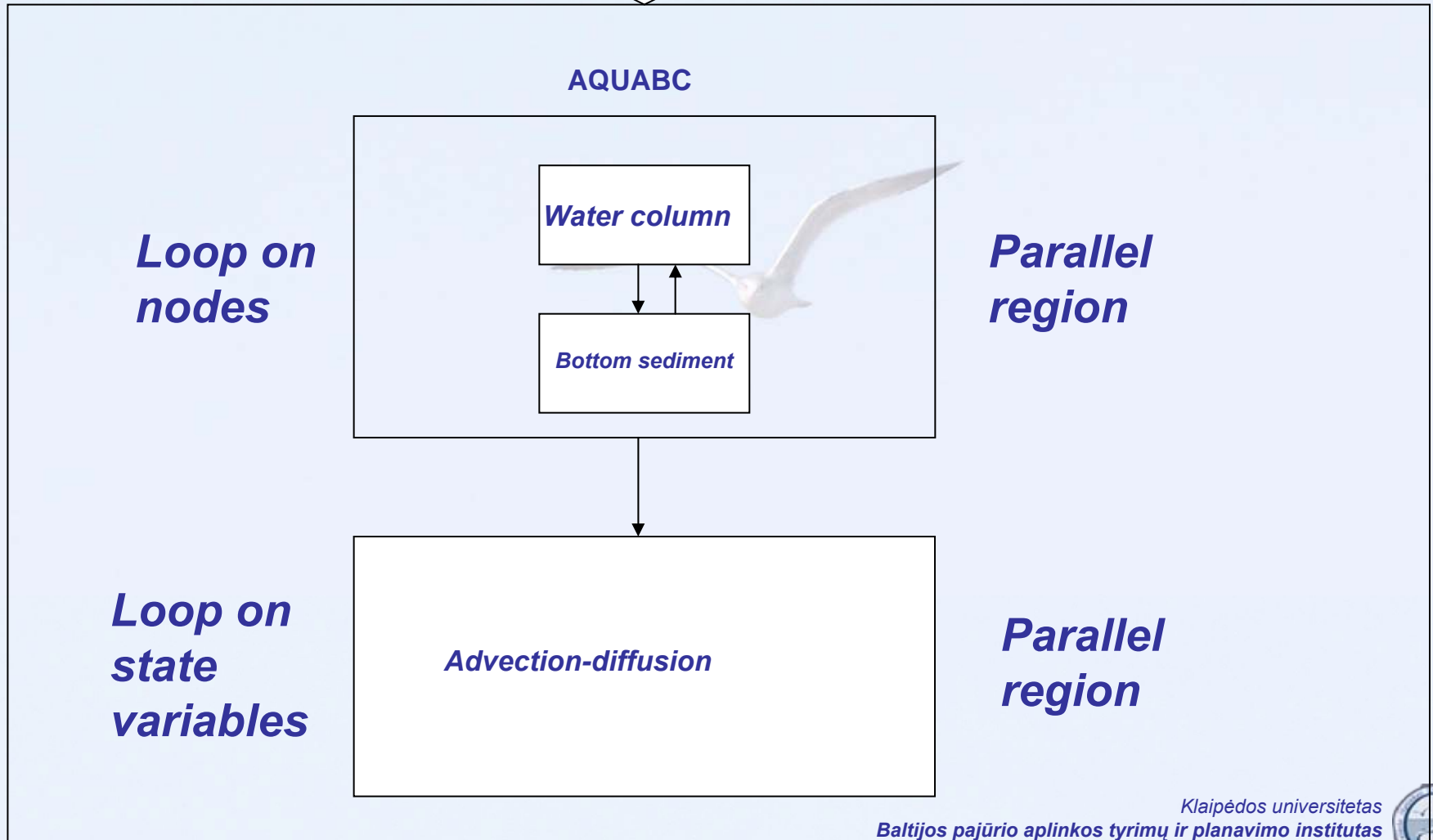


Parallelisation of SHYFEM/AQUABC

Hydrodynamic variables: velocity,
S,T, solar radiation...



AQUABC-FEM interface



Calculation speed

- One year run for the middle size grid (4524 nodes, 7687 elements) on server with 16 cores – 3h.

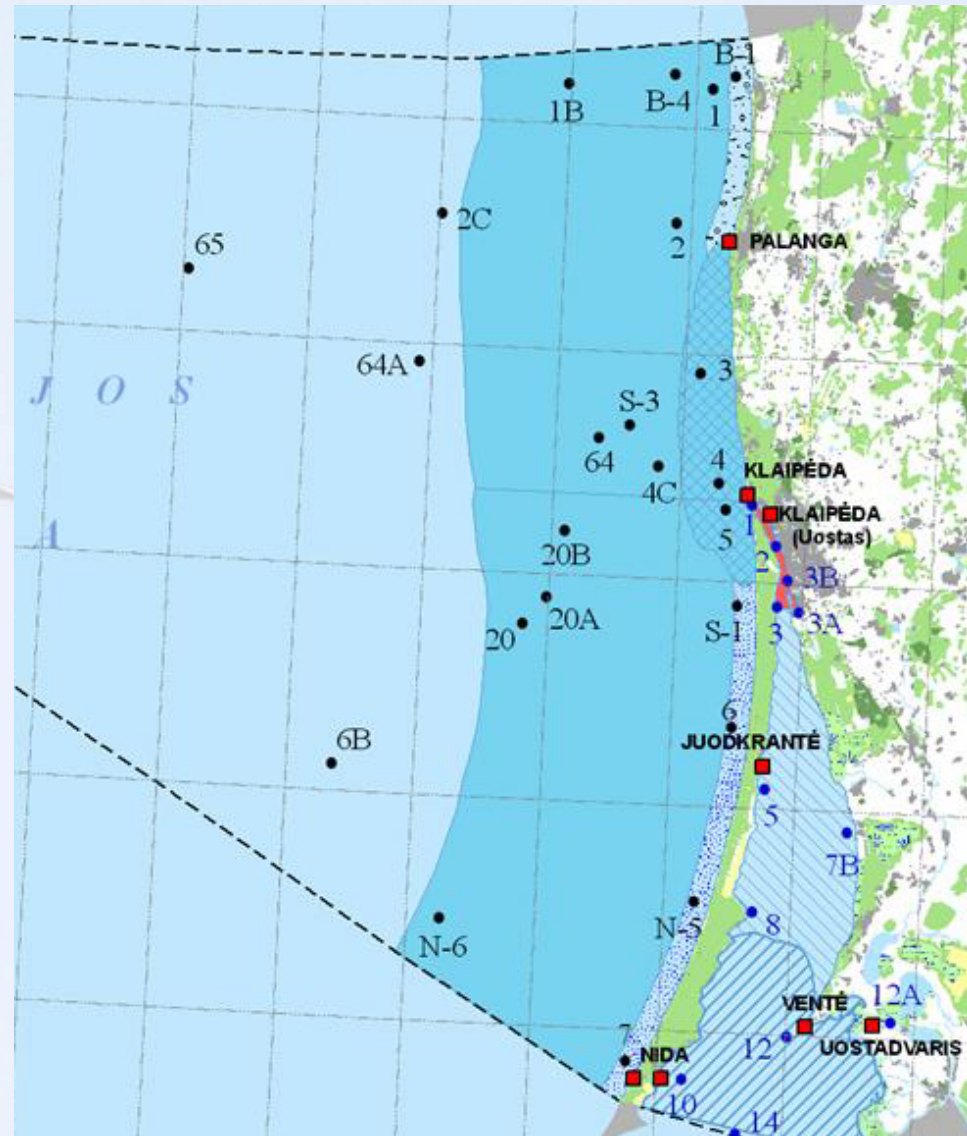


Performance. HYDRODYNAMICS

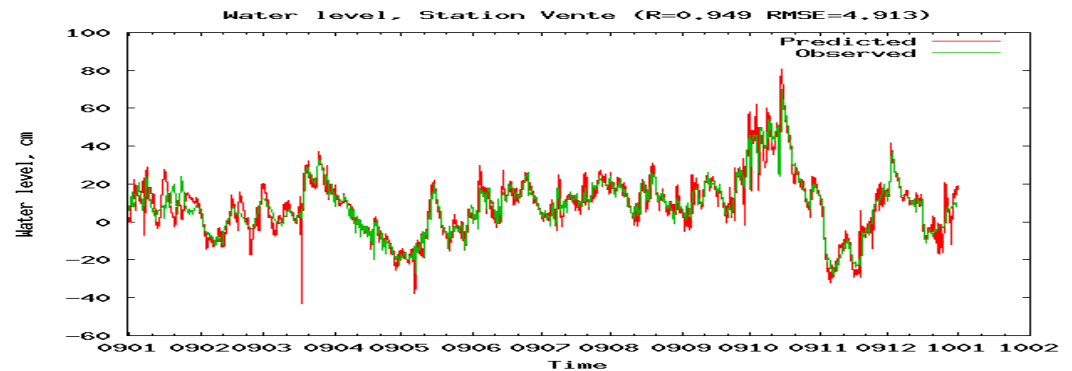
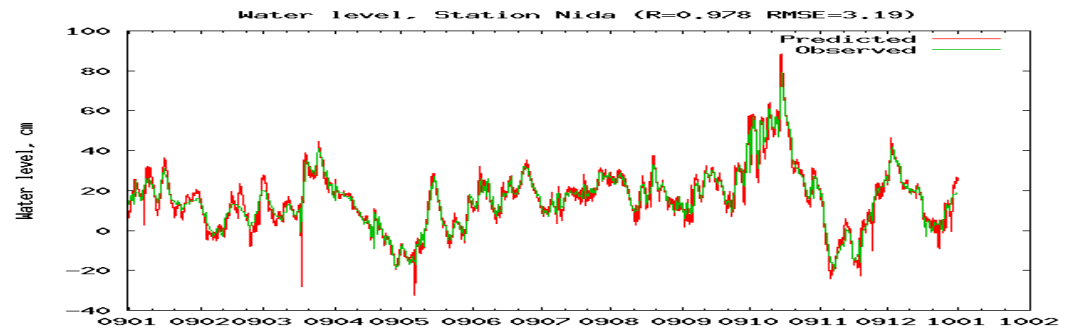
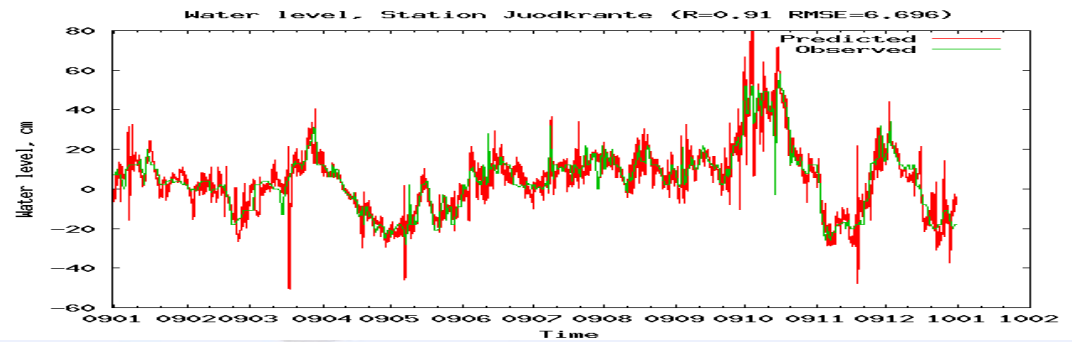
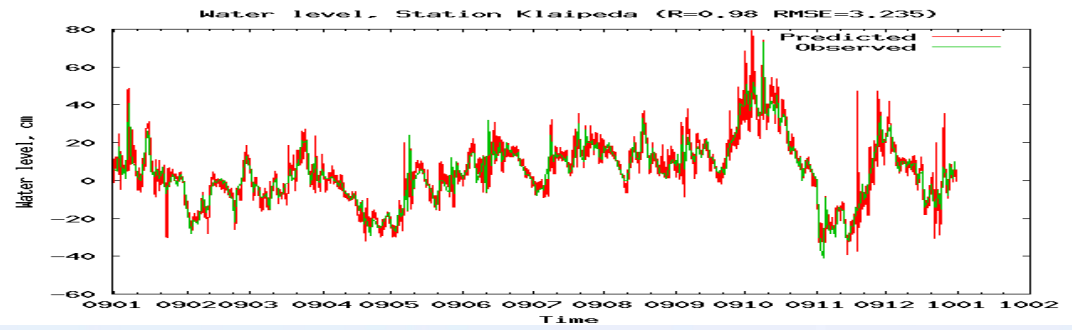


Measurements

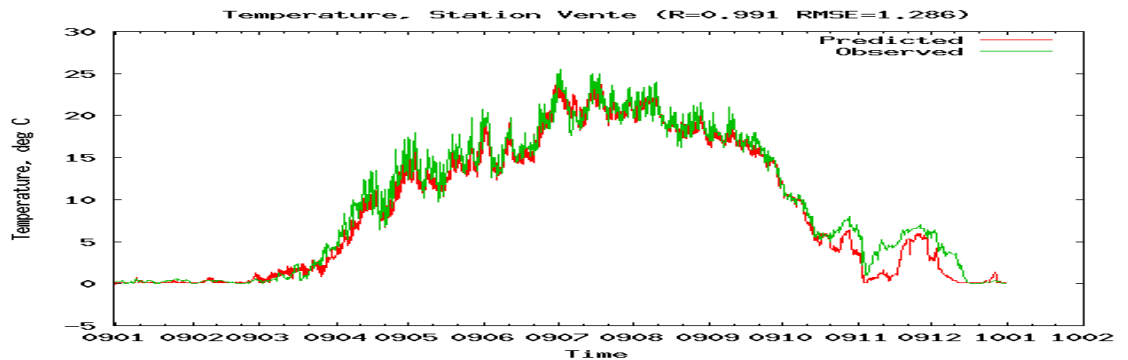
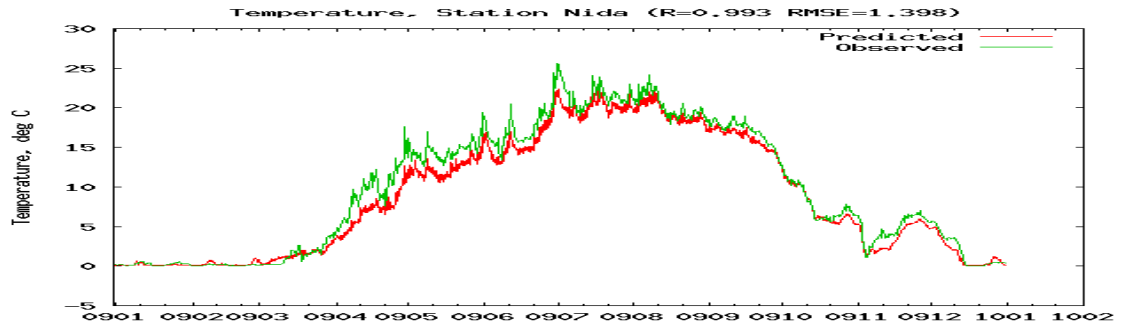
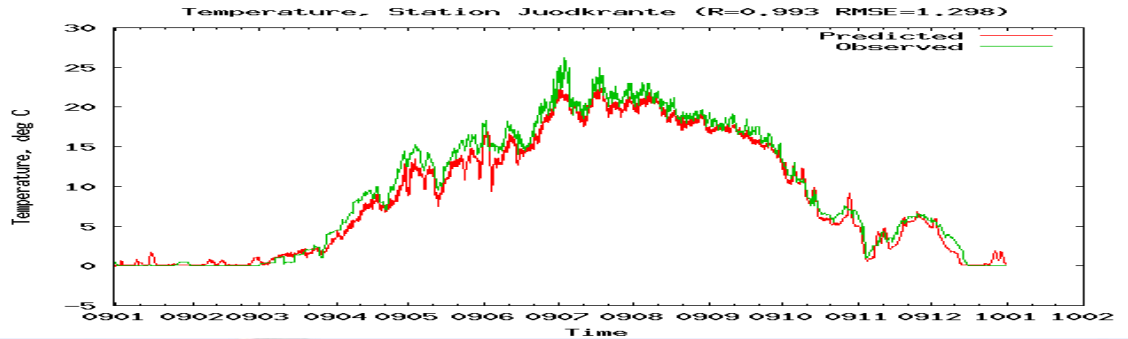
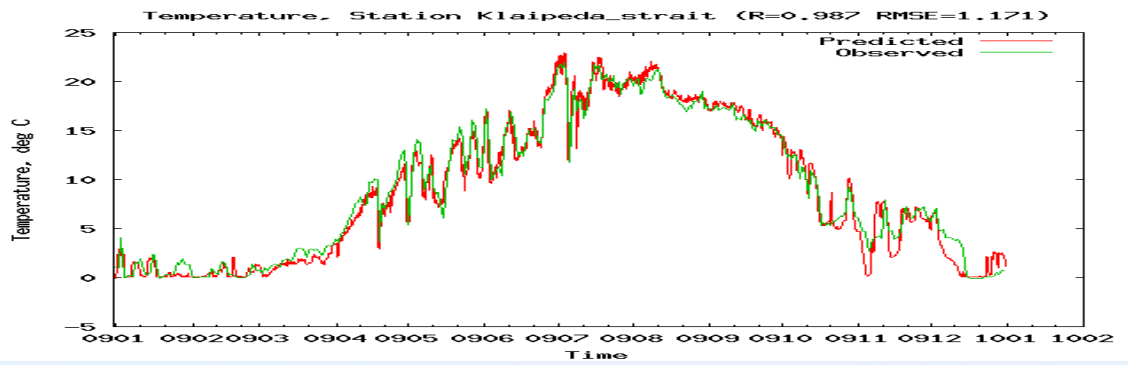
- Coastal monitoring stations (marked in red).
- Water levels measured inside of the Curonian lagoon.



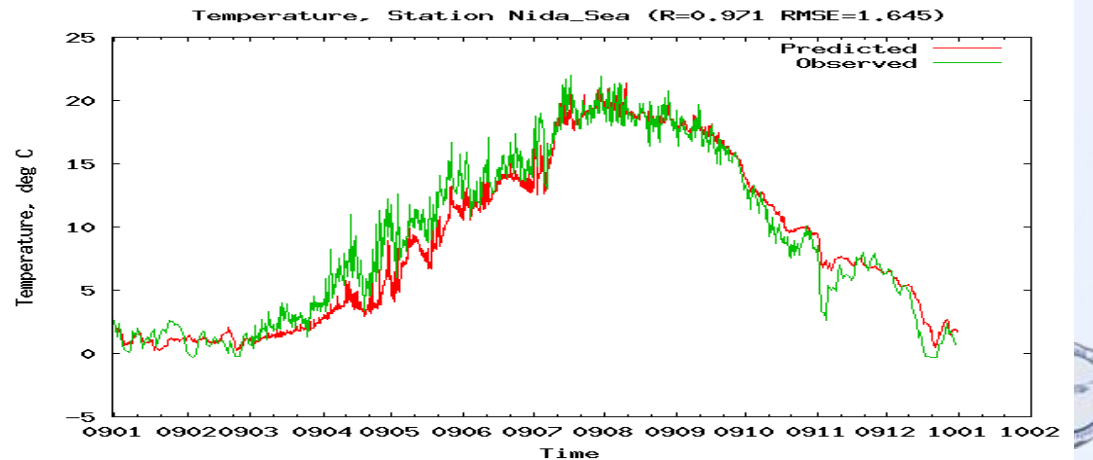
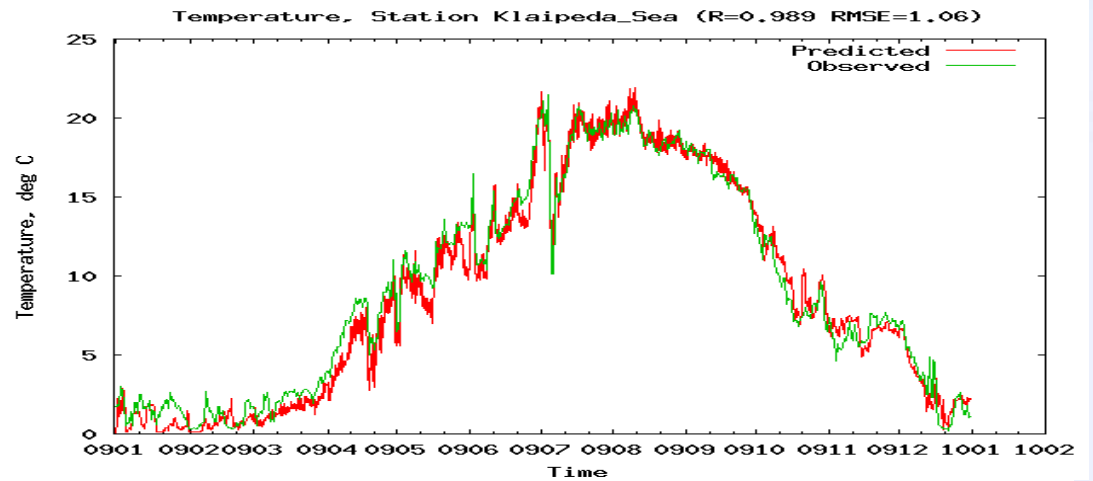
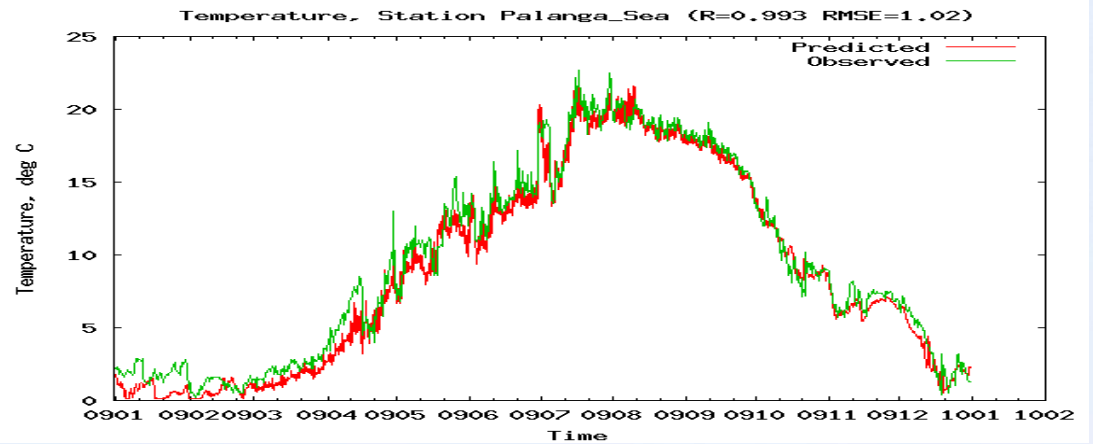
- Water level, 2009



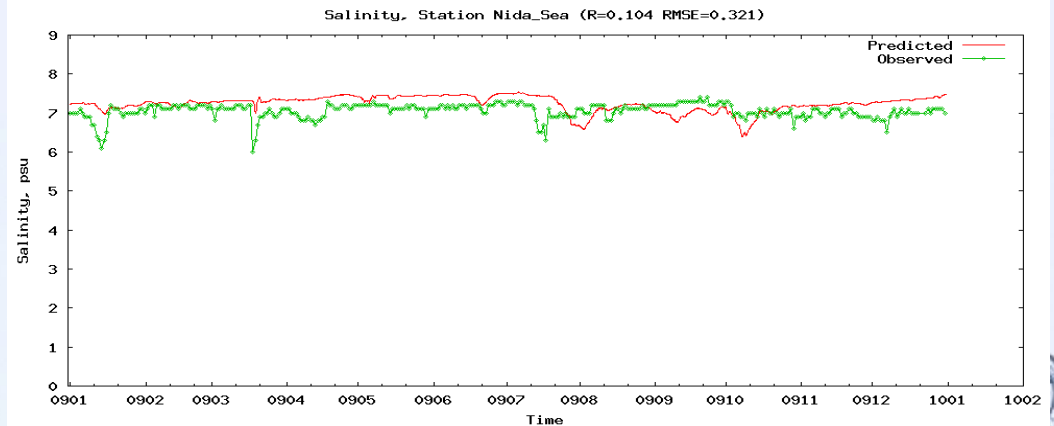
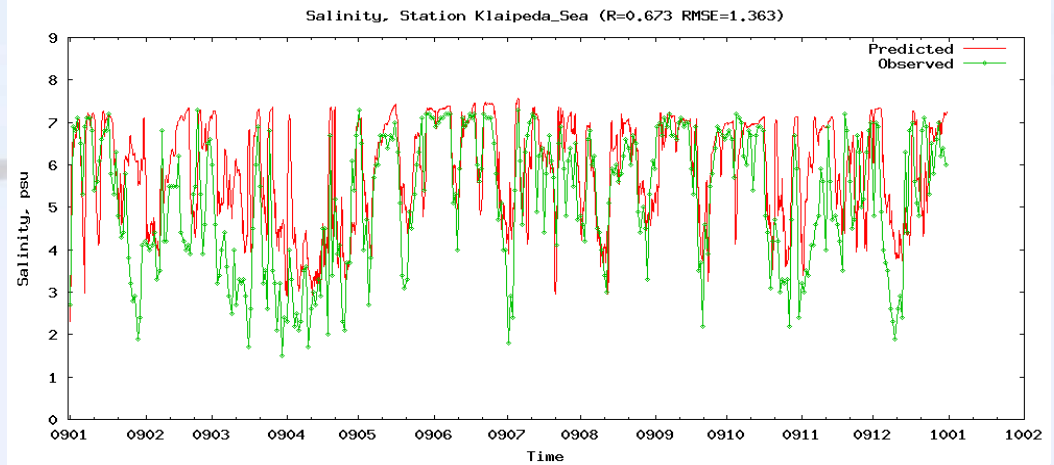
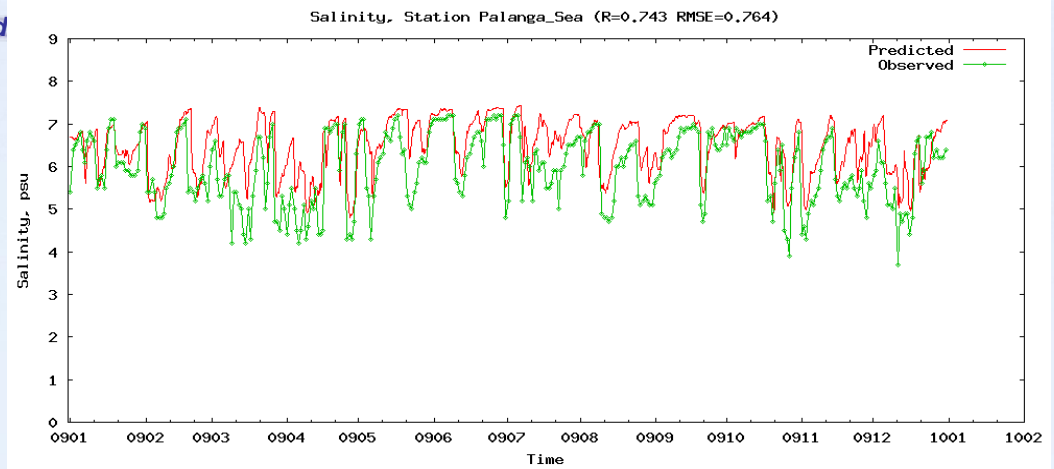
- Temperature, Curonian lagoon, 2009



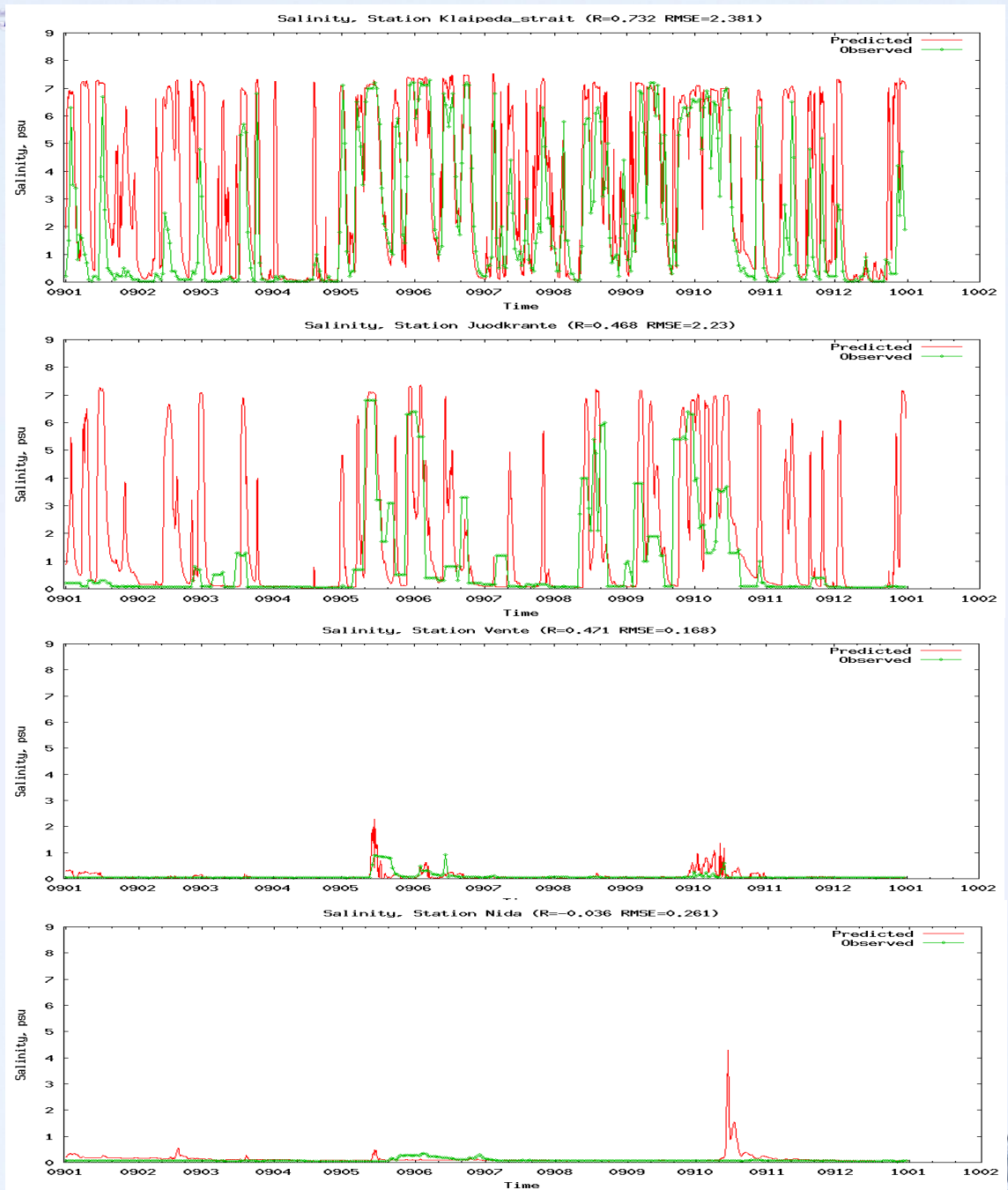
- Temperature, Baltic Sea, 2009



- Salinity, Baltic Sea, 2009



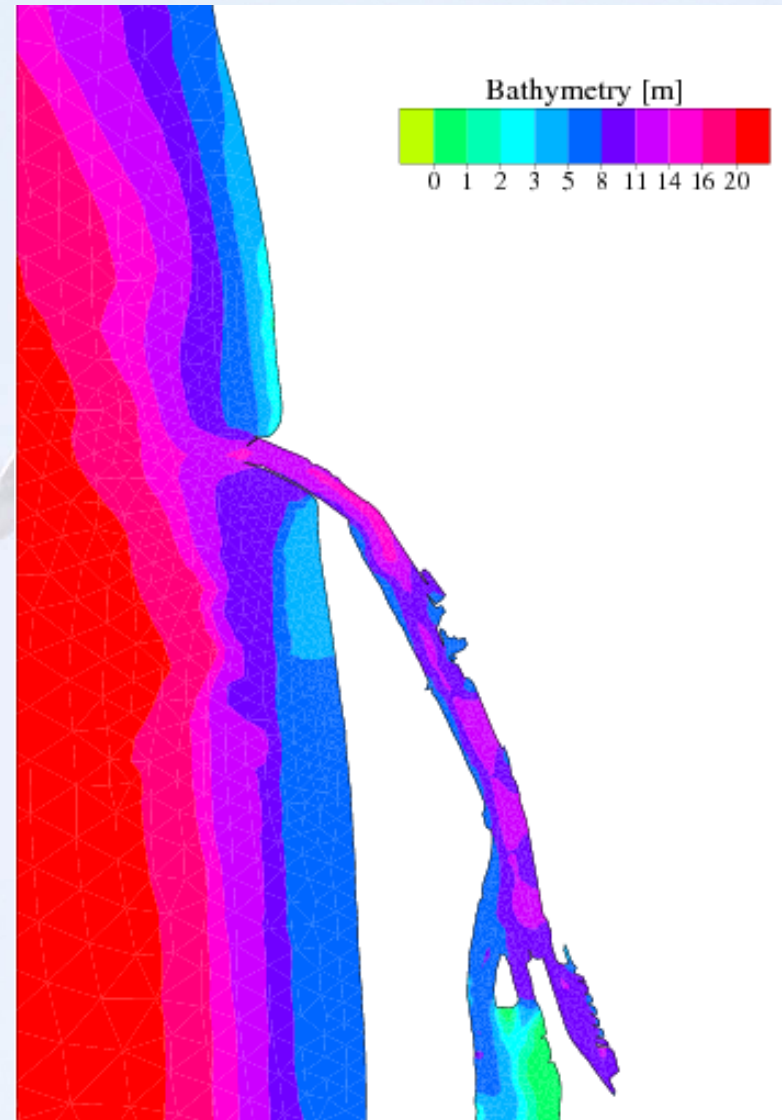
- Salinity, Curonian lagoon, 2009



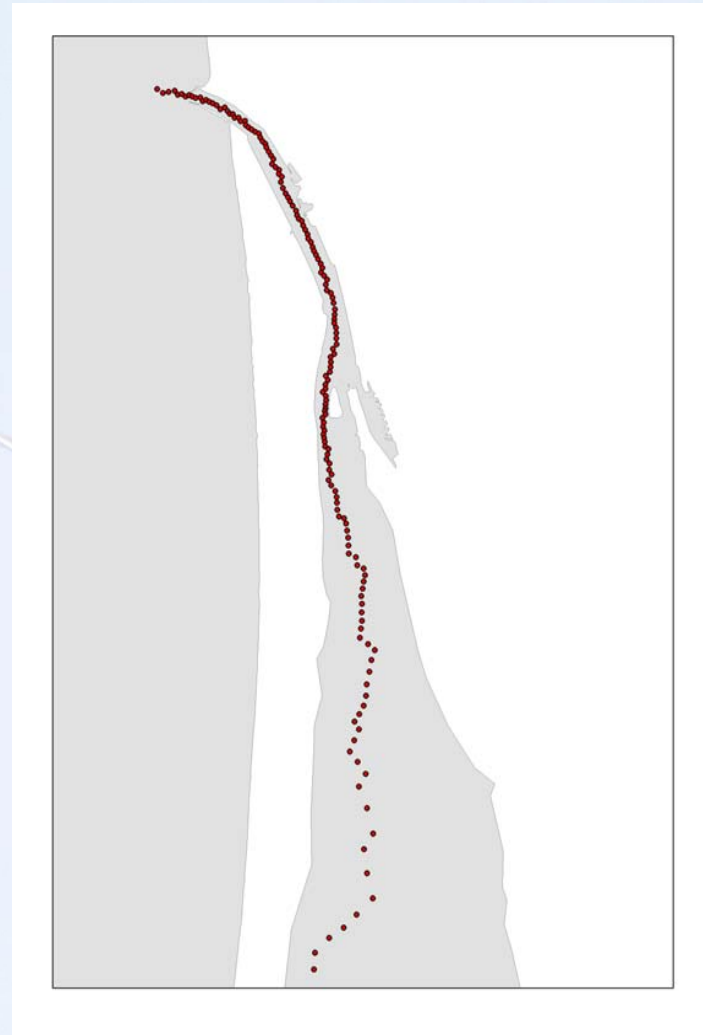
Vertical salinity distribution in the Klaipeda harbour area



- Klaipeda strait is the only a place where water exchange between lagoon and the Baltic Sea takes place.
- Max depth 16m.
- Also there is a place where salinity gradients may be expected.

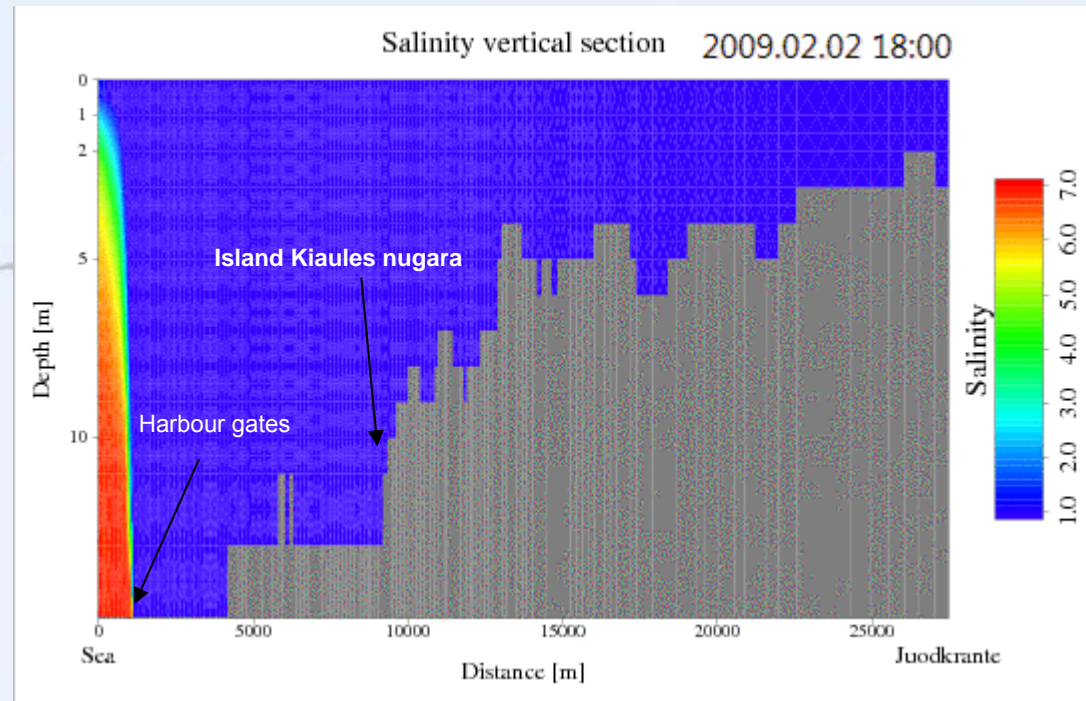


- The nodes of vertical section where model results were investigated

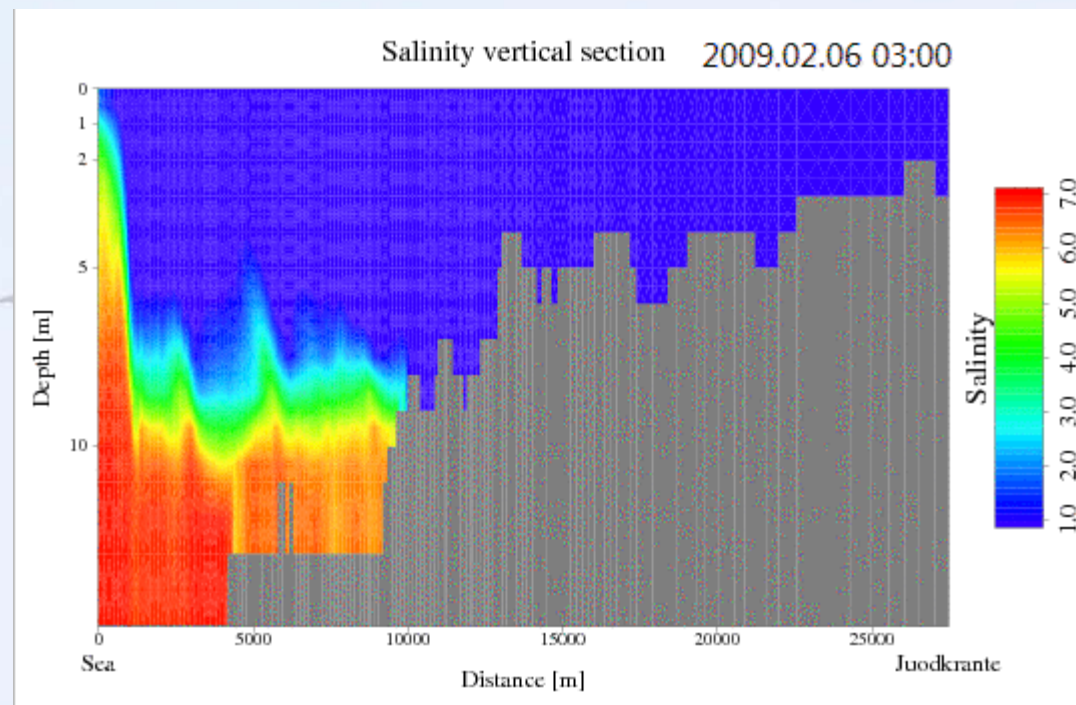


Types of salinity vertical distribution in Klaipeda strait

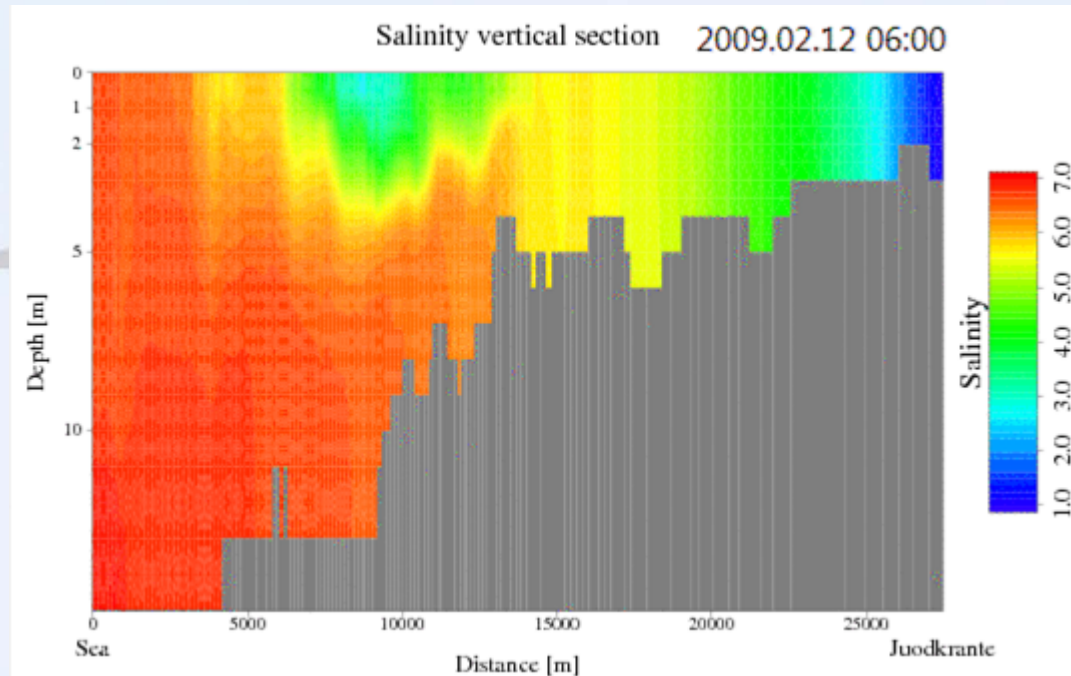
- **Type No 1** of salinity vertical distribution: only fresh water in the Klaipeda strait



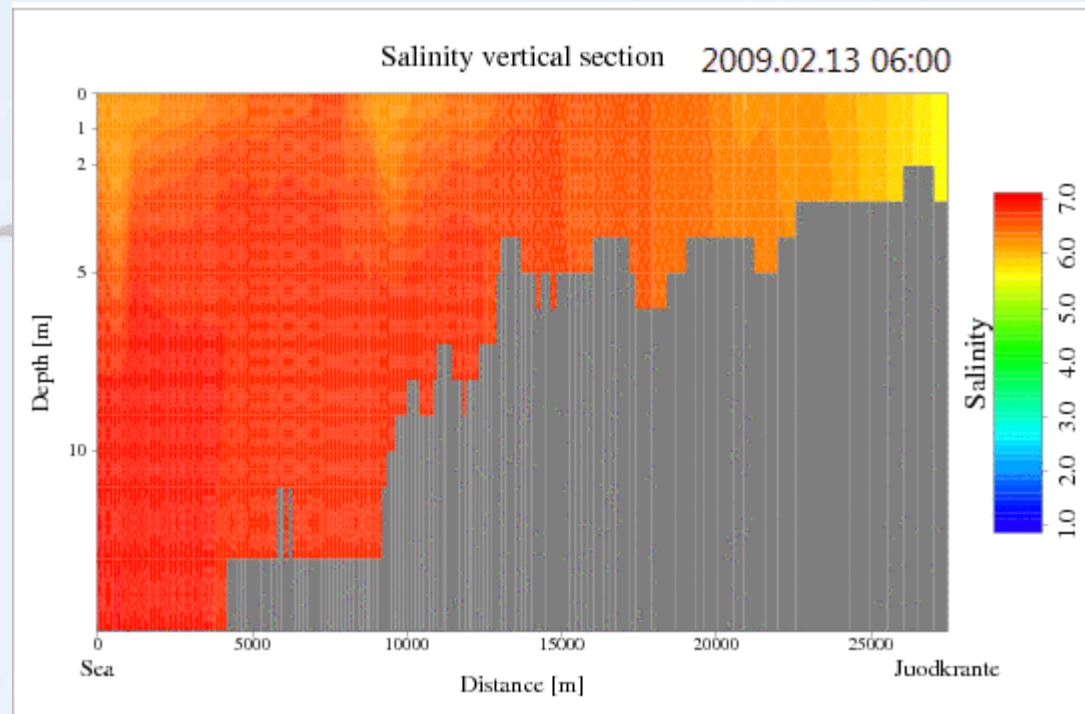
- **Type No 2** of salinity vertical distribution: stratification in the Klaipeda strait.



- **Type No 3** of salinity vertical distribution: stratification destruction (intrusion of saline water from the sea or start to push out saline water from the Curonian lagoon)



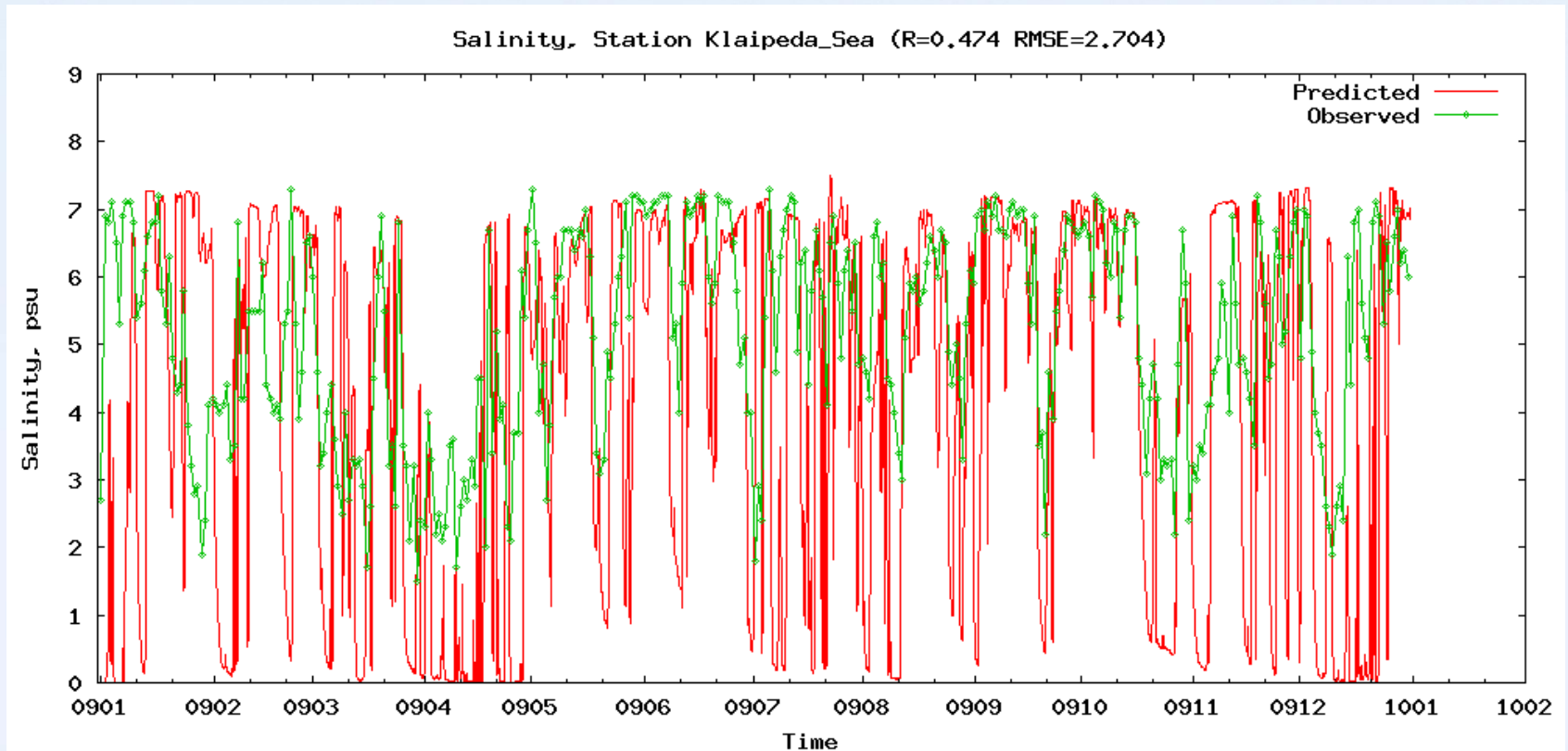
- **Type No 4** of salinity vertical distribution: deep intrusion of saline water into the Curonian lagoon, no stratification.

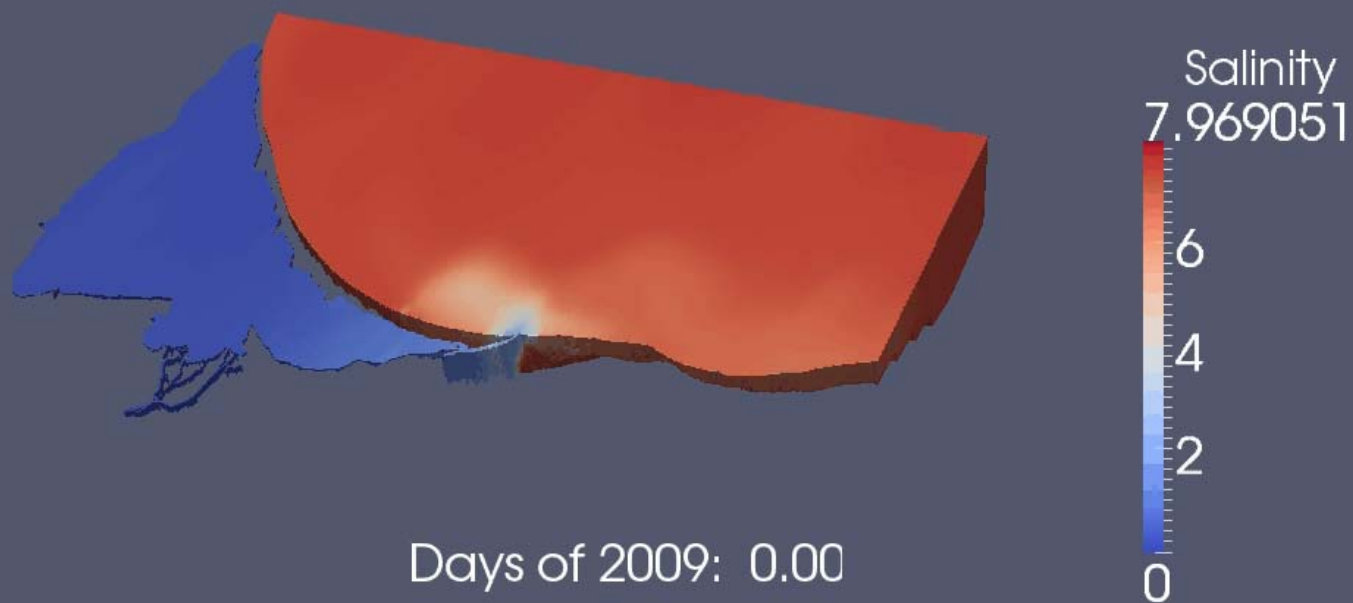


- No salinity gradients were observed to south of island Kiaules Nugara.
- Least frequent type of salinity vertical distribution is No 1.
- The total duration of this type during 2009 was only 20 days.
- Saline water is present in the Klaipeda strait the majority of time.



How wrong 2D model is around the Klaipeda strait?

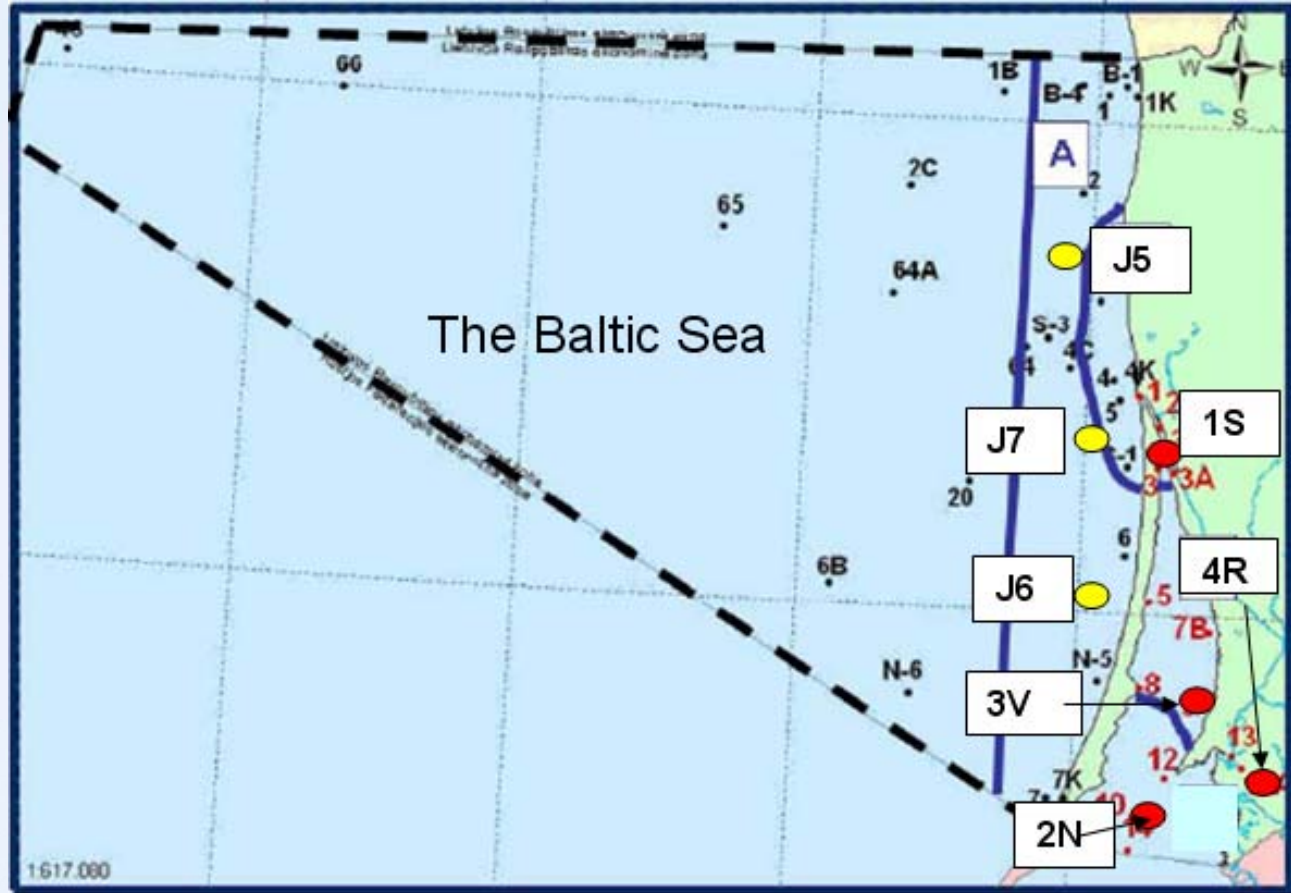




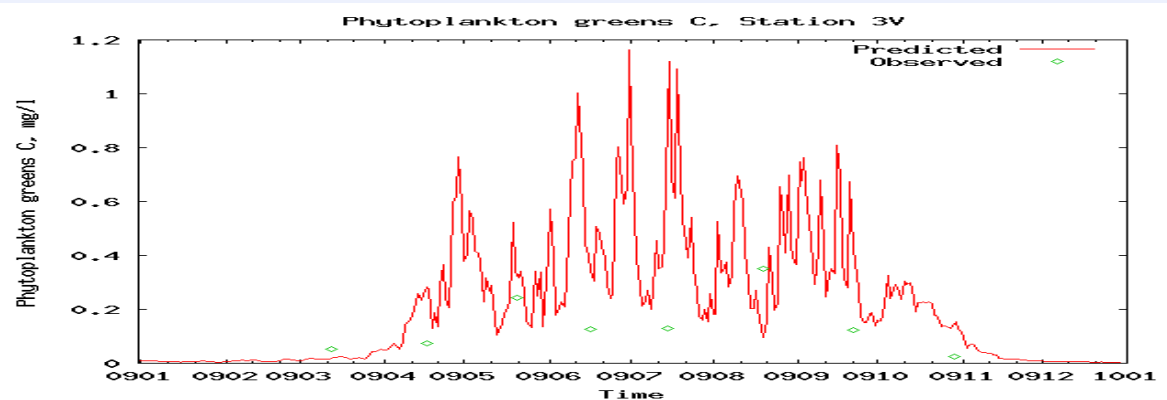
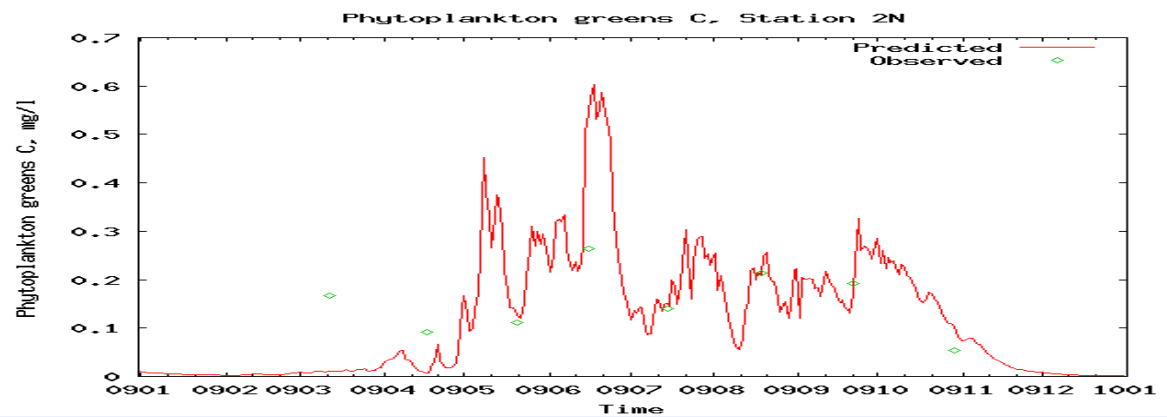
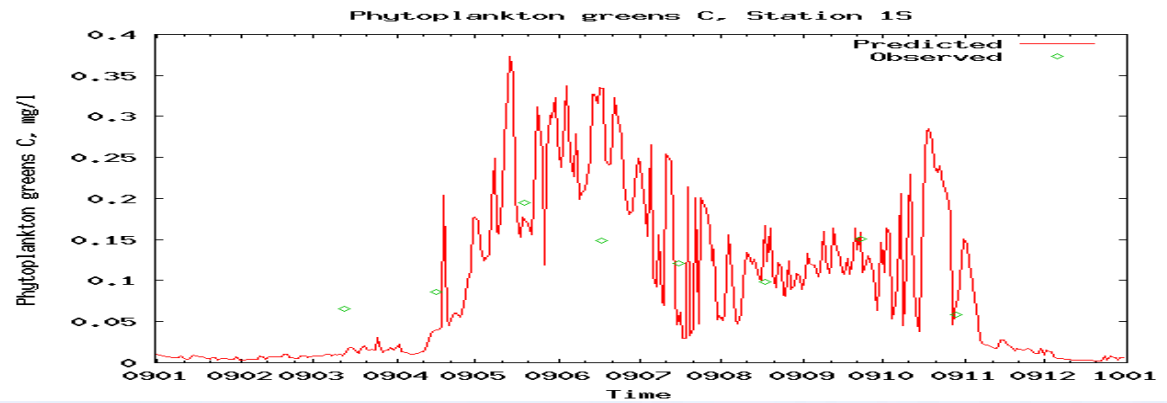
Performance of biogeochemical model



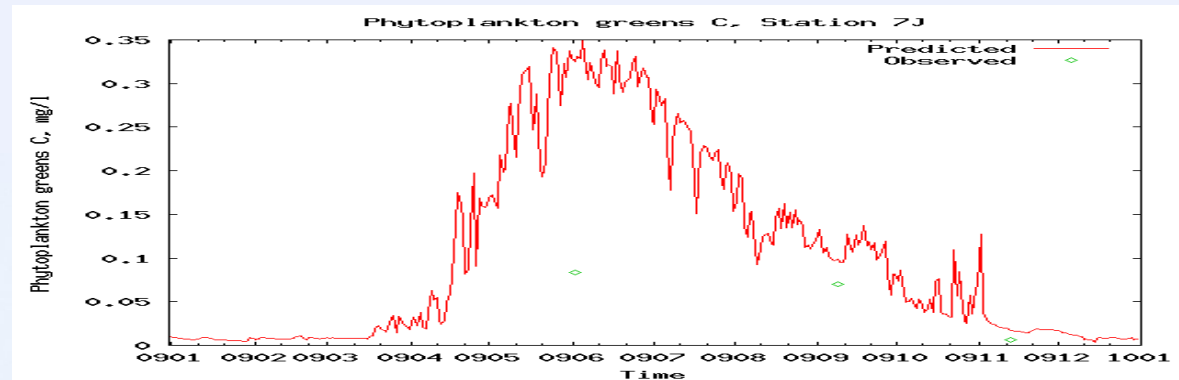
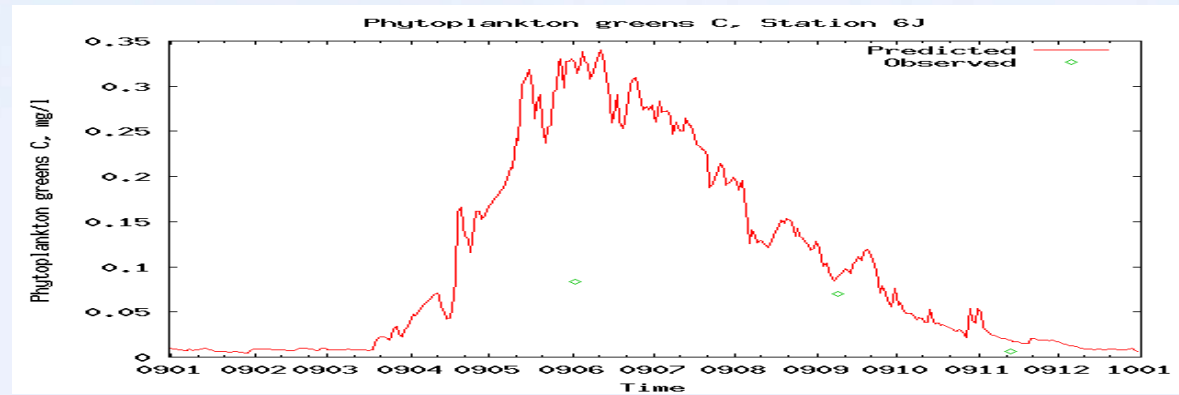
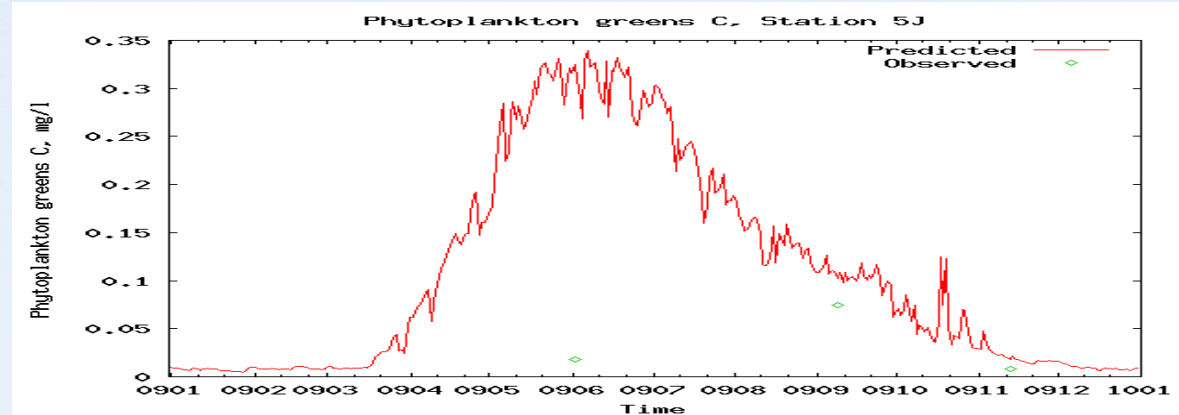
Monitoring stations



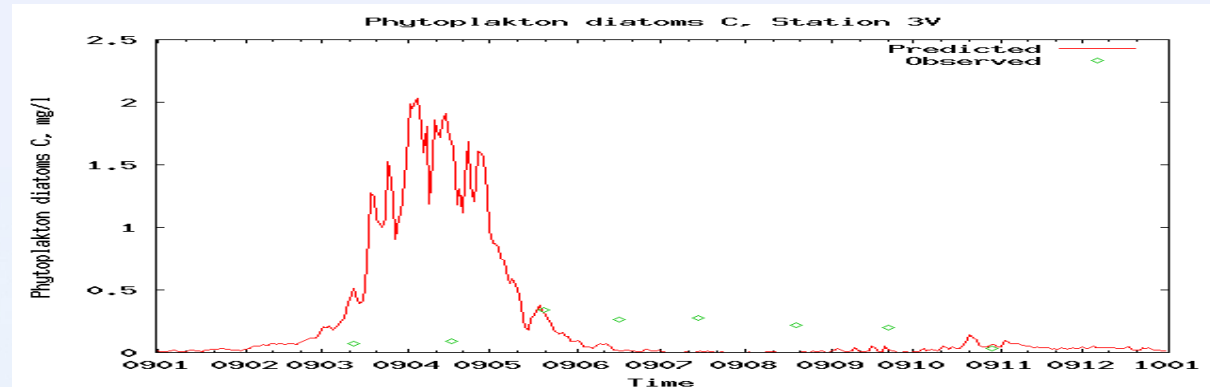
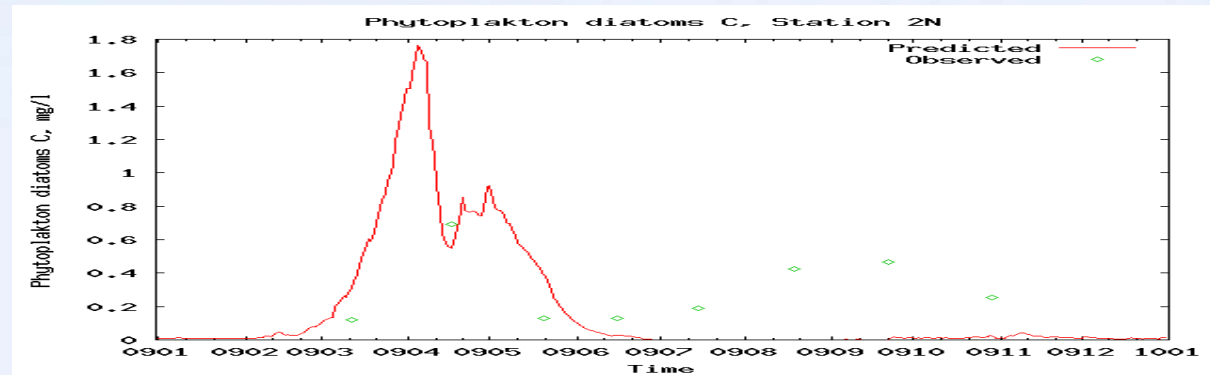
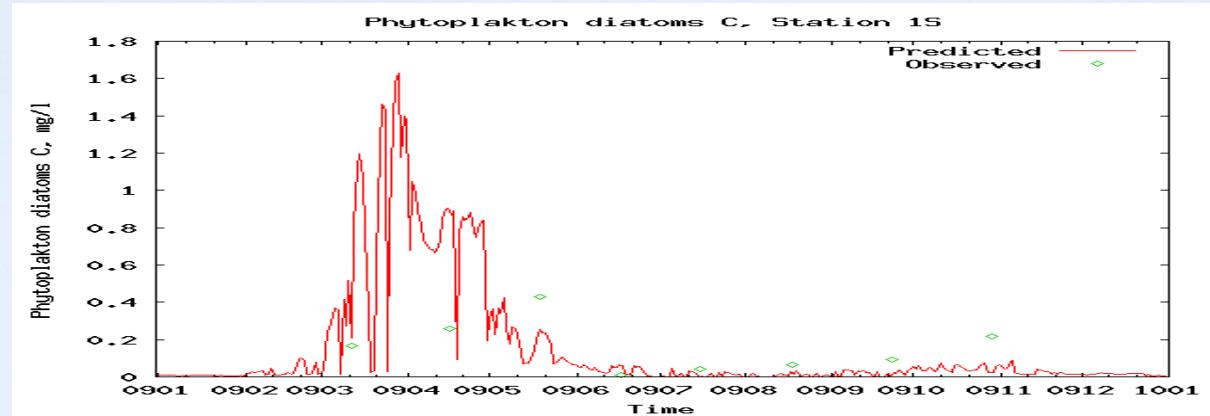
- Phytoplankton greens for stations located inside of the Curonian lagoon.



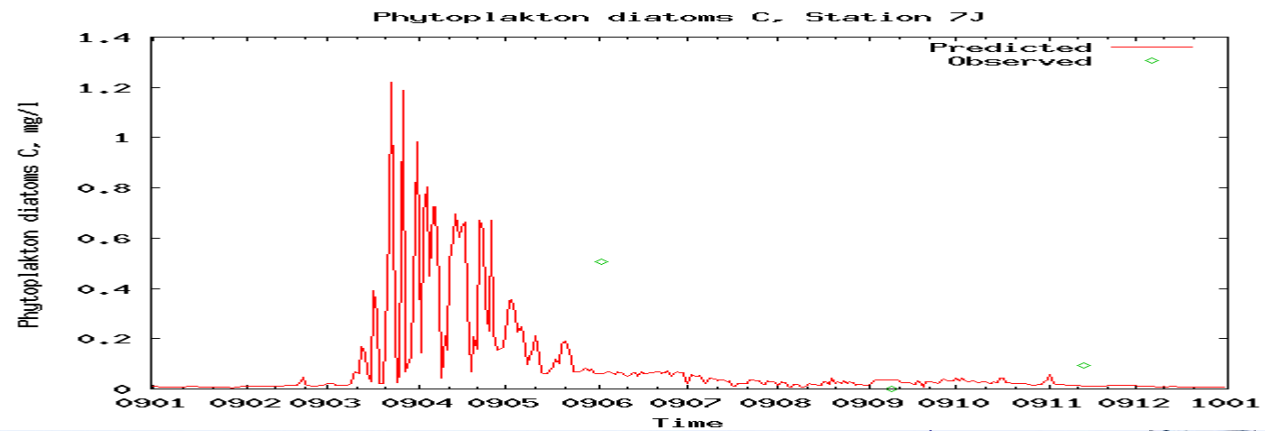
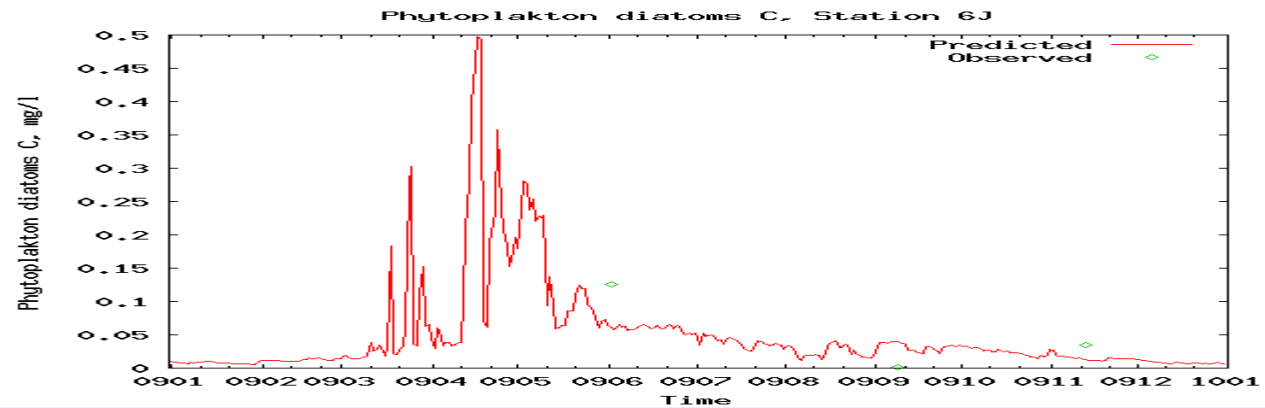
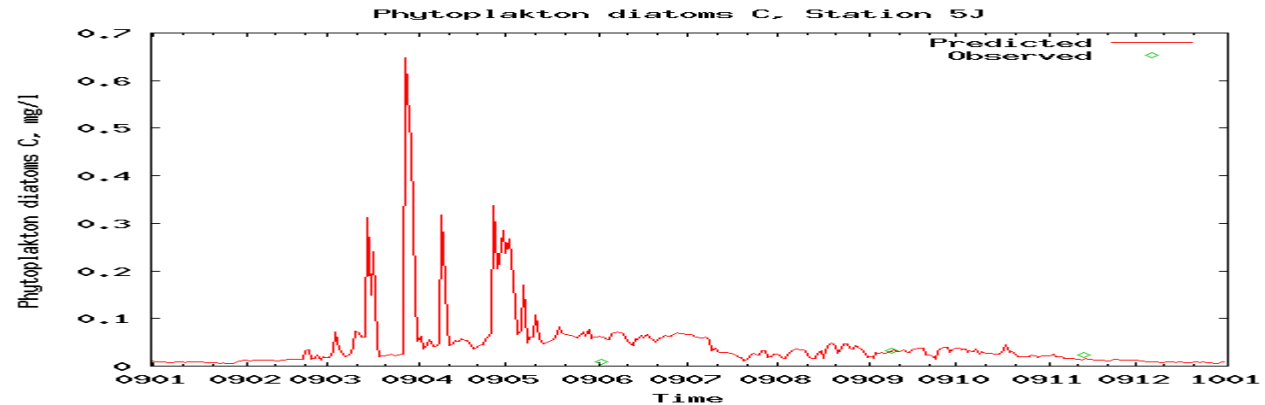
- Greens for stations located in coastal waters of the Baltic Sea.



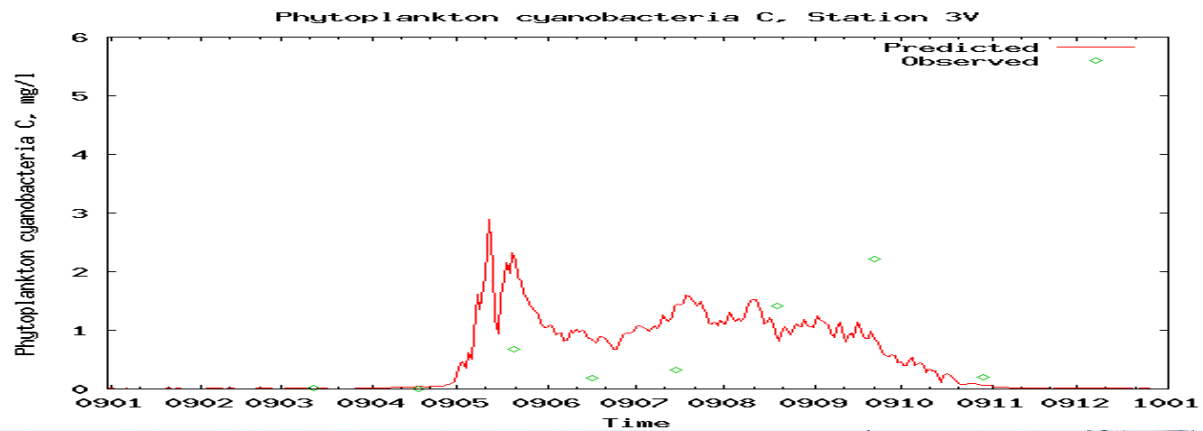
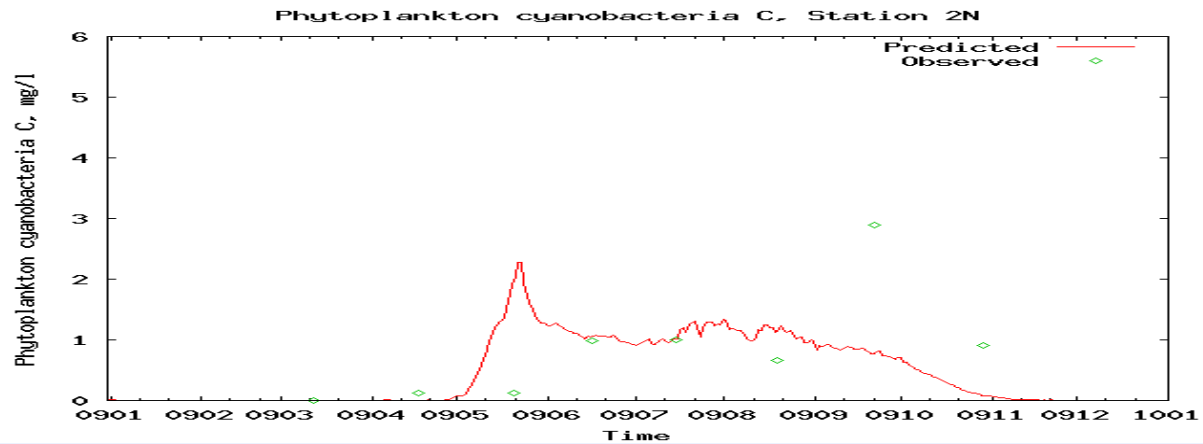
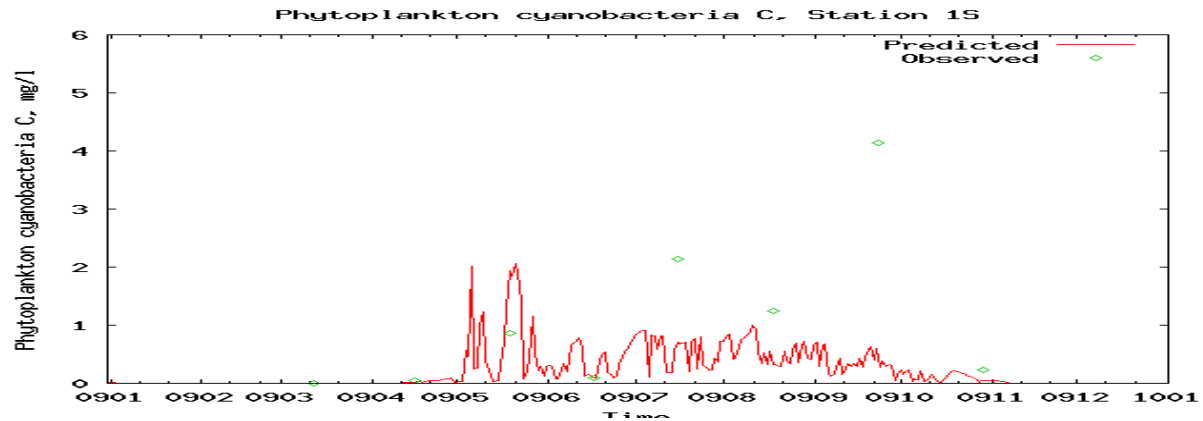
- Diatoms for stations located inside of the Curonian lagoon.



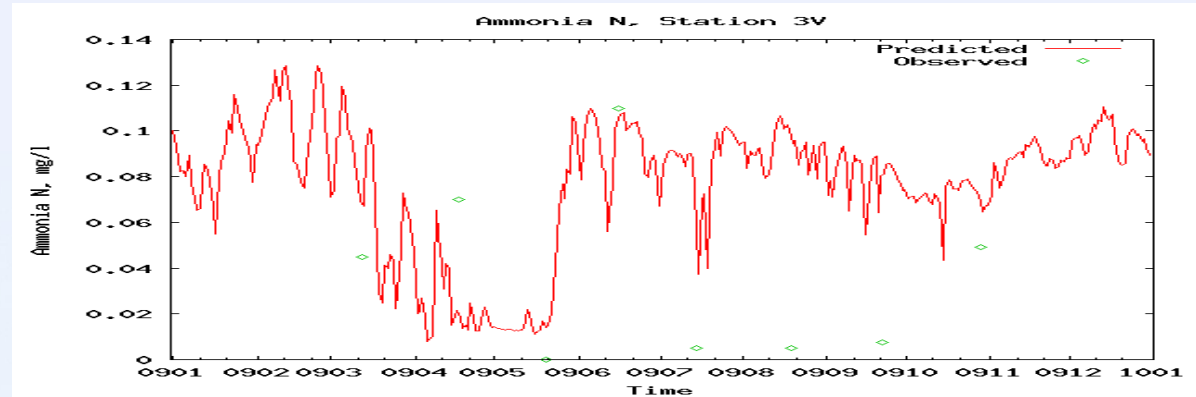
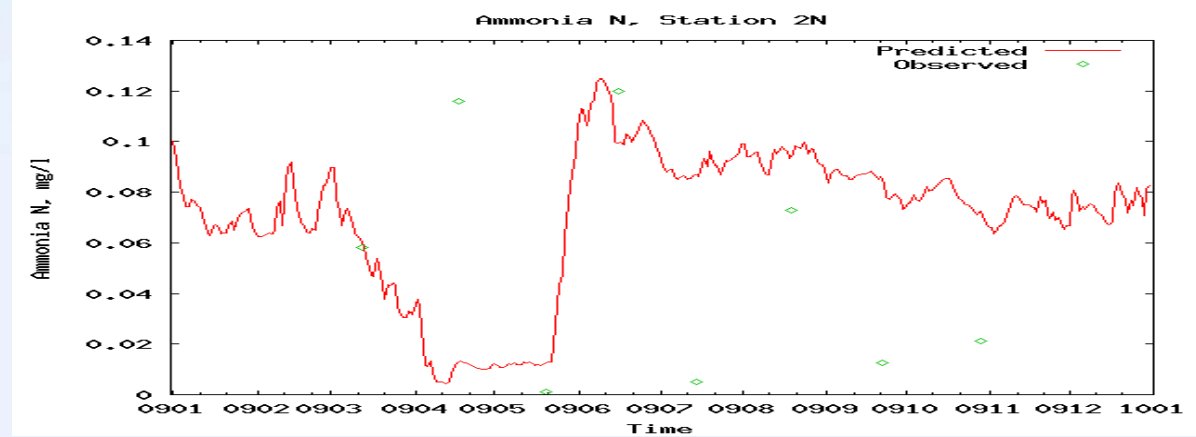
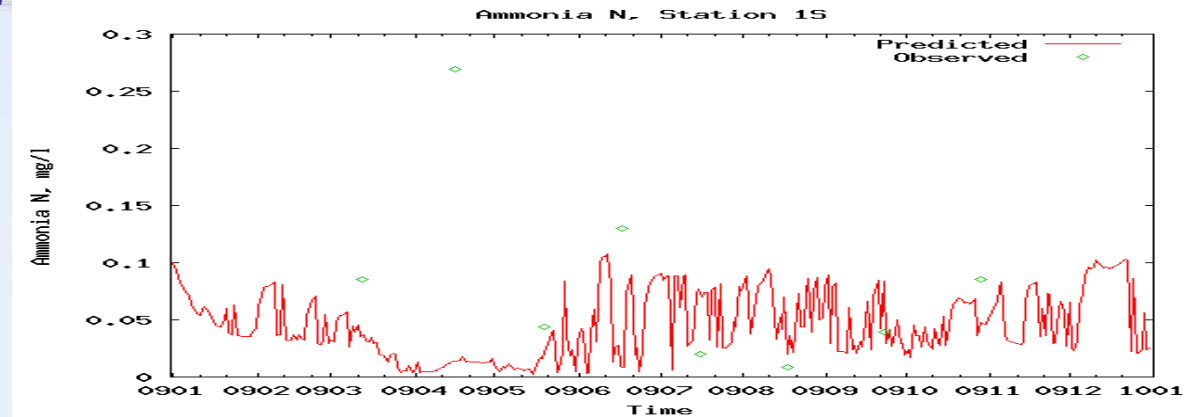
- Diatoms for stations located in coastal waters of the Baltic Sea



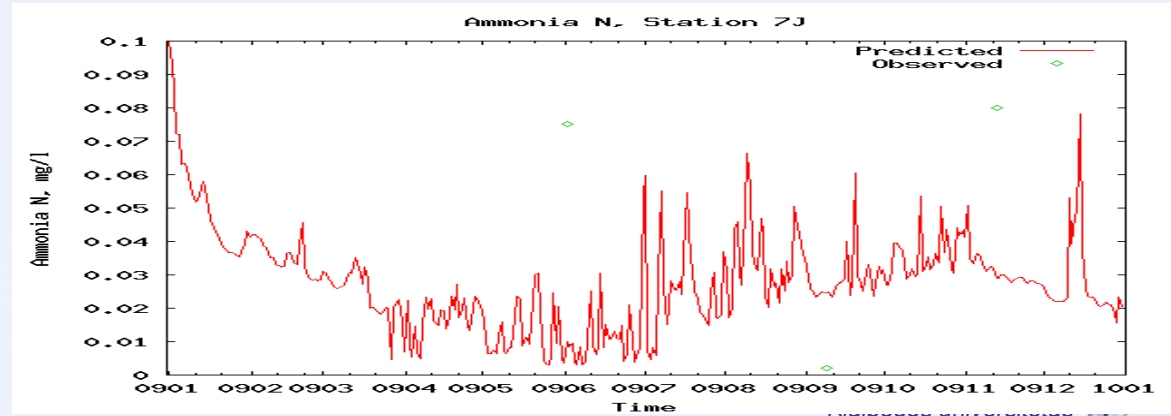
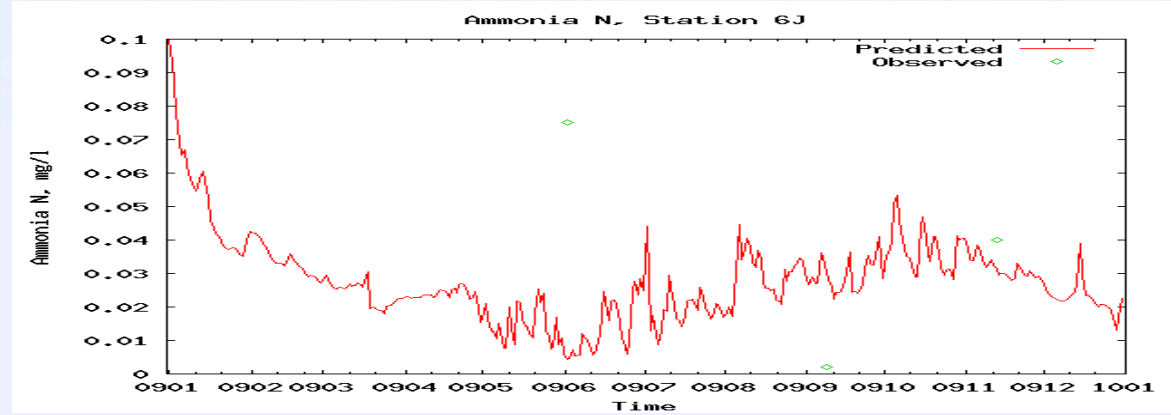
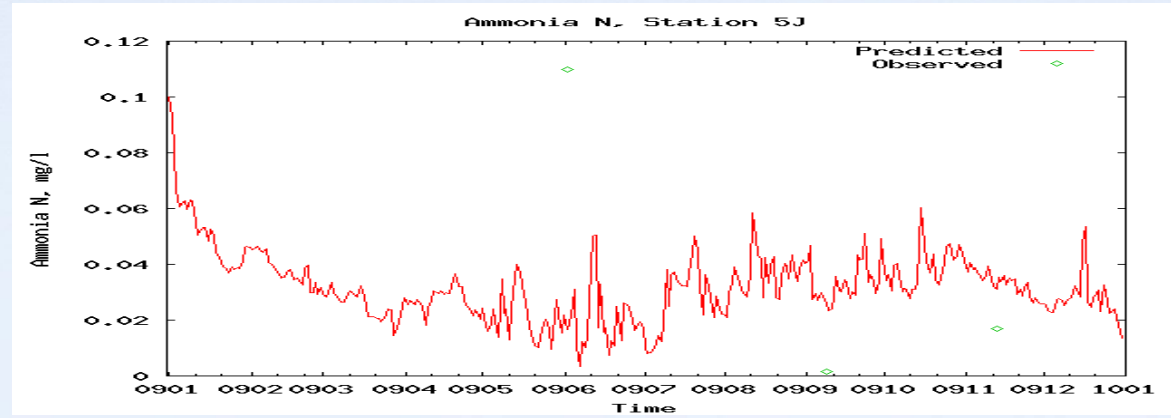
- Cyanobacteria for stations located inside of the Curonian lagoon



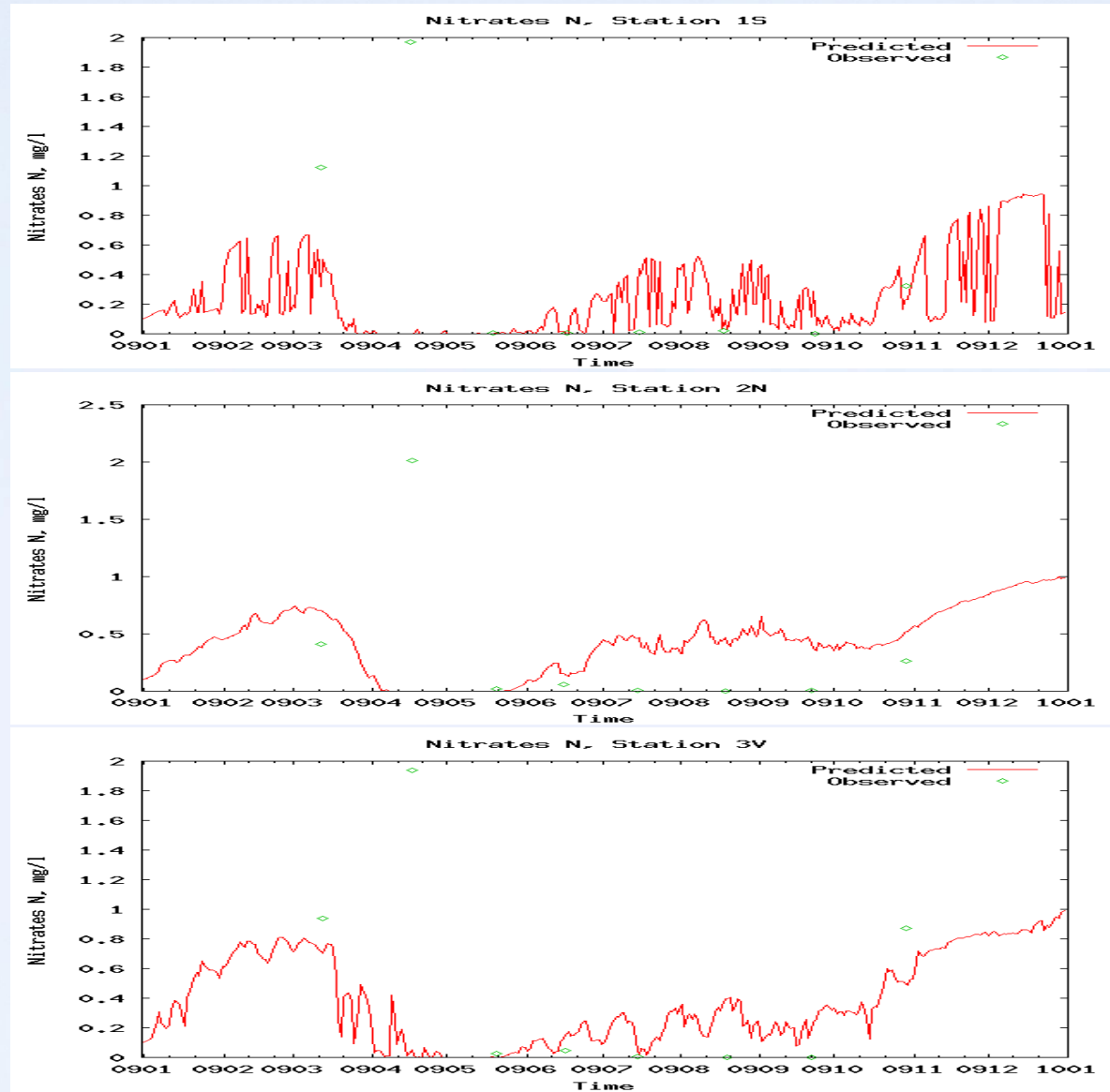
- Ammonia nitrogen for stations located inside of the Curonian lagoon



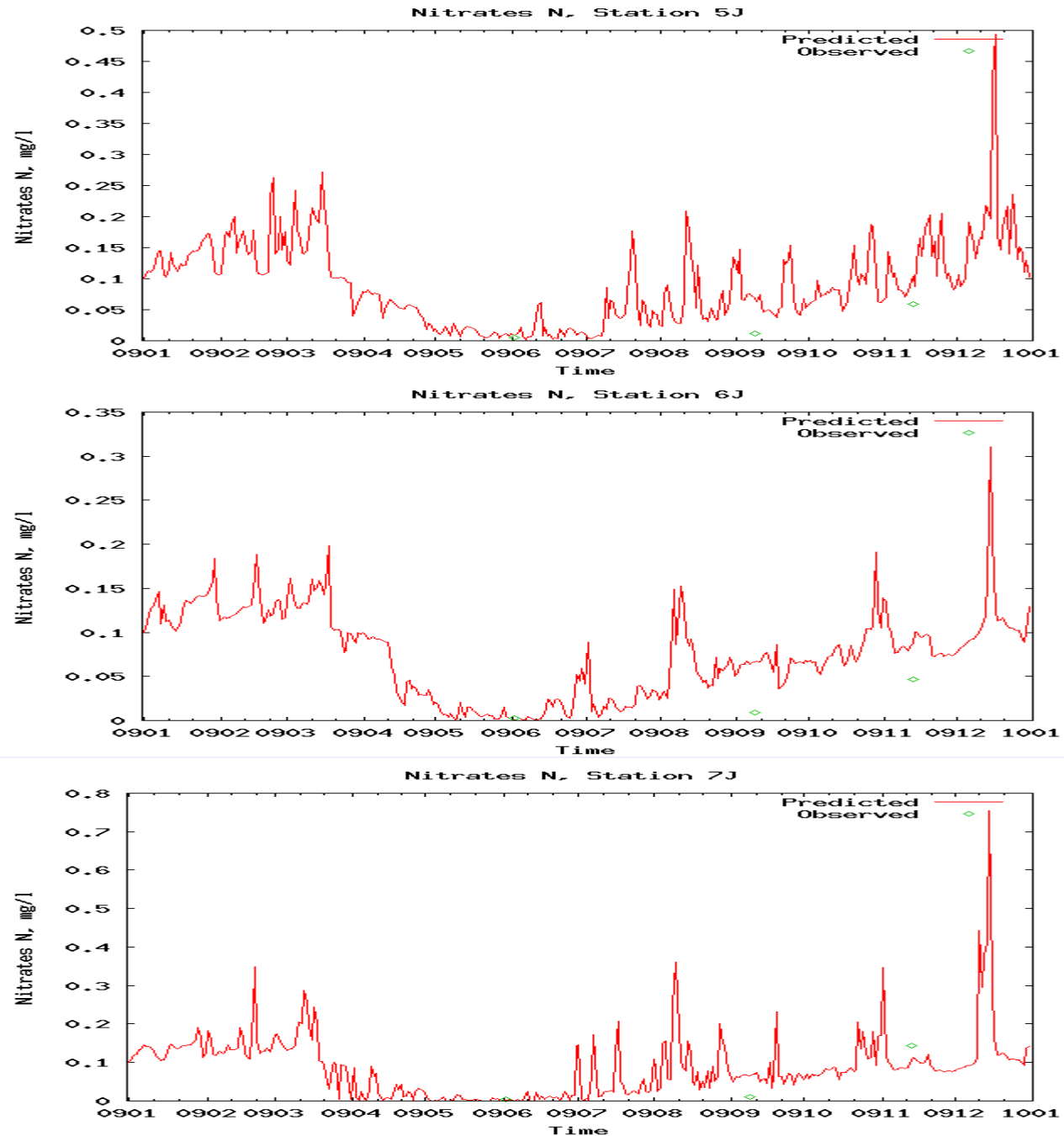
- Ammonia nitrogen for stations located in the coastal waters of the Baltic Sea.



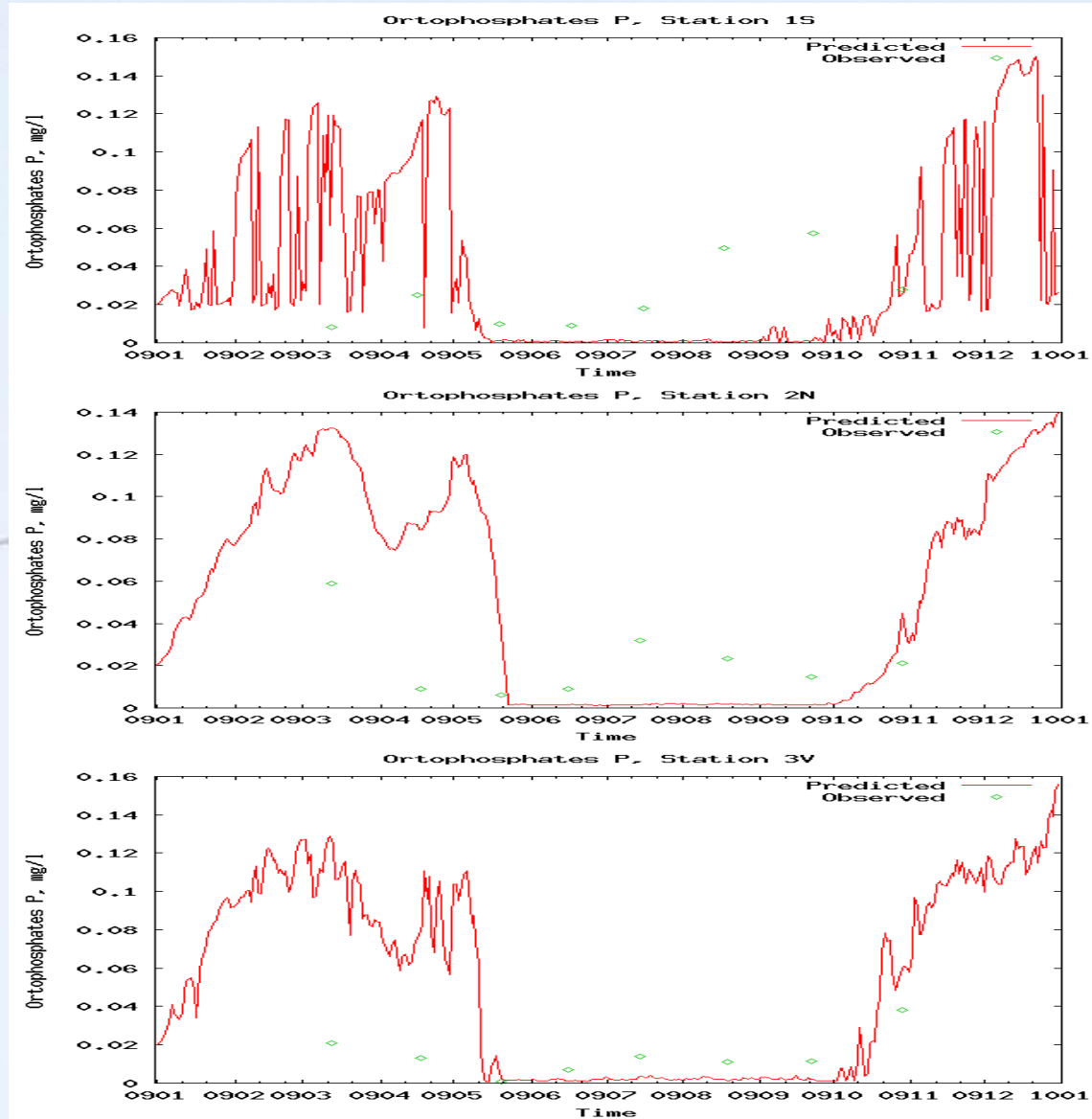
- Nitrates nitrogen for stations located inside of the Curonian lagoon



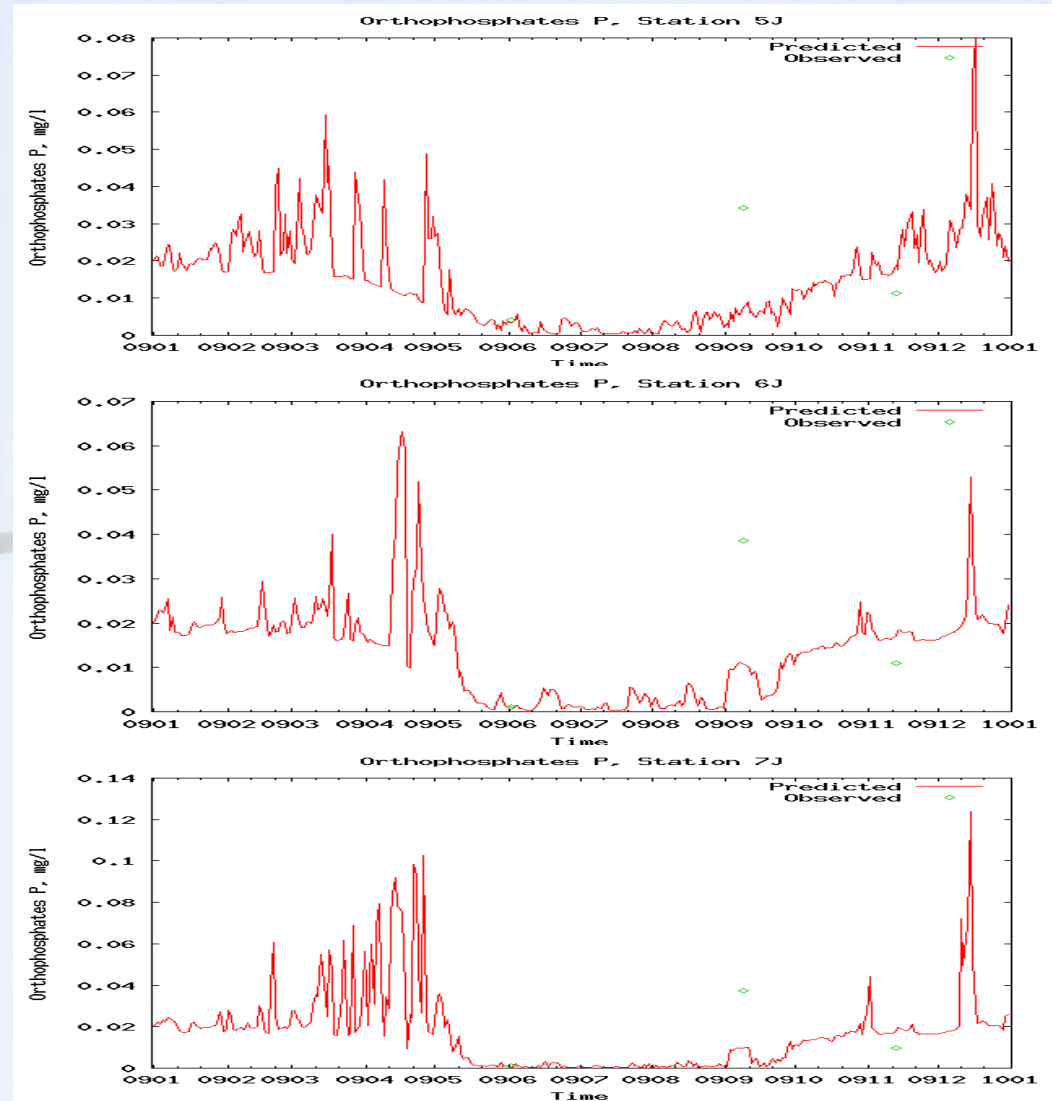
- Nitrates nitrogen for stations located in coastal waters of the Baltic Sea



- Orthophosphate phosphorus for stations located inside of the Curonian Lagoon.



- Orthophosphates phosphorus for stations located in coastal waters of the Baltic Sea



Future developments

- 2d->3d
- Bottom sediment model
- Coupling with sediment transport



The end

