

Ensemble forecasting of harmful algal blooms in the Baltic Sea

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Abstract

Operational marine environmental modelling has been considered notoriously hard; consequently there are very few operational models of the marine environment. Operational modelling of harmful algal blooms requires the modelling of individual species and is therefore harder still. The separation of algal species in models requires detailed knowledge of their behaviour (survival strategy through the life cycle), and in general, very little is known of harmful algal bloom (HAB) properties.

We present promising results of an ensemble approach to HAB forecasting in the Baltic, and discuss the applicability of the forecasting method to biochemical modelling. Ensembles were produced by running the biogeochemical model several times and forcing it on every run with different set of seasonal weather parameters from European Centre for Medium-Range Weather Forecasts' (ECMWF) mathematically perturbed ensemble prediction forecasts. The ensembles were then analysed by statistical methods and the median, quartiles, minimum and maximum values were calculated for estimating the probable amounts of algae. Validation for the forecast method was made by comparing the final results against available and valid in-situ HAB data. It turns out that it is possible to forecast HABs with useful accuracy.

Key words: Prediction, Algal blooms, Ensemble forecasting, Baltic Sea, (8.7° E 53.85° N), (30.3° E 65.85° N)

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1. Introduction

Modelling of non-linear variables always includes uncertainties from different sources. The initial conditions might be inaccurate, the model input has errors and the modelling of ocean conditions is not exact because of truncation errors and inaccuracies in the modelling of subscale phenomena (Leutbecher and Palmer, 2008). Therefore the solution deteriorates in time.

The deterioration of model forecasts with time is a well-known issue in weather forecasting, where the reliable forecast range is about a week. In oceans the predictability of some phenomena is typically longer. For example, the internal weather of the sea, the oceanic meso-scale, includes mainly phenomena which are occurring in temporal scales from days to months and spatial scales from kilometres to hundreds of kilometres (Lermusiaux, 2006). However, ocean predictability is rarely exploited to its useful limits. Most operational ocean forecasting is limited to ten day forecasts in the maximum, or to coupled atmosphere-ocean seasonal forecasts where the focus is nevertheless on the atmospheric forecast.

Physical ocean models are principally built on the same well-known and relied upon equations as atmospheric models, and have the same inherent limitations to their predictive skills. Biogeochemical models, on the other hand do

not enjoy a firm basis provided by e.g. the primitive equations of ocean motions. Furthermore, the initial condition for a biogeochemical forecast is often not well observed, or the uncertainties are large. While there are significant constraints to how the biogeochemical models are to be constructed (Redfield, 1958), the uncertainties involved in using biogeochemical models for forecasting appear to deserve an explicit treatment. This is particularly true with models that pursue to predict not only the overall biogeochemical processes, but also the behaviour of individual species.

In harmful algal (HA) bloom forecasts a relationship between phosphorus concentration and cyanobacterial blooms has been recognized for decades (Kahru et al., 2000). Various levels of utilization of this relationship have been employed for practical and even operational purposes. These operational estimates of cyanobacterial bloom probability and severeness have, however, been based mostly on the wintertime (January–February) nutrient concentration fields and best and worst case scenarios for summer weather conditions, without accounting for the actual weather development and forecasts.

Janssen et al. (2004) demonstrated with model experiments that a relationship between winter nutrients and summer cyanobacterial blooms, in agreement with the inferences of Kahru et al. (2000), is indeed replicated with biogeochemical 3-dimensional numerical model.

Biogeochemical ensembles offer a quantitative tool for the assessment of HA bloom related environmental risks

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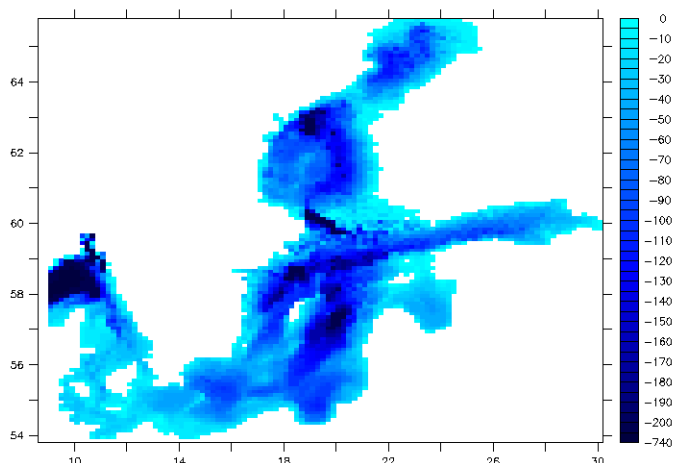


Figure 1: Bottom topography (m) of the Baleco model.

for a wide range of applications. Ensemble forecasts have been for long an essential tool in meteorology. In comparison with a single deterministic forecast, ensembles offer the benefit of estimates of bias, deviation and range of the modelled variables from real life situation. It is also possible to analyze the ensembles and recognize forecasts with low skill (Buizza, 1997).

There are several ways to dissect the ensemble. Variables can be studied by e.g. calculating the ensemble mean, which provides an estimate of the probabilistic expectation forecast. The ensemble can also be divided into smaller sub-ensembles to make alternative forecasts (Brankovic and Palmer, 1997) and even individual members can be used for prediction purposes. Ensembles can be used as a quantitative tool for risk assessment. The potential economic value can be much higher in many applications than the value of deterministic forecast (Richardson, 2000).

In this work we explore the predictability of ensemble harmful algal bloom modelling and present the usefulness of such forecasts in environmental policymaking and risk assessment.

2. Materials and methods

2.1. Model configuration

For forecasting we used FMI's operational 3-dimensional biogeochemical model, Baleco. The model consists of a general circulation model (Marshall et al., 1997a,b) and an ecological module. Model is realized on a spherical polar grid. The bottom topography (Fig. 1) is from Seifert and Kayser (1995). The spatial discretization is made with minimum filter at 6 nm intervals. The grid size is 6 nautical miles and the model domain reaches 120 grid cells in latitudinal, 108 grid cells in longitudinal and 21 grid cells in vertical direction. The model domain's most southwestern corner is located at (53.85° N, 8.7° E). The vertical resolution of the model is concentrated to the euphotic

zone so that the top most layer is 3 metres reduced to 2 metres in the cells hugging the coast (Kiiltomäki, 2008).

Ecological model is based on ecosystem dynamics formalized by Aksnes et al. (1995) and Tyrrell (1999). The model consists of three conceptual phytoplankton groups: diatoms, flagellates and cyanobacteria. These groups have constant mortality rates and they use phosphate, silicate and dissolved inorganic nitrogen. Diatoms are potentially limited by availability of silicate. Cyanobacteria can fix molecular nitrogen and therefore they are not limited by availability on DIN. Flagellates group represent autotrophic flagellates. Altogether the ecosystem model describes the essence of new production in the presence of three functional groups. The growth rates depend on nutrient concentrations, irradiation and temperature (Stipa et al., 2003). For model equations see Appendix A.

Model runs obtained their initial state from FMI's deterministic Baltic Sea forecast for the start date of the run. The deterministic forecast's initial conditions, both physical and chemical, were obtained from winter monitoring data of the HELCOM COMBINE program for the winter 2007–2008. The observations were interpolated in three dimensions with a robust nearest neighbour interpolation and then supplemented by climatological values for the North Sea from the World Ocean Atlas (Boyer et al., 2006).

2.2. Ensemble forecasts

The ensemble prediction system (EPS) is a technique to predict the probability distribution of forecast states, given a probability distribution of random analysis error and model error. Ensemble forecasts are formed by several slightly perturbed forecasts. A single forecast is called ensemble member and all members together form an ensemble forecast.

Ensemble forecasts include more information than single deterministic forecast and therefore the analysis can give us a deeper insight to many phenomena. Every ensemble member represents one possible evolution of system state in time and space. Therefore the variety of applicable analysis approaches is very wide, when compared to deterministic forecasts.

One of the oldest and simplest analysis methods is to calculate ensemble mean to find out the overall trend. It is also possible to calculate some statistical values for analysis. These values can be for example minimum and maximum values, which indicates the extreme values, and 25% and 75% quartiles, which give wider understanding of the ensemble uncertainties. Another useful approach is to interpret the percentage of ensemble members as the probability of exceeding some limiting value.

Ensembles in our study were created from an unperturbed initial condition by running the model several times with different sets of weather forcing parameters. The weather ensembles were made by ECMWF using singular vector method (Molteni et al., 1996). Weather parameters

used as external forcing for ocean model were 6 hourly 10 metre winds and 2 metre dew point temperature and 2 metre temperature, 12 hourly surface solar radiation and surface thermal radiation.

2.3. Chlorophyll-a conversion

As the model gives the amount of cyanobacteria in molar amount of nitrogen (N) we have used a special $C : N$ ratio, the molar mass number of carbon (12.01) and $C : Chla$ ratio to calculate the chlorophyll-a concentrations in mg m^{-3} . Since this work concentrates on the Baltic sea, we have used $C : N = 6.3$, which is based on studies made in the area: Walve and Larsson (2007) found out that $C : N$ ratio in the cyanobacteria in Western Gotland basin was $6.2-6.4 \pm 0.3$, highest ratio being 7.3. Another study made by Nausch (2009) supports these values as they found that the mean $C : N$ ratio was 6.2 in the Eastern Gotland basin. Carbon:chlorophyll ratio is also a non-constant variable, which depends most of all on the algal species studied, e.g. it is widely known that $C : Chla$ ratio is large in cyanobacteria. In this study we have used $C : Chla = 100$, which is an approximation based on study by Chang (2003). They found that $C : chla$ ratio was 94.4 when cyanobacteria dominated phytoplankton. With these configurations the chlorophyll-a (Chla) concentration in mg m^{-3} was calculated from the model results with formula:

$$Chla = \frac{N_c \cdot 6.3 \cdot 12.01}{100} \approx N_c \cdot 0.76,$$

where N_c is the molar mass of cyanobacteria produced by the model. As a limit for the cyanobacterial occurrence we used chlorophyll-a concentration of 2.0 mg m^{-3} which is an approximation based on studies by Seppälä (1999), Nausch (2004) and Kutser (2006).

3. Results

3.1. Case study: harmful algal blooms and upwelling in the Baltic Sea, June 2008

The summer weather of 2008 was cool and windy and thus large scale harmful algal blooms were absent. The total algal situation can be seen in figure (Fig. 2) In long term comparison June and August blooms were milder than usual, in July the situation was average. In the beginning of July the sea water temperature increased a few degrees and the concentration of cyanobacteria increased in the Gulf of Finland. Cyanobacteria was mainly mixed in the water column. The Sea of Åland had some blooms. From the middle July to end of July the algal blooms increased first in southern Sea of Archipelago, Sea of Åland, eastern Gulf of Finland and southern Bothnian Sea. In the end of July the blooms were more frequent and small blooms were present all along of the Gulf of Finland. The summer bloom culminated in the end of July, when the maximum extent (approximately $180,000 \text{ km}^2$) of algae

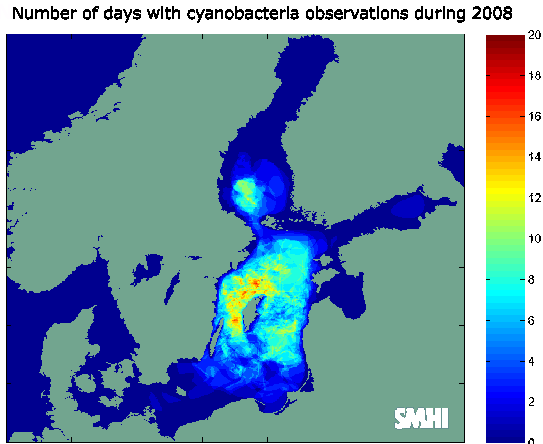


Figure 2: Number of days with cyanobacteria observations by NOAA-AVHRR satellite imagery during 2008 (HELCOM, 2009).

blooms was observed. However the normalized bloom indices for bloom extent ($6,575 \text{ km}^2$), duration (4.9 days) and intensity ($32,651 \text{ km}^2 \text{ days}$) were lower than the mean for the period 1997–2007 (HELCOM, 2009).

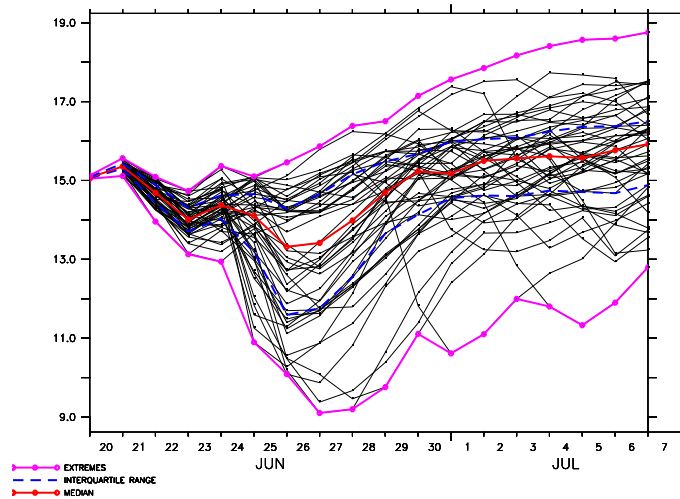
In our case study we observed upwelling on the west coast of Gotland on 24th of June. We show here how different weather scenarios affect ocean conditions and how ensemble forecasts see different biogeochemical phenomena.

Upwelling is very often strong enough for the sea-surface temperature be affected, and thus the low temperatures in thin strip to the coasts are a signature of upwelling. Upwelling can also be seen in the colour of the water and in the abundance of sea life (Gill, 1982)

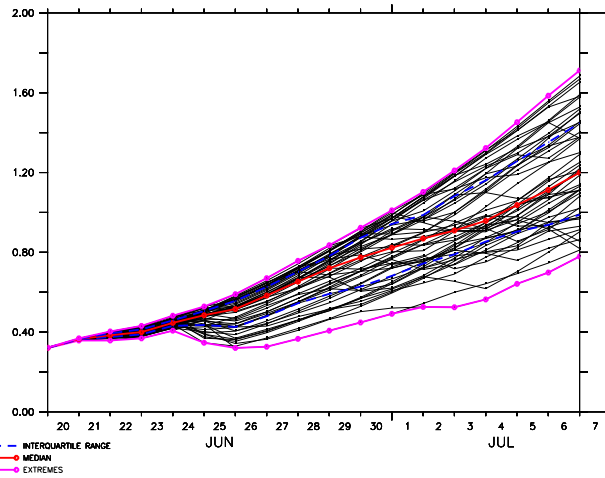
Temperature and nutrient ensembles (Fig. 5a), Fig. 5c and Fig. 5d) and cyanobacterial concentrations (Fig. 4) show an upwelling event in the area. We see that some weather scenarios may cause upwelling while other possible scenarios do not. Cyanobacteria ensemble (Fig. 5b) and Algaline biomass observations (Fig. 3) support this interpretation. We see that the lower cyanobacteria biomass concentrations observed near the coast are captured by large number of ensemble forecast members. This is an example of how ensemble forecasting brings added insight to our understanding of the situation.

3.2. Comparison between observations and forecast

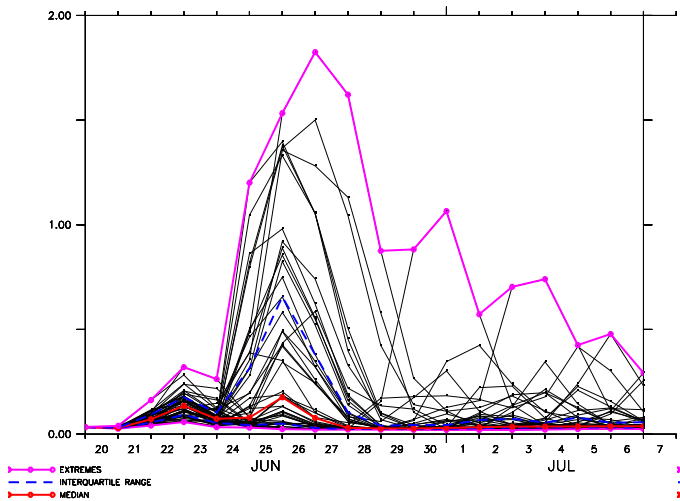
It is desirable to evaluate the quality of a probabilistic prediction system not only in terms of the intrinsic quality of the results it produces but also in terms of cost efficiency (Talagrand et al., 1999). In HA bloom verification the available observational data is very sparse and often qualitative in nature. Therefore the verification is especially challenging.



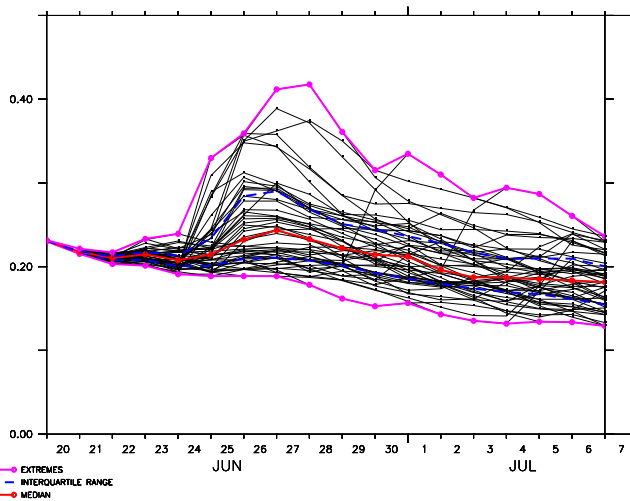
(a) Temperature ($^{\circ}\text{C}$)



(b) Cyanobacteria (mg m^{-3})



(c) Nitrate (mg m^{-3})



(d) Phosphate (mg m^{-3})

Figure 5: Monthly ensemble forecast plumes of biogeochemical parameters limited in the time frame from the beginning of the forecast 20th of June to 7th of July 2008 on the west coast of Gotland ($18.80^{\circ}\text{ E } 57.25^{\circ}\text{ N}$).

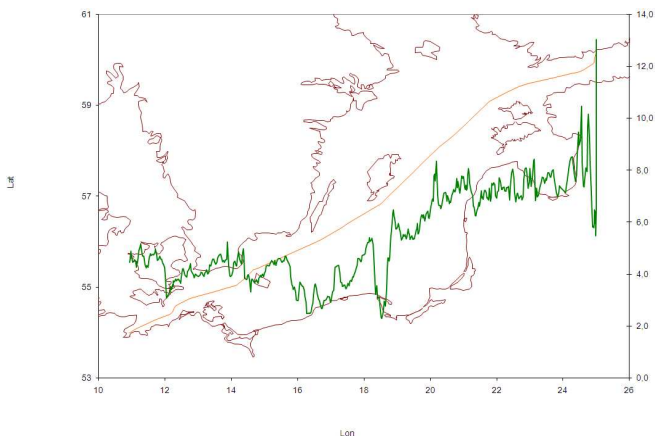


Figure 3: Algaline fycocyanin (blue-green algal biomass) observations (PC fluorescence) on 1st and 2nd of July 2008 on the route from Helsinki to Travemünde. On the west coast of Gotland the values are clearly lower.

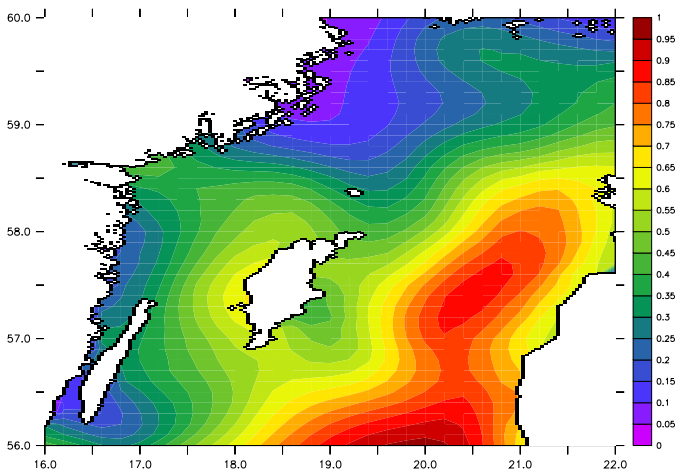


Figure 4: Cyanobacterial ensemble mean forecast (mg m^{-3}) for the 1st of July from the run beginning from 20th of June. Lower concentrations, on the coast of Gotland ($18.80^\circ \text{ E } 57.25^\circ \text{ N}$) indicates upwelling.

In Fig. 6a we see the observed situation in the end of July 2008, when the HA blooming had its peak. The observations are done by volunteers, environmental authorities and Finnish border guards. Several kinds of observations are combined in this Figure. Observations are mainly sensory especially near the Finnish coast and there is no data about biochemical variables during the phenomenon.

Contrast this with Figure 6b, a HAB probability map produced from an ensemble forecast for the same time. Unlike the observations, this map is based on probabilities of quantitative values of cyanobacteria chlorophyll-a as predicted by the model. Therefore, it is not predicting directly the concentration of chlorophyll-a but rather the possibility of the blooms.

From the Figures 6a and 6b we can see that in the Gulf of Finland are several observations of blooming in the areas where they were predicted. We can also see that in Northern Baltic Proper the predicted bloom area is considerably to the East from the observed blooms. Furthermore, there are no blooms forecasted for the Sea of Archipelago, yet there are several observations of blooms.

4. Discussion

Large parts of Baltic Proper and Gulf of Finland are nitrogen-limited, resulting an excess of phosphorus in the surface layer in late summer. This excessive DIP pool has the potential for blooms of nitrogen-fixing cyanobacteria. That is, the potential of late summer bloom is determined as early as February by the excessive DIP concentration in the surface layer. This correspondence has been studied in the beginning of the millennium by Kahru et al. (2000). In later studies Janssen et al. (2004) have reached the same conclusion with computational models and Lilover and Stips (2008) on their research on observational data.

Our ensembles demonstrate the sensitivity of HABs to nutrient fields, especially phosphate. Similarities can be seen in the shape of computational initial phosphate field after spring bloom in the end of May (Fig. 7b) and probability based forecast (Fig. 6b). The observed initial phosphate field (Fig. 7a) has similar high DIP concentrations in the Baltic Proper and western parts of Gulf of Finland, but concentrations in the Bothnian Sea are higher only in the initial winter DIP field.

The initial nutrient field plays an important role in algae growth and it appears at first that spatially the nutrient field is a more dominant factor in algal blooms than weather conditions. However, during the summer the meteorological variables have a great impact on timing, duration and intensiveness of the blooms as we see in Figure 5. For example Figure 5b shows that harsh weather conditions can delay the cyanobacteria growth for weeks. It is also seen that the concentration of cyanobacteria chlorophyll is strongly dependent on weather conditions.

As the initial condition data was based on somewhat sparse wintertime observations, it is quite possible that

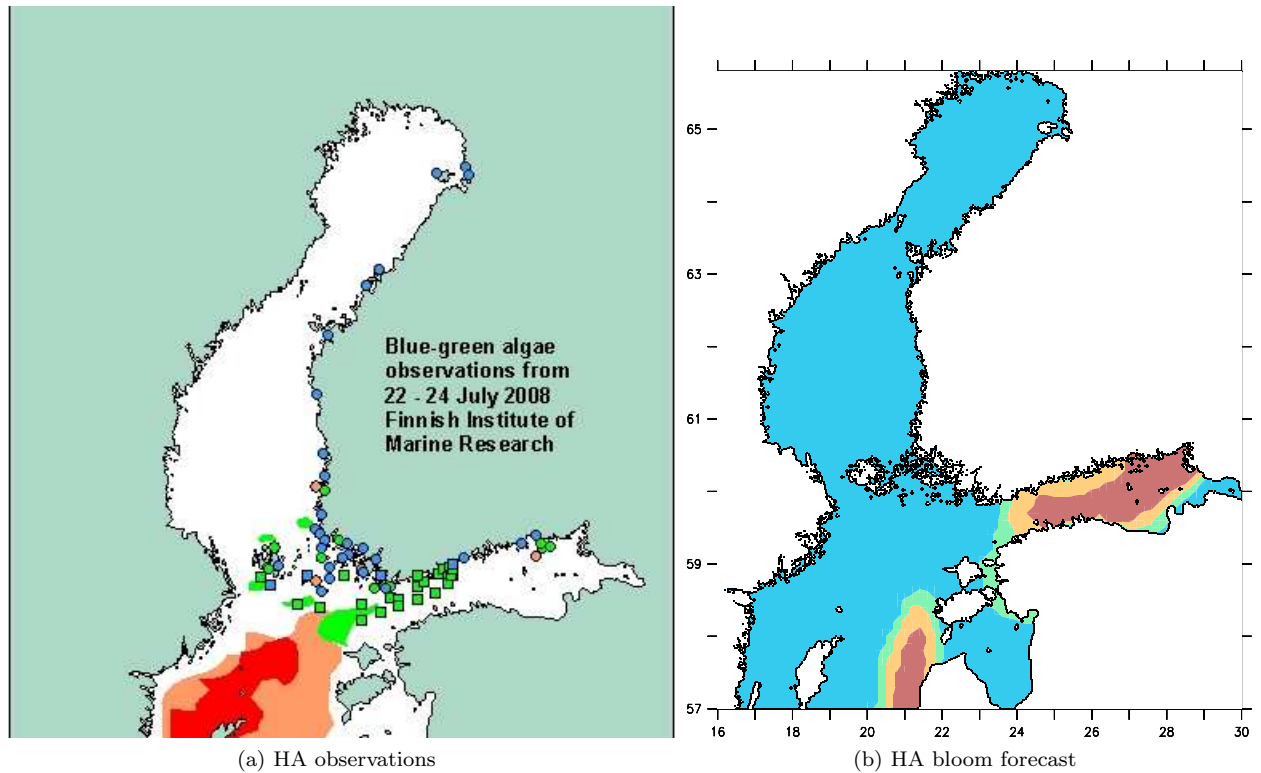


Figure 6: HA bloom observations and forecast. Figure 6a shows combined HA bloom observations from 22nd to 24th of July. Red colour is for very abundant blooms, orange is for abundant blooms, green means there is some algae and blue that there is no algae. This composite picture is based on qualitative sensory observations, there is no concentration data included. Figure 6b shows an ensemble HA bloom forecast with limiting value of 2 mg m^{-3} for blooming. This is a two week HA probability forecast formed from an ensemble run starting from 10th of July. Red colour indicates high probability of blooms ($> 75\%$), yellow considerable probability ($50\% - 75\%$), green moderate probability ($25\% - 50\%$) and green low probability ($< 25\%$).

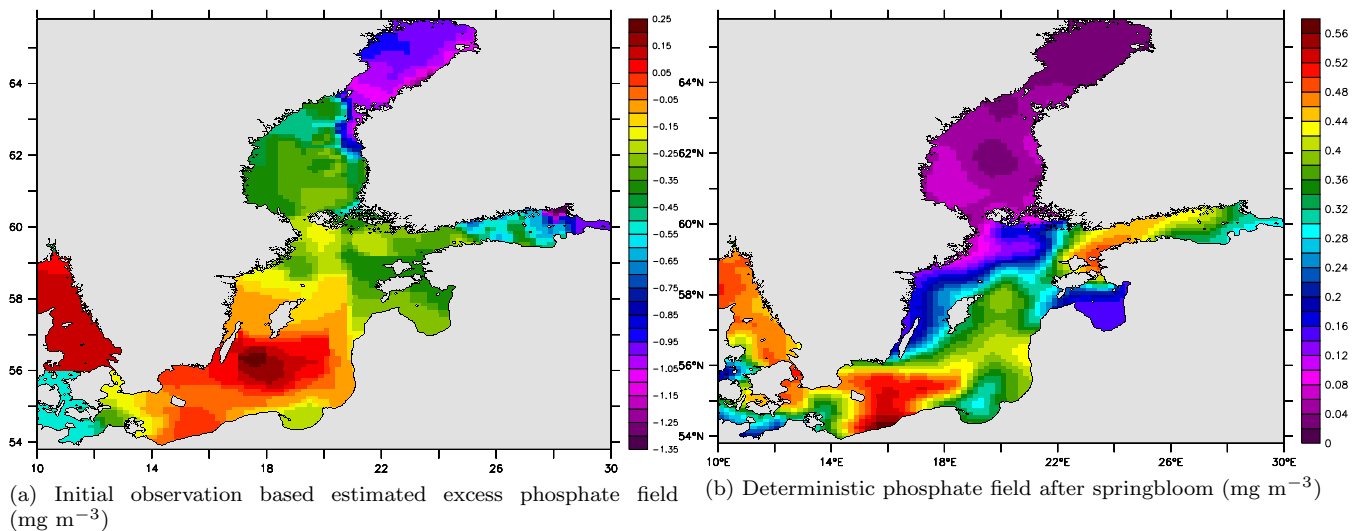


Figure 7: Figure 7a shows initial excess phosphate field interpolated and estimated from nitrate and phosphate observations made by R/V Aranda in winter 2008. Figure 7b shows phosphate field after spring bloom in the end of May 2008. Field is computed from observed initial fields by deterministic model.

there are significant areas where observations are not reliable or lacking altogether and therefore cause unestimated uncertainties in the model results. It will be interesting to further investigate whether perturbing the initial conditions could enable the quantification of the resulting uncertainty in the forecasts. However, a perturbation scheme for marine biogeochemical forecasts remains to be developed.

4.1. Applications

Ensemble forecasts of the marine environment have a variety of possible applications.

Environmental indicators, derived quantities describing state of the environment in an understandable manner, provide information needed for decision makers to mitigate environmental problems. The range of decision makers varies from individual consumers to politicians and the indicators should be helpful in making environmental decisions.

With ensemble forecasts it is also possible to illustrate how weather conditions affect HA blooms. It is a well-known fact that cold and windy weather prevents heavy blooms while sunny and calm weather promotes them. HA bloom maps can illustrate the probability of blooming instead of absolute amount of cyanobacterial biomass.

Applications developed by working with the users and recognizing their individual needs are essential when adding value for ensemble forecasts.

4.2. Illustrations of probability based forecasts

Because of the large information content of ensemble forecasts one major challenge is to communicate the results and their uncertainties to users. In deterministic forecasting we do not face these kind of problems simply because we have too little information on the uncertainties.

Recreational users need different kind of information than for example policy makers or commercial users. These differences should be taken into account in communication. There are different ways to solve the problem with probability based forecasts and in this work we have presented some of them. For instance, commercial users may benefit from the more detailed information provided by plume graphs in Fig. 5, while recreational users appreciate the more easily approachable map based presentation like the one in Fig. 6b. Customization of communicated message to suit end user needs often works for the benefit of all partners.

4.3. Carbon–Nitrogen stoichiometry

As discussed in Section 2.3, we used $C : N$ ratio of 6.3 for chlorophyll-a conversions. Carbon:nitrogen stoichiometry is one of the most discussed topics in marine chemistry and no final agreement on this relationship has yet been found. Most widely used ratio is so called Redfield ratio, $C : N = 106 : 16 = 6.625$. There has been many studies about the subject and it has been pointed out by

Arrigo (2005) that Redfield ratio is more an average than an universal constant, and a single measurement especially if made in coastal region can differ significantly from it.

The uncertainties in the nitrogen to chlorophyll-a conversion has its effects also on the accuracy of the forecast when verified against observations. Variation in conversion values adds uncertainties which could not be observed by this model setup. A biased conversion value will also cause bias to the results irrespective of actual model skill.

4.4. Warning limit for HABs

In Section 2.3, we determined a chlorophyll-a concentration of 2 mg m^{-3} as a limit for a possible visible cyanobacterial occurrence (see Section 2.3) Defining such a limit, however, for cyanobacterial bloom is difficult due to the lack of standards and especially because most bloom observations are based on visual approximation. However there are some studies where measurements have been done during cyanobacterial blooming in the Baltic Sea area (Seppälä, 1999; Nausch, 2004; Kutser, 2006; Mazur-Marzec, 2006). Kutser (2006) suggested that blooming can be defined as chlorophyll-a concentration exceeding 4 mg m^{-3} . Mazur-Marzec (2006) found that chlorophyll-a concentration was round 10 mg m^{-3} or more during blooming in Gulf of Gdańsk summer 2004. Therefore, taking into account the uncertainties in the nitroge-chlorophyll conversion, 2 mg m^{-3} is a conservative limit for a level of biomass that could be perceived as a harmful or nuisance bloom.

5. Conclusions

Ensemble forecasting appears to be a promising tool in operational biogeochemical oceanography. The probability based approach better illuminates the behaviour of modelled phenomena. Stable conditions create more unanimous ensembles and vice versa.

Spring-time phosphorus fields are a relatively good predictor for the spatial, basin-level distribution of HAB blooms in the summer. The spatial variation of forecasted blooms is relatively small.

The weather conditions, however, clearly have an impact on timing, duration and intensity of HA blooms. This variation can be observed from and quantified with the ensemble forecasts in a manner that lends itself to supporting pre-emptive actions, at least against adverse health effects.

When developing tools for marine policy making the quality of the modelled results should be well known and the quantification of errors should be considered. Quantitative verification of the HA bloom ensemble forecasts, however, is very challenging because of the limited amount of observational data, and the difficulties in matching the observed variables with the predicted variables.

Both the model's sensitivity to initial conditions and the challenges faced with verification suggest that HAB modelling would greatly benefit from an increased amount

of relevant observations. Verification would become much easier if quantitative information about biomass concentrations in the Baltic Sea during the summer was available. Gaps in the winter time phosphate monitoring measurements can lead to notable shortcomings in summer's bloom forecasts, and would need either more observations or a highly sophisticated assimilation scheme to fill. Should these kind of measurements and better assimilation schemes become available, we expect the benefits of the ensemble approach to become even more pronounced.

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A. Ecological equations

The equations in the ecological model are

$$\frac{\partial c_d}{\partial t} = c_d(\mu_d - e_d - m_d c_d) \quad (1)$$

$$\frac{\partial c_f}{\partial t} = c_f(\mu_f - e_f - m_f c_f) \quad (2)$$

$$\frac{\partial c_c}{\partial t} = c_c(\mu_c - e_c - m_c c_c) \quad (3)$$

$$\frac{\partial c_N}{\partial t} = -c_d(\mu_d - e_d) - c_f(\mu_f - e_f) - c_c(-e_c) \quad (4)$$

$$\frac{\partial c_P}{\partial t} = r_{PN}(-c_d(\mu_d - e_d) - c_f(\mu_f - e_f) - c_c(\mu_c - e_c)) \quad (5)$$

$$\frac{\partial c_S}{\partial t} = r_{SN}(-c_d(\mu_d - e_d)), \quad (6)$$

where c_d , c_f and c_c are the biomasses of diatoms, flagellate and cyanobacteria, respectively. Concentrations of nitrogen, phosphate and silicate are c_N , c_P and c_S . The constant ratios for cyanobacteria nutrient intake are r_{PN} and r_{SN} . Mortality rates are m_d , m_f and m_c . The specific rates of exudations are dependent exponentially on temperature by equation $e_{d,f,c} = e_0^{a_2 T}$.

The phytoplankton growth rates $\mu_{d,f,c}$ depend on nutrient concentrations, irradiation and temperature:

$$\mu_{f_{max}} = \mu_{f0} a^{dT} \quad (7)$$

$$\mu_f = \mu_{f_{max}} \frac{I}{I + k_{fI}} \left(\frac{c_P}{c_P + k_{fP}} \frac{c_N}{c_N + k_{fN}} \right), \quad (8)$$

where $I = I(z)$ is the illumination, μ_{f0} is the maximum growth rate at 0°C . $k_{fP,fN} = \mu_{f_{max}} / \alpha_{fN,fP}$ are the half saturation functions as used by Aksnes et al. (1995) with constant but species and limitation dependent affinities α . $I(z)$ depends on the amount of biomass between the depth z and the surface (shelf-shading).

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