SPECIAL PROJECT PROGRESS REPORT

All the following mandatory information needs to be provided. The length should *reflect the complexity and duration* of the project.

Reporting year	……07/2022-06/2023…………………………….……
Project Title:	Black Sea Ensemble forecasting system
Computer Project Account:	…spebulc…………………………………….……
Principal Investigator(s):	…Luc Vandenbulcke……………………….……
	………………………………………………….……
Affiliation:	……Université de Liège, Belgium………………
Name of ECMWF scientist(s) collaborating to the project (if applicable)	…………/……………………………………….……
	………………………………………………….……
Start date of the project:	……01/01/2021………………………………….……
Expected end date:	……31/12/2023………………………………….……

Computer resources allocated/used for the current year and the previous one

(if applicable)
Please answer for all project resources

		Previous year		Current year	
		Allocated	Used	Allocated	Used
High Performance Computing Facility	(units)	2.400.000	/	16.150.000	2.334.291
Data storage capacity	(Gbytes)	5000	/		

Summary of project objectives (10 lines max)

The aim of the project is to convert a deterministic NEMO implementation used in the CMEMS Black Sea Forecasting Center, into an ensemble model. The ensemble members will have different initial conditions, scalar model parameters e.g. in the turbulence module, the light penetration scheme, the surface bulk formulae, etc The uncertainty obtained from the ensemble will be quantified and the ensemble reliability and consistency will be studied.
Next, SST and in situ temperature and salinity will be assimilated using an EnKF method.
The impact of the uncertainty coming from the physical model, on a coupled biogeochemical will also be investigated. In particular, it will be analyzed if spurious adjustments of the vertical velocity lead to artificial nutriment upwellings. Finally, some biogeochmical variables will be assimilated in the coupled biogeochemical model as well.

Summary of problems encountered (10 lines max)

N/A

Summary of plans for the continuation of the project (10 lines max)

During the first half of 2023, 30 ensemble simulations of 10 members each were realized. In each ensemble, 1 specific model component was perturbed. This work is detailed further in the report.

During the remainder of the project, ensembles with all perturbations applied together will be run at reduced (15 km) and nominal (3 km) horizontal resolution, leading to the total consumption of the allocated SBUs. The results will then be evaluated using stochastic metrics (CPRS, RCRV…).

List of publications/reports from the project with complete references

N/A

Summary of results

If submitted **during the first project year**, please summarise the results achieved during the period from the project start to June of the current year. A few paragraphs might be sufficient. If submitted **during the second project year**, this summary should be more detailed and cover the period from the project start. The length, at most 8 pages, should reflect the complexity of the project. Alternatively, it could be replaced by a short summary plus an existing scientific report on the project attached to this document. If submitted **during the third project year**, please summarise the results achieved during the period from July of the previous year to June of the current year. A few paragraphs might be sufficient.

Although this report is submitted during the third year, given the delay of the tasks foreseen during the second year, and ultimately realized during the third year, the report is somewhat longer than a few paragraphs.

This first task, realized during the first years, consisted in selecting model components that are subject to uncertainty in the coupled Black Sea physical-biogeochemical modelling system, and generating corresponding perturbations that will be applied in ensemble simulations.
38 model components were selected to undergo perturbations in subsequent tasks, and are listed below in Table 1. Components 1-6 affect the physical model, the remaining affect the biogeochemical model. In anticipation of subsequent tasks, the corresponding recommended method of generating the perturbation is also indicated in the table.
The first 6 components concern uncertainty on the physical model inputs at the atmospheric interface, the land interface (rivers), and the bottom. The next 2 components concern the biogeochemical model at the atmospheric and land interfaces. All 8 components are perturbed using 2D fields with relevant spatial and temporal correlations (see later, task 1.3). The remaining components are scalar parameters of the biogeochemical model, which will be perturbed uniformly in space and kept constant in time (i.e. the deterministic scalar parameter is replaced with another scalar value).
These biogeochemical parameters are selected from the literature. Grégoire et al (2008) contains the original description of the BAMHBI model, and includes a sensitivity study. Wang et al (2020) and Garnier (2006) both contain a sensitivity study and ensemble simulations of different biogeochemical models. Capet (private communication) realized a sensitivity study of the BAMHBI biogeochemical model in the Black Sea, based on Morris screening. Various biogeochemical parameters appear in multiple studies among the 4 cited above; in that case, in Table 1, they are attributed only once.

	Component	Source	Perturbation method and intensity
1	River water flux		2D AR1
2	Bottom drag coefficient		2D AR1
3	Wind at 10 meter		0D * Fourier modes
4	Temperature at 2 meter		0D * EOFs
5	Total cloud coverage		0D * EOFs
6	Precipitations		0D * EOFs
7	River nutrient flux		2D AR1
8	Atmospheric nutrient deposition		2D AR1
9	Maximum grazing rate of mesozooplanktong	Grégoire et al (2008)	Γ [20%]
10	α_π of diatoms		Γ [30%]
11	Assimilation efficacity on carbon		β [20%]
12	Efficiency of growth (mesozooplankton)		β [10%]
13	Nonlinear mortality rate (mesozooplankton)		Γ [50%]
14	Half-saturation of mortality (mesozooplankton)		Γ [0.67 %]
15	Capture efficiency of mesozooplankton by gelatinous		β [20%]
16	Maximum grazing rate of gelatinous		Γ [20%]
17	Capture efficiency of diatoms by mesozooplankton		β [10%]
18	Assimilation efficacity of nitrogen		β [10%]
19	μ_{max} (diatoms)		Γ [30%]
20	Si:N ratio (diatoms)		Γ [5 %]

21	Minimum N:C ratio (diatoms)		Γ [10%]
22	Mortality rate (diatoms)		Γ [50%]
23	Messy feeding ratio (microzooplankton)		β [20%]
24	Messy feeding ratio (mesozooplankton)		β [20%]
25	Minimum sinking rate (diatoms)	Wang et al (2020)	Γ [50%]
26	Maximum sinking rate (diatoms)		Γ [50%]
27	Mortality (flagellates)		Γ [50%]
28	Mortality (Emiliana)		Γ [50%]
29	k_s (NHS)		N [50%]
30	μ_{max} (flagellates)	Garnier (2006)	Γ [50%]
31	μ_{max} (Emiliana)		Γ [30%]
32	Q10 (flagellates and Emiliana)		logΓ [20%]
33	Q10 (diatoms)		logΓ [idem]
34	Q10 (zooplankton)		logΓ [idem]
35	$Dzeta_{bio}$ (light absorption model parameter)	Capet (private communication)	Γ [5 %]
36	eta_{bio} (idem)		Γ [5 %]
37	Light absorption rate B (idem)		Γ [5 %]
38	Q10 (chemical reactions)		logΓ [20%]

Table 1. list of perturbation candidates, corresponding literature reference, recommended perturbation method and intensity = σ/μ where μ is the parameter's expected value, and σ is the expected parameter standard deviation

The next task, also realized during the second year of the project, required to update the stochastic module of NEMO, as well as the (physical and biogeochemical) modules using it. The work was realized in NEMO 3.6 and 4.0.6.
The NEMO STORNG module allows to initialize (seed) the random number generator, and to draw random numbers from specified statistical distributions.

In the publicly-available NEMO code, the random number generator is initialized from hard-coded values (e.g. 1234567890987654321) with the idea that ensemble members are run concurrently (double MPI parallelization on both members and space). However for practical reasons, on mid-size (tier-1 and tier-2) high-performance computing (HPC) machines, it is not possible to run ensembles of 50 members using ~200 cpu cores each. Members have to run (at least partly) sequentially. Therefore, a new option (controlled from the model namelist) was implemented in STORNG to allow a different seed for different members, based on the unix system time.

STORNG already contained routines to draw random numbers from the uniform, gaussian and gamma distributions. Code was added to also draw from the beta distribution.

The STOPAR module then builds various methods for generating the actual perturbations. The general idea of the original module is to build 2D or 3D fields with given temporal and spatial correlation lengths by means of autoregressive random processes, and filtering.

The new version adds 0D (scalar) fields (with given temporal correlation length) and the ability to load fields from netcdf files and combine them in random sums.

These fields are specified from the model namelists. The user could choose to use temporal lags (i.e. model states at different instants), data assimilation increments (for observed variables in a data-assimilative model run), empirical orthogonal functions (EOFs), Fourier modes…

During the project, the method was applied to generate perturbations for atmospheric fields such as the air temperature at 2m above the sea. 100 EOFs are computed from a time-serie extracted from the ECMWF ERA5 product over 2015-2020. At model initialization, these EOFs are loaded from netcdf files (including the on-the-fly spatial interpolation coefficients if EOFs are provided on a different horizontal grid than the model). During model integration, at each timestep, 100 random numbers are drawn and multiply the EOFs in a linear combination that is added to the original field. In the case of air temperature, the random numbers have a temporal correlation of 5 days.

The same methodology is applied to air humidity or to precipitation, with temporal correlations of respectively 2.5 days and 1 day.

The method described above relies on the hypothesis that the EOFs (or other 2D spatial fields that can be used to characterize the model error in space) have a unique temporal correlation length.

It is well known that the first EOFs generally correspond to large-scale spatial structures, which tend to evolve over longer time scales; whereas higher-order EOFs tend to represent smaller scales; at the limit, the highest-order EOFs are mostly random noise.

Regarding the wind perturbation, the following variant is used. Fourier modes are computed from the original time-serie of U and V wind fields (2015-2020), leading to a huge amount of modes (over 100.000). The 75 most important modes (in the statistical sense) were selected; the most important one was identified as having a 24-hour period (i.e. the daily mode). Only 4 modes were automatically selected with a relatively short period (shorter than 96 hours), although it is expected that these “fast” modes may have relevant contributions to the error. Therefore, 25 supplementary modes with short periods were randomly selected. The selection procedure is illustrated in Fig. 1.

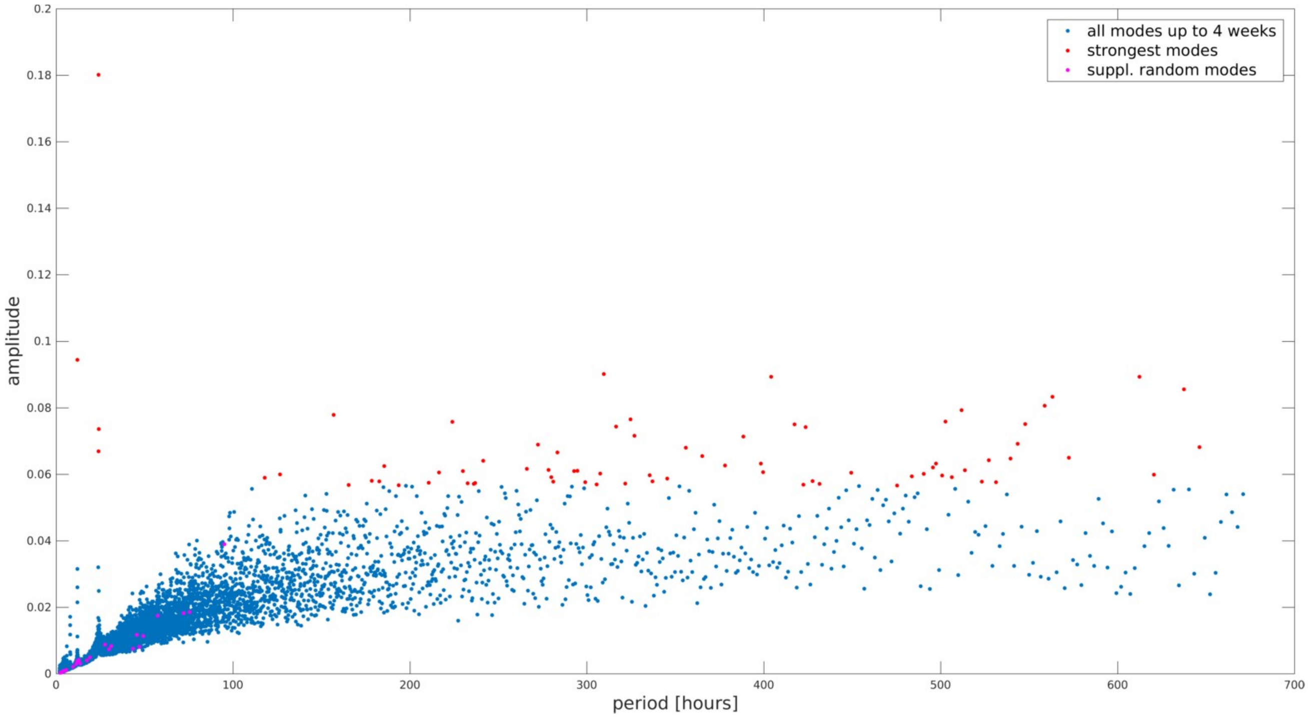


Figure 1. basin-wide average of the amplitude of the Fourier modes, as a function of the period. The 75 modes with highest amplitudes are selected (red dots). 25 modes are selected among the modes with short periods (pink dots).

These 100 (75+25) modes are loaded at model initialization. During the model run, the random coefficients that multiply the modes each have a different temporal correlation length, corresponding to the period of the respective modes. Large (spatial) scale error modes will vary more slowly than small scale error modes.

The intensity of the perturbation is tuned so that it corresponds to the expected error of the respective product, e.g. for the wind field, the expected error can be estimated by comparing the actual wind forecasts (provided by ECMWF) to satellite wind measurements.

Regarding the method used to perturb the scalar biogeochemical model parameters, the approach of Prieur et al (2019) was used. Unconstrained parameters are drawn from normal (i.e. Gaussian) distributions. Parameters required to be positive (or negative) are drawn from Gamma distributions. Parameters required to be in the [0,1] interval are drawn from Beta distributions. Finally, parameters required to be larger than 1 are drawn from the log-Gamma distribution. The distribution parameters are chosen in order to obtain the required mean and standard deviation; the latter is specified in the NEMO namelist corresponding to the biogeochemical model and its perturbation.

It should be mentioned that other perturbation candidates exist, and methods are readily available in the standard NEMO branch to apply the corresponding perturbations, e.g. the perturbations of the equation-of-state or the variables trend with respect to sub-grid processes. These model components have not yet been perturbed during the project, but may be examined later. Perturbations of the initial conditions are also not explicitly considered.

The next task aims at validating the choice of perturbation candidates described above, and validate the chosen perturbation intensities, by running 1 ensemble simulation for each perturbation. Thus, 38 ensembles of 10 members of low-resolution (15 km) models were run for 1 year, on the HPC during the first half of 2023.

1 year simulations were realized, in order to cover all hydrodynamic and biogeochemical regimes. The drawback of simulating 1 full year at once, is that no perturbation of the initial condition is required, whereas it could be necessary in non-subsequent short-term forecasts. However, it is expected that perturbed initial conditions can be obtained off-line (i.e. before starting the model), e.g. by building a random linear combination of model states around the real forecast start time, or by adding random combinations of data assimilation increments obtained from previous simulations.

Some examples of ensemble spread are given below, first for the physical variables and then for the biogeochemical ones.

In sub-ensemble 1 (perturbed river water flux, as indicated in Table 1), as expected the surface salinity is largest at the river mouths, in particular the Danube. The salinity spread is also large in deeper layers of the shelf (20-40 meters depth). Interestingly, the velocity spread is large at the shelf break, indicating that the river flux influences the export from shelf to open sea (Fig 2).

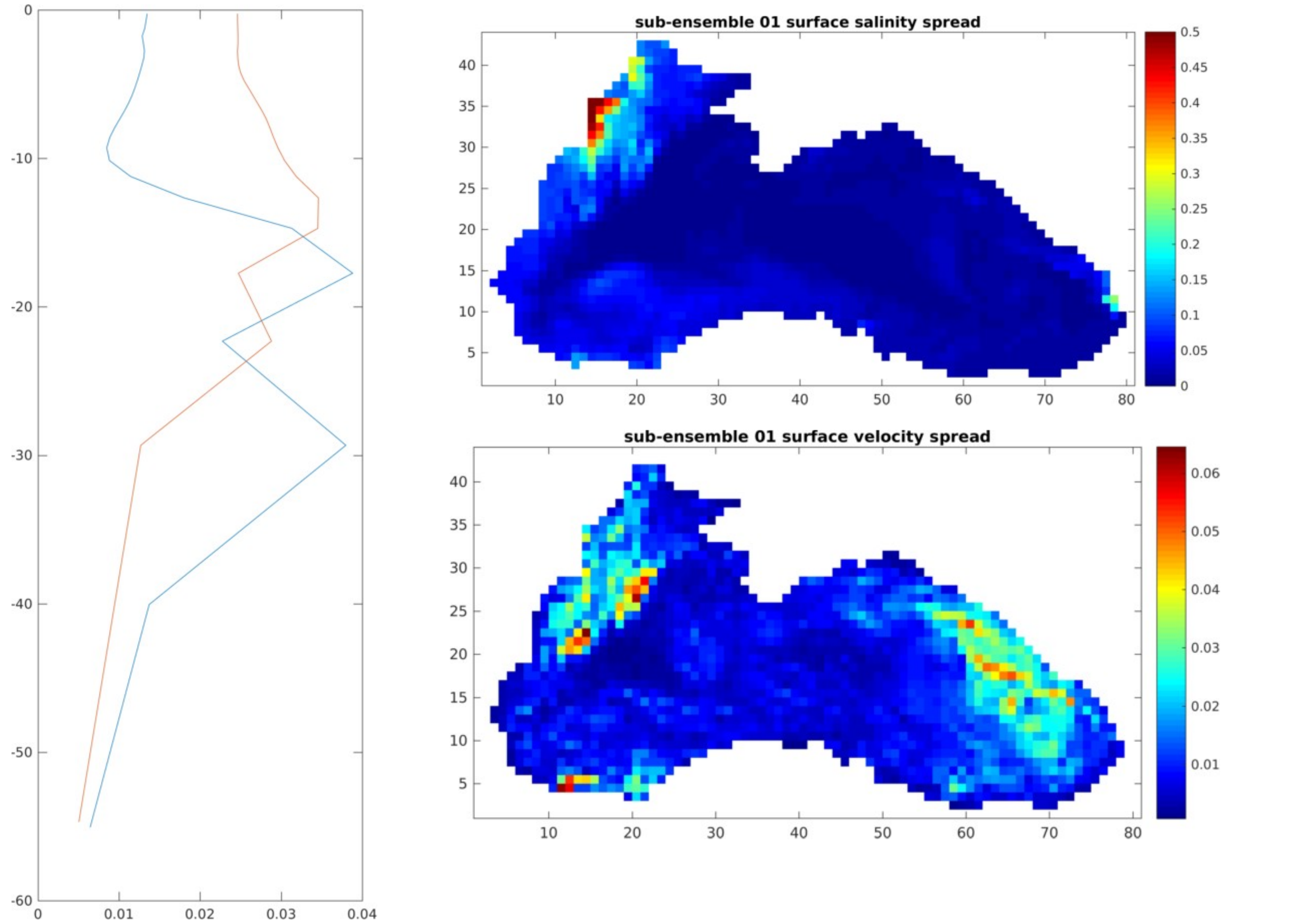
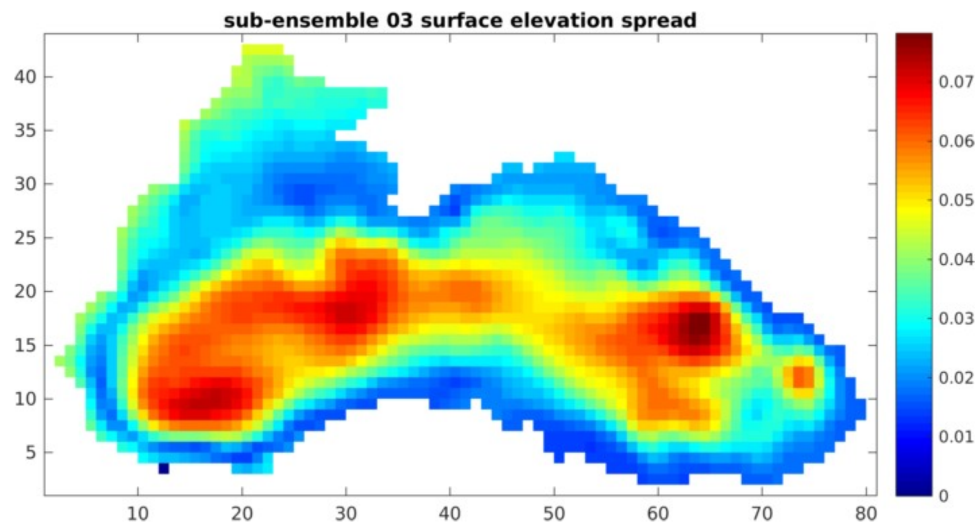


Figure 2. ensemble spread in ensemble 1 (perturbed river flux) : (left) 2 vertical profiles of ensemble spread of salinity in the deep part of the basin, limited to the upper 60 meters. (top right) ensemble spread of surface surface salinity (bottom right) ensemble spread of surface velocity module.

The sub-ensemble corresponding to perturbations of the wind yields the largest impact on the spread of physical variables (as expected from numerous examples in the literature), and particularly the sea surface height, with spread locally over 7 cm (Fig 3). The color range in Fig. 3 is about 3 times larger than in the corresponding panel of Fig. 2; the velocity spread is largest in the Rim Current but also on the coast (especially on the shelf), with values frequently over 10 cm/s.



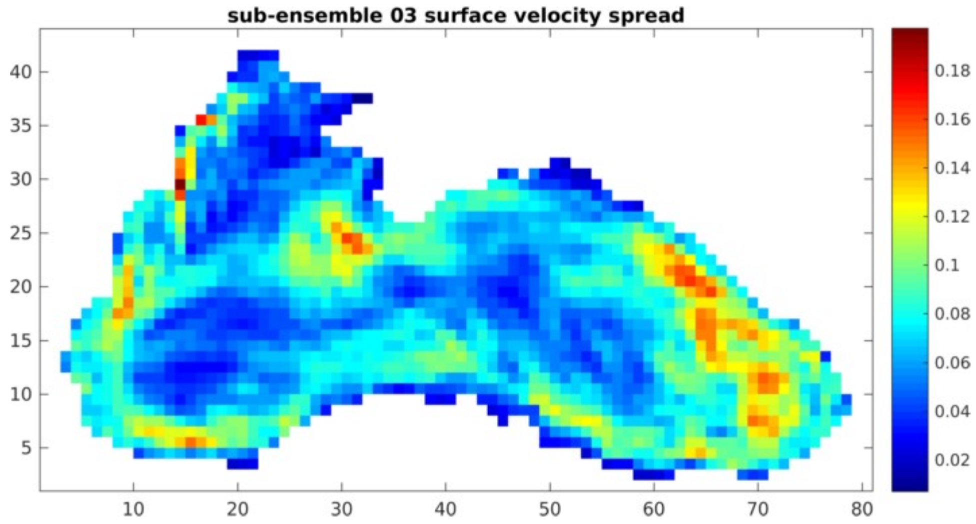


Figure 3. Ensemble spread in ensemble 3 (perturbed wind) : (top) surface elevation spread, (bottom) surface velociry module spread

Compared to river water flux perturbations, perturbations of the air temperature at 2m does lead to surface salinity spread slightly larger in the open sea, but (as expected) much smaller on the shelf areas. The corresponding sea surface temperature spread is (naturally) much higher in sub-ensemble 5 with a spread in winter of 0.2°C. The surface elevation spread is more-or-less uniform over the basin, with the exception that is is higher in the semi-permanent eddies at the Rim Current margins.

Perturbations of the total cloud coverage moderately influence surface salinity and temperature, particularly on the shelf break. Surface elevation spread is small (less than 1 cm). Perturbations of the precipitation influences the surface salinity (locally the spread is larger than 1 psu) and also temperature.

A more detailed impact study may reveal the influence of the different physical perturbations on particular processes, e.g. the Turkish coastal upwelling events as characterized by the BS-MFC Ocean Monitoring Indicator (OMI) and may be studied later.

Perturbation of the biogeochemical model does not influence the physical fields in the current version (the feedback of chlorophyll on temperature propagation to depth is not activated); this will be modified after inclusion of the radiative transfer model.

Dissolved oxygen concentration is mainly characterized by the physical model, with an additional effect of the biogeochemical processes. The perturbation of the wind field leads to ensemble spreads of up to 10 mmol/m3 at the surface, and over 30 mmol/m3 at the depth of the oxycline (when the latter is shoaled or deepened due to the perturbation). River water flux, bottom drag, air temperature, and cloud coverage all lead to much smaller ensemble spread, although not negligible.

Chlorophyll concentration is also most strongly influenced by the wind, with, in winter, values of 0.1 mg/liter at the surface and in the mixed layer, and up to 0.4 mg/liter at the depth of the deep chlorophyll maximum (DCM). On the north-western shelf, the ensemble spread is even higher, and reaches values over 1 mg/liter at the surface or below it. Similarly as for oxygen, the other physical perturbations also have an impact, although smaller. For example, perturbations of air temperature yield a spread of 0.01 mg/liter at the surface and in the mixed layer, and 0.03 mg/liter at the DCM depth.

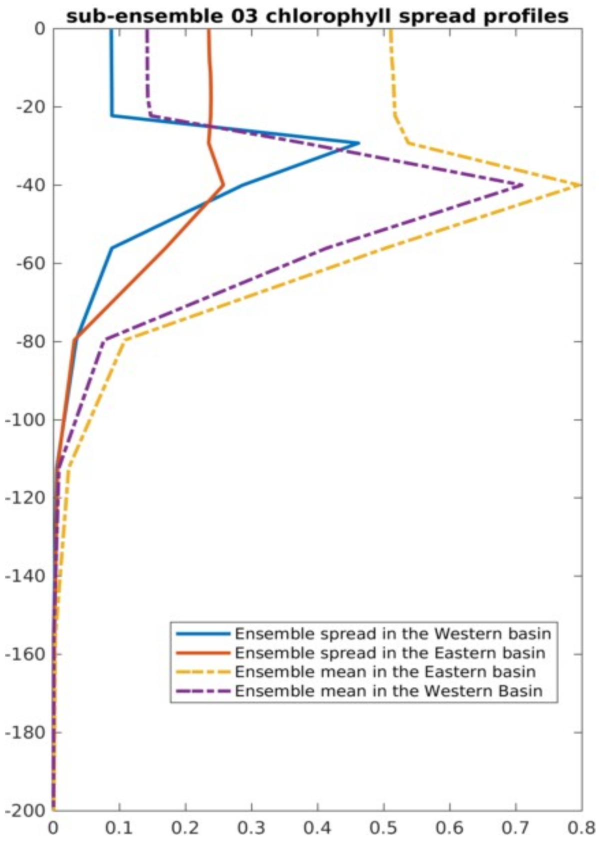
The impact of river nutrient concentrations is huge at the river mouths, with spread values for chlorophyll reaching 1.3 mg/liter close to the Danube mouth and over 0.5 mg/liter further away (on the shelf), but less than 0.002 in the open sea surface and 0.012 at the DCM depth.

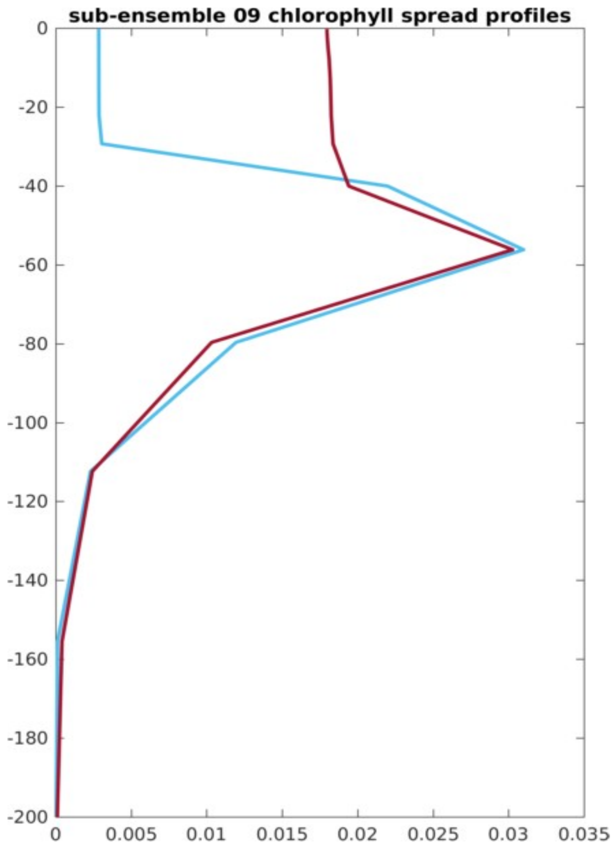
Surprisingly, the atmospheric deposition perturbation effect is small everywhere, and this particular perturbation is probably too small and will be re-estimated (and the corresponding ensemble re-run). Uncertainty on atmospheric deposition of nitrate and phosphate is actually huge, with estimates for phosphate varying by a factor of 10 (JRC, private communication), i.e. much larger uncertainty than what is currently considered in current study.

The impact of the (perturbation of the) 30 biogeochemical scalar model parameters cannot be briefly summarized; it would require a separate description for each of them.

Generally speaking, perturbations of some parameters have rapid and short-term effects, or have an effect only during specific periods (e.g. bloom) while the impact of others can only be seen after longer periods.

However, all of them have a clear impact, which can be (periodically) more important than the ones coming from physical parameter perturbations (except the wind). Logically, the impact is always most visible where the biogeochemical acivity is the most intense, e.g. the shelf areas close to river mouths, or at the DCM depth in the open sea, or in the mixed layer during winter/spring blooms.





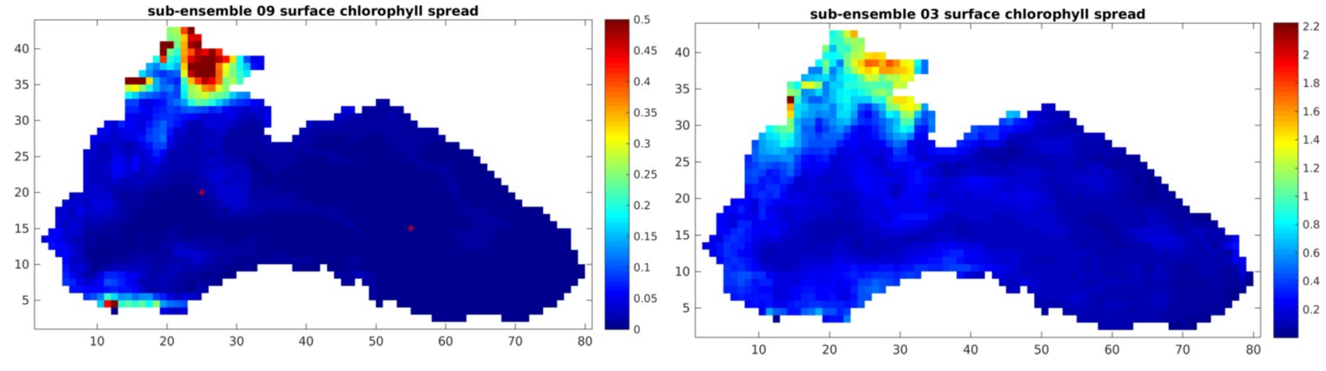


Figure 4. Ensemble chlorophyll spread : vertical profiles (top) and surface values (bottom) in sub-ensembles (left) 3 (perturbation of the wind) and (right) 9 (perturbation of the maximum grazing rate of the mesozooplankton). On the upper left panel, the ensemble mean chlorophyll profiles are indicate for reference, as dashed lines. The location of the vertical profiles is indicated by red starts in the lower left panel