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Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

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Abstract

Operational prediction of the marine environment is recognised as a fundamental research issue for Europe. We present a pre-operational implementation of a biogeochemical model for pelagic waters of the Mediterranean Sea, as developed within the framework of the MERSEA-IP European project. The OPATM-BFM coupled model is the core of a fully automatic system that weekly delivers analysis and forecast maps for the Mediterranean Sea biogeochemistry. The system in the present configuration has been working since April 2007 with successful execution of the fully automatic operational chain in the 87% of the cases, and in the remaining cases the runs were successfully accomplished after operator intervention. A description of the system developed and a comparison of the model results with satellite data are also presented, with Spearman correlation on surface chlorophyll temporal evolution equal to 0.71. Future studies will be addressed to the implementations of a data assimilation scheme for the biogeochemical compartment in order to increase the skill of the model performances.

1 Introduction

Environmental risks of natural or anthropogenic origin may be prevented or managed by the use of short-term forecasts as those provided by an operational forecasting system. In this regard, operational oceanography constitutes a powerful tool to monitor, analyse and predict the state of the marine resources as well as the sustainable development of coastal areas (Fleming et al., 2002).

The progress of short-term forecasts for the marine ecosystem to be employed within an environmental monitoring system is one of the main objectives pursued by the Global Monitoring for Environment and Security initiative (GMES; http://www.gmes.info/). The Marine Environment and Security for the European Area (MERSEA) Strand-1 Project was launched in 2003 in order to assess the European capabilities to put in

OSD

6, 1223–1259, 2009

Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

action the proposals of the marine GMES (Johannessen et al., 2006). This effort has been then followed in 2004 by the MERSEA Integrated Project (MERSEA-IP; http://www.mersea.eu.org/), whose primary objective was the deployment of a pan-European operational system for monitoring and forecasting the ocean physics, biogeochemistry and ecosystem on global and regional scale. The purposes of MERSEA are going to be further developed during the MyOcean initiative (http://www.myocean.eu.org), the implementation project of GMES Marine Core Service, started in April 2009.

An application of the operational monitoring and forecasting system expected by MERSEA-IP is particularly needed for the Mediterranean Sea, a basin which is characterized by a natural variability and an intense human pressure, and represents a region extremely vulnerable to the environmental threats (Pinardi et al., 2006; Pinardi, 2007). These goals are fostered by the association of operational and research institutes collaborating within the Mediterranean Operational Oceanography Network (MOON; http://www.moon-oceanforecasting.eu/). MOON is the coordinating body of EuroGOOS Mediterranean Task Team, who has developed the Mediterranean ocean Forecasting System (MFS; http://gnoo.bo.ingv.it/mfs/; Pinardi et al., 2003) starting from the MFSTEP project (http://www.bo.ingv.it/mfstep/).

The object of the present work is the implementation of the OPATM-BFM (Océan PArallelisé Transport Model – Biogeochemical Flux Model) for the Mediterranean basin, leaded by OGS in the framework of MERSEA, and constituting the zero-version of the MyOcean services catalogue.

Other examples of biogeochemical and ecosystem-level short-term predictions for some European regional seas include the TOPAZ system for the North Atlantic and Nordic Seas (http://topaz.nersc.no/), operated by the Mohn-Sverdrup/Nansen Center and the Medium Resolution Continental Shelf model for the north-west European continental shelf (http://www.ncof.co.uk/Ecosystems-Model-Forecast.html), managed by the National Centre for Ocean Forecasting.

Operational forecasting in the Mediterranean Sea has greatly improved during the last decade, but the biogeochemical applications have been less pursued with re-

OSD

6, 1223–1259, 2009

spect to those related to marine physical state (Pinardi et al., 2006). MOON aims at improve the capacity of operational modelling of the biogeochemical cycles in the Mediterranean Sea, both at regional and basin scale.

As the marine ecosystem component of MFS, the coupled eco-hydrodynamic model OPATM-BFM, initially conceived to supply boundary conditions for the coastal biogeochemical models developed under MOON, has become one of the most promising results of MERSEA-IP. During this project, this model successfully delivered via web pre-operational short-term hindcasts/forecasts of some key biogeochemical variables for the Mediterranean basin.

The present work widely illustrates the preparation, the implementation and a positive evaluation of the first pre-operational system devoted to routinely provide short-term forecasts for the Mediterranean Sea biogeochemistry. The technological and scientific results obtained so far illustrate that the system has properly worked during the testing phase, satisfactorily reproducing the features of the chlorophyll seasonal cycle in the Mediterranean basin during the period under study, as well as the dynamics of a localized chlorophyll bloom event. The interdisciplinary effort under the OGS coordination in the framework of the Italian GNOO (Gruppo Nazionale di Oceanografia Operativa – National Group of Operational Oceanography; http://gnoo.bo.ingv.it/) has assured the development of all the components constituting the OPATM-BFM system.

Section 2 describes the model structure, Sect. 3 deals with the multi-disciplinary infrastructure behind it, Sect. 4 resumes some results obtained over one year of pre-operational activity and a discussion about the on-going development of the system is finally presented. The conclusions are resumed in Sect. 5.

2 OPATM-BFM model overview

OPATM-BFM is a transport-reaction model that numerically solves the time evolution of chemical and biological state variables in the marine environment. It is based on the coupling between the OPA Tracer Model version 8.1 (Madec et al., 1998) and the

Biogeochemical Flux Model (BFM; Vichi et al., 2007a,b).

The governing equations are formulated as advection-diffusion-reaction equations, one for each variable:

$$\frac{\partial c_i}{\partial t} = -\boldsymbol{U} \cdot \nabla c_i + (-1)^{n+1} k_h \nabla_h^{2n} c_i + \frac{\partial}{\partial z}\left[k_v \frac{\partial c_i}{\partial z}\right] + w_{si} \frac{\partial c_i}{\partial z} + R_{\mathrm{bio}}(c_i, c_1 \ldots c_N, T, I \ldots) \quad (1)$$

where $c_i = c_i(\boldsymbol{x}, t)$ is the biogeochemical concentration of the i-th state variable, $-\boldsymbol{U} \cdot \nabla c_i$ is the advection term ($\boldsymbol{U}$ is the circulation field), $k_h (-1)^{n+1} \nabla_h^{2n} c_i$ is the horizontal diffusion term, with k_h the horizontal eddy diffusivity and n= 1,2 according to, respectively, the Laplacian or bi-Laplacian scheme, and $\frac{\partial}{\partial z}\left[k_v \frac{\partial c_i}{\partial z}\right]$ the vertical diffusion, with k_v the vertical eddy diffusivity. The previous term allows to simulate the vertical mixing, a fundamental environmental process for the ecosystem evolution. The fourth term on the RHS represents the sinking process, and w_{si} is the particulate sinking velocity, while the last term R_{bio} is the biological reactor. The initial and boundary conditions are:

$$c_i(\boldsymbol{x}, t = t_0) = c_i^0 \quad (2)$$

$$c_i(\boldsymbol{x} \in \partial D, t) = BC(\boldsymbol{x} \in \partial D, t) \quad (3)$$

where ∂D is the boundary of the domain D where the boundary conditions (BC) hold.

In the present work, BFM implements the generic term R_{bio}. BFM is based on cycles of carbon and macronutrients (phosphorous, nitrogen and silica), and is targeted on the phytoplankton/nutrients and microbial loop. Key aspects of the BFM are its potential for limitation by macronutrients (nitrogen, phosphate and silicate), the use of adjustable C:N:P:Si ratios in zooplankton and phytoplankton compartments, and the chlorophyll to carbon variable dependency.

The simulations are carried out by coupling OPATM-BFM with an high resolution Ocean General Circulation Model (OGCM). The coupling between the OGCM and BFM is described in the following.

2.1 The biogeochemical-physical coupling and the physical forcing

In the present case the coupling allows the integration of Eq. (1), providing the physical fields (e.g. $\boldsymbol{U}$, T, I) to the advection, diffusion and reaction terms. It is worth noting that the advection and diffusion terms are linear. Conversely, BFM depends non-linearly on wind, temperature and PAR.

The coupling can be implemented in two ways: on-line or off-line. In the on-line approach a synchronous solution of the OGCM equation and transport-reaction equation is carried out, thus meaning that the two models are simultaneously running. The on-line approach is the "standard" way of coupling (Crise et al., 1998), but for operational purposes not always represents the best choice. In the off-line approach the physical fields are considered as an external forcing so they must be already computed before the integration of the transport-reaction equation. One of the hypotheses of the off-line approach is that the generic biogeochemical concentration c_i does not influence the physical fields, therefore c_i is passively transported by the current. This hypothesis holds because, generally, the physical processes are mostly independent of the biology (Mann and Lazier, 1991).

For the present application, the off-line approach was decided. The principal motivations can be summarized in the following points:

1. In off-line operational applications, any upgrade in the OGCM model (e.g. evolution of the data assimilation skill, advancements in the numerical scheme or in the parameterizations) is directly reflected in an improvement of the physical forcing for the biogeochemistry.

2. The BFM parameters have been estimated mainly through experiments defined by constant light and external conditions (Baretta-Bekker, 1995), and this approach is therefore consistent with daily mean forcings used in the present off-line coupling.

3. In case of very complex models such OPATM-BFM the off-line approach allows to reduce the computational burden. Moreover, the integration time-step for physics and biology are decoupled, therefore the biogeochemistry equations can be integrated using larger time-step, dramatically improving the performances.

4. It is possible to implement new versions of the OPATM-BFM code on different computational infrastructures using exactly the same stored physical forcings.

In the pre-operational infrastructure started during the MERSEA project, the physical forcing fields have been provided, by the MFS-SYS2b ocean forecasting system managed by INGV (Istituto Nazionale di Geofisica e Vulcanologia, Bologna, Italy). This system is based on the OPA8.2 model (Madec et al., 1998) implemented on the Mediterranean Sea (Tonani et al., 2008) and includes as assimilation scheme the System for Ocean Forecasting and Analyses (SOFA; Dobricic et al., 2007). The MFS was chosen since this model has been intensively validated and today represents one of the most advanced tools to simulate the circulation in the Mediterranean Sea.

The INGV circulation model supplies three-dimensional and two-dimensional surface physical forcing fields for the Mediterranean Sea (Fig. 1): the first are zonal, meridional and vertical current speeds, vertical eddy diffusivity, temperature and salinity, the second are solar short-wave irradiance and wind speed. The three velocity components are necessary to calculate the transport term for each passive tracer. Eddy diffusivity is relevant to reproduce the vertical mixing processes of the tracers along the water column. Temperature, salinity, irradiance and wind speed enter as regulating terms in the biogeochemical reaction term R_{bio} of Eq. (1).

The OPATM-BFM has 1/8° horizontal resolution and a numerical configuration characterized by an affordable computational load. However, the horizontal resolution of the INGV model is higher (1/16°) than that of the tracer model, therefore to reduce the finer grid to the coarser one an interpolating interface is necessary.

The interpolation is implemented by a mesh merging technique: the coarse grid is obtained by merging (by a cell surface weighted average) four adjacent cells of the

OSD
6, 1223–1259, 2009

finer grid. Horizontal velocity fields are calculated with the constraint of preserving fluxes along the same vertical cross-sections:

$$\int_A \boldsymbol{u}_h^A \cdot d\boldsymbol{A} = \int_B \boldsymbol{u}_h^B \cdot d\boldsymbol{B} \tag{4}$$

where A and B are the discretization of the same vertical cross-section defined respectively on the INGV model grid and on the OPATM-BFM grid, $\boldsymbol{u}_h^A$ and $\boldsymbol{u}_h^B$ are the original and interpolated horizontal velocity, $d\boldsymbol{A}$ and $d\boldsymbol{B}$ are the vectors normal to the surfaces A and B.

Interpolated vertical velocity fields w are then derived integrating the horizontal divergence of the velocity field:

$$w(z) = -\int_{\text{Bottom}}^{z} \text{div}_h(\boldsymbol{u}_h^B)dz \tag{5}$$

The vertical resolution is left unchanged in order to maintain a good reproduction of the vertical dynamics and mixing of the water column, which is known to be of great relevance for biogeochemical processes (Mann and Lazier, 1991).

For what concerns the time resolution, the forcing data are stored as daily means, filtering out all the fast gravity waves which do not contribute substantially to the general circulation. The tracer model of the OPATM-BFM system, that has an integrating time step of 30 min, computes the values of the forcing fields between each frame by a linear interpolation in time.

The skill of the spatial interpolation scheme has been checked on the advective and diffusive processes. In Fig. 2 we show the water mass inflow, outflow and net flow for the Gibraltar and Sicily Straits sections (see Fig. 1), evaluated on the period under study: the net horizontal fluxes of mass computed after the interpolation (1/8°) are equal to the original ones (1/16°) for the condition imposed in Eq. (4). The slight differences between IN and OUT fluxes are caused by the resolution-dependent sections

OSD
6, 1223–1259, 2009

Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

used in the two estimates. These differences can be evaluated as nearly the 1% of the IN and OUT fluxes.

In Fig. 3 we show four monthly profiles of the vertical eddy diffusivity coefficient (k_v) spatially averaged over two sub-basins of the Mediterranean Sea, NWM and EME (see Fig. 1). The interpolation acts on each level and the vertical profiles of k_v before and after the interpolation remain preserved throughout the period considered, with small discrepancies observed in May (around 100 m depth in NWM and around 40 m in EME).

2.2 The BFM customisation

The BFM has been tailored to be more specifically suitable for our purposes, in particular since the effect of the bottom fluxes is negligible with respect to the simulation time scales, the benthic compartment has been switched off. In the present configuration, the no-flux boundary condition for the generic tracer holds at the bottom level and no specific formulation is prescribed to all the organic variables in the mesopelagic and batipelagic compartments. The living functional groups implemented in the model are presently:

- phytoplankton (diatoms, flagellates, picophytoplankton, dinoflagellates);
- mesozooplankton (carnivorous and omnivorous mesozooplankton);
- microzooplankton (microzooplankton, heterotrophic nanoflagellates);
- bacteria.

Each functional group can be represented as a vector of state variables, whose components represent the dynamically adjustable concentration of carbon and macronutrients. The OPATM-BFM has 51 prognostic variables, which are divided in living components (pelagic bacteria, diatoms, flagellates, picophyotplankton, dinoflagellates, microzooplankton and mesozooplankton) and non-living components (dissolved oxygen, macronutrients as phospate, nitrate, ammonium, silicate, dissolved and particulate organic matter). The diagnostic variables are gross/net primary production and bacterial production.

The number of parameters is larger than 120: for such a high number of degrees of freedom, a brute force approach to estimate the sensitivity in a three-dimensional environment is therefore not feasible. The model was initially calibrated by testing empirically the sensitiveness of its implementation, confirming what already found out for the other models: the most sensitive parameterisation was that related to the photosynthesis and respiration processes (Varela et al., 1995), with a relevant role played by the bacterial activity. The model parameters were then tuned for the Mediterranean Sea in the framework of the MFSTEP project (see details in Lazzari and Crise, 2006).

The same tests showed the importance of light parameterisation: the light model adopted in the present configuration is the Lambert-Beer non-spectral approximation that is commonly used for Mediterranean Case 1 water (e.g. Allen et al., 2002; Crise et al., 1998).

2.3 Initial and boundary conditions

The time scales explored by the operational models are typically short and therefore deserve to have accurate sets of initial and boundary conditions. This procedure substantially reduces the spin-up time and helps the convergence toward a realistic solution. Emphasis has been put in the collection and definition of the initial conditions for the described forecasting system.

The nutrient pools (nitrogen, phosphate, silicate) and oxygen for the biogeochemical model BFM were initialised with the vertical profiles provided by a retrospective reanalysis carried out during the MFSTEP project over the MEDAR-MEDATLAS 2002 data set (Crise et al., 2003). The data considered in that analysis concern dissolved oxygen (from 1948 to 2002), nitrate (from 1987 to 2002), phosphate (from 1987 to 2002) and silicates (1987 to 2002). A nutrient vertical profile was assigned to each of the eleven sub-domains of the Mediterranean basin discussed in Crise et al. (2003). The other

OSD
6, 1223–1259, 2009

Title Page
Abstract Introduction
Conclusions References
Tables Figures
◂◂ ▸▸
◂ ▸
Back Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

biogeochemical state variables were initialised homogeneously in the photic layer (0–200 m) following the standard BFM values, and with low values in the deeper layers. A smoothing algorithm was applied to manage the discontinuity between the different sub-domains.

The model presents two kinds of boundary conditions: at the Gibraltar Strait with the Atlantic buffer zone and in correspondence of the riverine inputs. A seasonal nudging for phosphate, nitrate, silicate, dissolved oxygen is forced at the Gibraltar Strait, consisting of a longitude dependent Newtonian relaxation term based on the climatological MEDAR-MEDATLAS fields. The time scales used in the nudging vary from 90 d (in proximity of the outer boundary) to 2 d (near Gibraltar strait). The riverine input takes in account the climatological nutrient load of three major Mediterranean rivers, Po (Palmeri et al., 2005), Rhone (Moutin and Raimbault, 2002), Nile (Nixon, 2003) together with the input from Dardanelles (Polat et al., 1997), accounting for 40% of the total land-based freshwater input. In addition their plumes can detach from the coast and influence the open sea, thus reducing the filtering effect of coastal processes. The riverine loads are currently parametrized on a seasonal base similarly to the Atlantic box, using a climatological relaxation to the nutrient load quoted above with time scale equal to 1 h.

2.4 The numerical implementation

The numerical integration of Eq. (1) in time is divided in two phases, the first one based on a first order forward time scheme, and the second one by an implicit scheme:

$$c_i^* = c_i^t + \Delta t \left\{ -\boldsymbol{U} \cdot \nabla c_i^t + (-1)^{n+1} k_h \nabla_h^{2n} c_i^t + w_{si} \frac{\partial c_i^t}{\partial z} + R_{\text{bio}}(c_i^t, c_1^t \ldots c_N^t, T, I \ldots) \right\} \quad (6)$$

$$c_i^{t+1} = c_i^* + \Delta t \frac{\partial}{\partial z} \left[k_v \frac{\partial c_i^{t+1}}{\partial z} \right] \quad (7)$$

where the time step Δt is 1800 s.

In the first phase advection, horizontal diffusion, sinking term and biogeochemical reactions are computed, while in the second phase only the vertical diffusivity is computed.

The Smolarkiewicz advection scheme (Smolarkiewicz, 1983) is adopted to reduce the intrinsic numerical diffusion of the advection scheme, and a bi-Laplacian horizontal diffusion ($k_h = -3 \times 10^9$ m^4 s^{-1} constant in space and time, $n=2$ in Eq. 6) was chosen to preserve the sharpness of the propagation fronts associated to the biogeochemical concentrations. For more details please refer to Lazzari et al. (2005).

The geographical domain covered is the Mediterranean Sea and part of the Atlantic Ocean, from 8.78125° W to 36.3438° E and from 30.2188° N to 46.0938° N, with an uniform horizontal resolution of 0.125° and 72 vertical z-levels (18 levels from surface to 100 m depth, 7 between 100 and 200 m depth, 12 between 200 and 500 m depth, 9 between 500 and 1000 m depth, 10 between 1000 and 2000 m depth and 16 below 2000 m). The output data are released as daily means.

The three-dimensional computational domain resolved by the OPATM-BFM system has more than 3×10^6 cells and each run produces almost 2.7 Gb of data per day of integration. In particular, the weekly run launched for the pre-operational forecasting system (see the following section for details) produces more than 113 Gb of data.

The OPATM-BFM code has been parallelized by means of the message passing paradigm (using the MPI library) through the domain decomposition approach. This method consists in splitting the computational domain in smaller sub-domains: each processor works exclusively on one of the sub-domains assigned at the initialisation, exchanging the necessary cells only with its neighbours. The default algorithm for the splitting of the horizontal domain is a simple, automatic and static decomposition that subdivides the domain in regular sub-domains. When such a two-dimensional partitioning is applied on an irregular domain as the Mediterranean basin, it produces a computational load imbalance among processors due to the very different number of sea grid points that every processor has to compute. To reduce the unbalance related to the default decomposition, we introduced allocatable memory in the structure of the code and a pre-processing procedure that computes the best domain decomposition through an iterative algorithm that equally distributes the computational cells among processors. Such adaptive domain decomposition maintains the load balance efficiency to an acceptable 80% even increasing the number of processors from 32 to 64, a configuration that in the default algorithm accounts for a load balance efficiency lower than 10%.

The production runs object of this paper have been executed using 32 processors of the IBM-sp5 facility hosted at CINECA (Bologna, Italy), with a memory request of 1.5 Gb for each processor. The weekly run that performs a total of 17 d of simulations is configured with a total of 816 time steps.

3 The pre-operational system

The OPATM-BFM coupled eco-hydrodynamic model is the core of the pre-operational procedure embedded in the OGS operational system, which aims at producing analyses and forecasts of the Mediterranean Sea biogeochemistry on a weekly basis.

The products of the simulations are the concentrations of key variables (macronutrients, chlorophyll, phytoplankton and bacterial productivity) and are routinely delivered from the OGS website (http://poseidon.ogs.trieste.it/cgi-bin/opaopech/mersea) in order to track temporal and vertical evolution of the basin biogeochemical properties. Surface maps and vertical sections have been made available starting from 1st April 2007 (beginning TOP2, Toward Operational Phase 2), during the MERSEA-IP development.

The pre-operational system (also referred as operational chain) is today a multidisciplinary effort that involves four different Italian scientific institutes:

- OGS, that manages the OPATM-BFM model and is responsible of the correct functioning of the whole system;

- INGV, that provides the physical forcing fields needed to drive the biogeochemical model as outputs from the MFS_Sys2b OGCM model;

- CINECA, that hosts the computational facility (IBM-sp5) where the whole system runs weekly fully automatic and unattended (an external intervention from OGS or CINECA staff is necessary only in case of failure due to broken communication between the INGV server, where the physical forcing fields are stored, and CINECA server, where OPATM-BFM runs, or due to technical problems at CINECA);
- ISAC CNR, that provides the MODIS satellite images necessary for the comparison with the model results (at present, this institute is not actively involved in the pre-operational forecasting system but a quality control of the chlorophyll surface maps with satellite images is under study and will be included in the operational development).

INGV and ISAC CNR make available data on their own FTP sites and OGS disseminates the products on its web site. These activities are in principle not synchronized, being carried out independently in geographically remote sites.

The collating element that sets the proper timing and synchronization of fluxes information is the operational chain. More in detail, the operational chain is basically organized as a collection of programs and files implementing the following main functionalities:

- coordinating the input, production and dissemination stages necessary for the execution of OPATM-BFM that are described below;
- monitoring the status of the execution;
- obtaining diagnostics about any previously executed run, through the log files in order to investigate possible causes of failure;
- minimizing human intervention after system failures.

The operational chain creates a job command file for each run, that is submitted to the available scheduler (LoadLeveler in the case of the IBM-sp5 cluster, but eventually LSF or other schedulers available on other clusters).

Most of these tools are implemented as Korn shell scripts. The operational chain contains also the sources of the model, all the Unix commands needed for the execution and the OPATM-BFM configuration files. Moreover, the operational chain defines a directory structure for the log files, model execution and data archiving. All the files necessary for the chain to operate are managed through a versioning system, that permits a full control of any development of the system components.

A specific protocol has been defined to preserve the correct version of the whole chain and consequently the integrity of the model simulations, in order to make every run completely reproducible. Indeed, it is possible to restore the same release of the chain that was in production in any time in the past, and thus reproduce exactly any run.

As cited above, the chain is composed by three main sequentially dependent steps (Fig. 4), that implement the three stages of the run that are described below.

3.1 The setup of the physical forcing

This stage includes the download of the input data from the INGV server to the CINECA server and the horizontal interpolation of the physical forcing fields (velocity, temperature, salinity, eddy diffusivity coefficient, PAR and wind speed) from the 1/16° grid of the OGCM model to the 1/8° grid of the OPATM-BFM. The INGV-OGCM outputs are organized in 7 d of analysis starting from Tuesday of the previous week (day A1) to Monday of the current week (day A7) and 10 d of forecast starting from Tuesday of the current week (days F1, F2, ..., F10), with a total of 17 daily fields (Fig. 5). The computational time needed to complete this stage is presently about 30 min.

3.2 The OPATM-BFM production

This stage first sets the initial conditions and the ancillary files necessary to the code running, and then executes the OPATM-BFM production. The model is initialised in its biogeochemical state variables with the model output fields relative to day A7 of

OSD

6, 1223–1259, 2009

Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

the previous run (Fig. 5). The ancillary ("namelist") files set the parameters necessary for the model running (domain decomposition, time step, horizontal diffusivity coefficient, etc.). The results of the present stage are 7 d of analysis, where the 7th day corresponds to Monday of the current week, and 10 d of forecast (Fig. 5). The computational time needed for the model execution in the current configuration is about 4.5 h on 32 processors of the IBM-sp5.

The OPATM-BFM code is purely prognostic: no assimilation scheme has been implemented so far. The absence of such a scheme implies that the OPATM-BFM analyses are the result of INGV assimilated forcing only, without any type of assimilation of biogeochemical fields.

3.3 The data dissemination

The last stage includes the post-processing applications that generate the graphical plots and the ftp transfer of the maps from CINECA to OGS server. When this step is completed (currently order one hour), the output fields become available at the OGS web page and are organized in:

1. surface maps of chlorophyll, phosphate, nitrate, ammonia, silicate, bacterial, gross/net primary production (produced by the OPATM-BFM model), temperature and salinity provided by the INGV model for 7 d of analysis and 10 d of forecast;

2. temporal evolution along the whole run (17 d) of the vertical profiles of chlorophyll and phosphate and of temperature and salinity for selected sub-basins of the Mediterranean Sea;

3. mean vertical cross-sections (for 7 d of analysis and 7 d of forecast) of chlorophyll and phosphate along: 5.5° E, 19° E, 28° E, 35° N, and 40° N.

This step includes also the data archiving, which consists of the storage of the model outputs and of all the files needed to an eventual re-run of the simulation (restart files

OSD
6, 1223–1259, 2009

and physical forcing fields). These files are compressed and stored at CINECA, with an amount of memory for each weekly run of about 5 Gb.

4 Results and discussion

The OPATM-BFM system achieved two kinds of results: a technological and a scientific one. The technological results regard the implementation and successful functioning of the OPATM-BFM system. The scientific results are related to the comparison of the model outcomes with experimental data.

Since April 2007, the pre-operational infrastructure has offered short-term forecasts of meaningful biogeochemical variables in the Mediterranean basin (chlorophyll, nutrients, productions) on a weekly basis. Starting from July 2007 the whole infrastructure has been fully automatized and unattended. This main achievement has been demonstrated by the continuous update of the web page hosted at the OGS server, featured by more than 3000 visits and 17000 page views from September 2007. The deployment of a pre-operational forecasting system for the Mediterranean biogeochemistry based on the multiple platform, eco-hydrodynamic off-line coupling, one of the objectives of MERSEA-IP, has been completed successfully.

Considering the period from August 2007 to April 2009, 93 weekly runs have been executed by the operational chain. In the 87% of the runs the procedure effectively started automatically at 12 a.m. of each Wednesday, for the remaining 13% of the runs it was necessary to manually operate in order to solve some issues of different nature (technical problems on the High Performance Computing cluster or internet connection failures) and re-submit the procedure.

The procedure usually takes less than 24 h to be fully completed (72% of the runs, with an average length of 11.5 h). The threshold of 24 h has been exceeded in the remaining 28% of the runs, the reason for such delay being imputed to the technical problems above mentioned or to the time spent in queue to wait for the available resources. In particular, the longest waiting times are mostly related to the OPATM-BFM production which is the most computational demanding phase.

4.1 Analysis of surface chlorophyll results

The operational system has also demonstrated the capability to provide reliable information on the Mediterranean Sea biogeochemistry. We checked the results provided by the OPATM-BFM by analysing and comparing them with the remote satellite data provided by ISAC-CNR. In particular the model surface chlorophyll, evaluated as the chlorophyll concentrations averaged over the first optical length, is easily comparable with the remotely measured data. Since we do not assume any specific statistical distribution for the surface chlorophyll, we use in the comparison non-parametric indicators such as median, 25th, 75th percentiles, minimum and maximum values, all of them evaluated over the whole Mediterranean basin or over selected sub-basins (coastal areas are masked out).

As described above, the OPATM-BFM daily fields (both forecasts and analyses) are available starting from April 2007. For the following analyses we consider the period from April 2007 to September 2008, since the post-processed satellite data are available for this time interval.

4.1.1 Comparison between forecast and analysis

We evaluated firstly the difference between the surface chlorophyll results forced by prognostic physical fields Fn, (n=1, 7; see Fig. 5) and those from assimilated physical fields An (n=1, 7). In this case the investigation is extended to December 2008.

In Fig. 6 we show for each day of the period under evaluation the data relative to F1, F2, ..., F7 and those corresponding to A1, A2, ..., A7 that cover the same 7 d (see Fig. 5). All over the simulation period the forecast-analysis difference (FAD, computed for every week as Fn−An with n=1, 7) shows no evident discrepancies. The average relative FAD for the median, the 25th and the 75th percentile are equal to 0.8%, 1.2% and 1.6%, respectively. The impressive agreement not only for the median but also for

OSD
6, 1223–1259, 2009
Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry
P. Lazzari et al.

the two percentiles (Fig. 6) evidence a similar overall distribution. This is maintained almost constant all over the simulation period, that guarantees that the FAD is clearly not time-dependent. Therefore, because of the very small FAD observed for the OPATM-BFM, the following remarks on the model results will be made using the data relative to analyses (A1, ..., A7) of each weekly run.

4.1.2 Comparison between model and satellite data on the Mediterranean basin

The model results have been compared with remote sensing chlorophyll values measured by MODIS-Aqua satellite sensor (Fig. 7). The satellite and model data illustrated in Fig. 7 have been geometrically averaged over a 5 d interval.

MODIS-Aqua data were processed by the Satellite Oceanography Group of the Rome Institute of Atmospheric Sciences and Climate – CNR (GOS-ISAC-CNR). Level-0 data were acquired via ftp from the Goddard Space Flight Center (NASA) at full resolution (1 km) and processed up to Level-3 with the SeaWiFS Data Analysis System (SeaDAS) software package version 5.1.5 available from NASA website (seadas.gsfc.nasa.gov). Standard flags and Siegel's atmospheric correction algorithm were applied to Level-1A raw data. Chlorophyll concentrations were computed from Level-2 water leaving radiances, using a validated regional algorithm called MedOC3 that takes into account the peculiar characteristics of the Mediterranean Sea (Santoleri et al., 2008).

The temporal evolution of the median of the surface chlorophyll concentration simulated by OPATM-BFM presents characteristics similar to those provided by the remote sensing measurements. As shown in Fig. 7 the satellite measurements are characterized by the typical mid-latitudes seasonal cycle (Longhurst, 2001; Bosc et al., 2004) with summer lower values (July–August 2007 and 2008), a growth between October and November 2007, and a winter plateau with higher values (January–March 2008). The model is able to reproduce the seasonal cycle with summer lower values (June–July 2007 and 2008) a growth in August 2007 and winter higher values (February–March 2008), thus showing a time lag in the seasonal chlorophyll cycle. During the

OSD
6, 1223–1259, 2009

Title Page
Abstract | Introduction
Conclusions | References
Tables | Figures
◀I | ▶I
◀ | ▶
Back | Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

summer periods the model median and variability are in good agreement with MODIS data, while from August 2007 to April 2008 OPATM-BFM overestimates the satellite data. Overall the agreement between the temporal evolution of the data and model median can be evaluated by means of the Spearman correlation coefficient (R_S), which is equal to 0.71.

The MODIS maximum estimates of surface chlorophyll concentration over the whole basin generally range 1–10 mg chl/m^3, the same holds for the model results.

Being the surface variability of the chlorophyll signal over the whole basin quite heterogeneous, we selected two sub-basins, characterized by opposite regimes: Northwestern Mediterranean and Eastern Mediterranean (respectively NWM and EME in Fig. 1). NWM is a mesotrophic sub-basin influenced by Rhone outflow on the coastal area and subjected to vigorous convection during late winter, while EME is an oligotrophic sub-basin that exhibits a quasi-tropical regime with semi-permanent stratification and chronic shortage of nutrients in the euphotic zone (Figs. 8 and 9).

As observed for the entire Mediterranean basin, also the two selected sub-basins well reproduce the surface chlorophyll concentrations during the summer periods. During the September–February semester NWM shows an agreement with satellite estimations better than EME, where model strongly overestimates MODIS data.

The model variability (25th–75th percentile area) remains almost constant throughout the simulation for both the sub-basins whilst the satellite estimations show an increase of variability during spring, especially in NWM where is related to spring bloom events. The R_S for chlorophyll median is equal to 0.71 and 0.70 for NWM and EME, respectively.

Both maximum and minimum model values are satisfactorily in agreement with the respective satellite data in the two sub-basins.

The time-lag between the data and model above observed for the Mediterranean basin is also a common feature of the two selected sub-basins. The East-West chlorophyll gradient of the Mediterranean basin observed by many authors (e.g. Longhurst, 2001) is reproduced by OPATM-BFM, since in the period considered the surface chlorophyll in NWM are mostly higher than the values simulated in EME. This result confirms the validity of the BFM generic formulation, able to self-adjust to quite different environmental conditions without any specific parameterization.

The OPATM-BFM model is a powerful instrument to produce forecasts of the Mediterranean biogeochemistry not only for large scale averages, but also for relevant localised events, whose dynamics cannot be captured by spatially and temporally filtered data processing as that adopted for example in Figs. 7, 8 and 9 or by climatological averaging.

Figure 10 presents the surface chlorophyll concentration maps for some selected days between February and March 2009 in the Gulf of Lions. As shown by the satellite images (Fig. 10, top), the mixing in the centre of the Lions Gyre (probably ascribed to deep convection) is already present at the end of February and characterized by a surface chlorophyll concentration with values lower than 0.1 mg/m^3. This minimum appears still evident on 12 March, when increasing chlorophyll concentration is observed in the south-western area of the image. Between 15 and 17 March a bloom event develops, clearly visible by the surface patches with chlorophyll concentration higher than 3 mg/m^3, that expand and cover the area characterized by the lowest values. On 26 March the event results mostly concluded.

OPATM-BFM model demonstrates its good performance by satisfactorily forecasting the temporal dynamic, the location and the intensity of the event (Fig. 10, centre). The qualitative comparison between the two sets of images confirms the capability of the model to provide forecasts of local chlorophyll bloom events in the Mediterranean Sea, the only evident discrepancy being a bloom on 17 March that is slightly shifted south-westward with respect to the correspondent satellite image. Furthermore, the slight difference between the forecast (Fig. 10, centre) and the analysis (Fig. 10, bottom) confirms what already discussed in Sect. 4.1.1 relative to the surface chlorophyll statistics evaluated on the Mediterranean basin.

The bloom events in NWM are well known and their dynamics is recurrently reproduced by the model, mainly because this signal is very energetic and has a strong time dependency on physical forcings. Conversely, the intensity of blooms is directly dependent on the nutrient supply, that can be quantitatively demonstrated to be hyperbolically dependent on the mixing depth. This non-linear response reduces the impact of the uncertainty of the mixing depth on the vertical nutrient fluxes and consequently on the bloom intensity.

5 Conclusions and future development

A pre-operational, unattended and fully automatic procedure that provides public short-term forecasts of the Mediterranean biogeochemistry on weekly basis has been developed in the framework of the MERSEA-IP project. This can be considered as the first example of such a system applied to the Mediterranean Sea.

The implementation has been coordinated by OGS with the cooperation of INGV and ISAC CNR. The need for a sustained and truly operational approach for the forecasts led to involve CINECA, the largest supercomputing centre in Italy, as the technical partner and computer services supplier.

Maps of biogeochemical key variables (e.g. chlorophyll and nutrients) have been disseminated via web since April 2007. The results obtained so far can be considered from the technological and scientific point of view.

Firstly, the fully automatic and unattended execution of the whole pre-operational procedure (job submission, model production, archive and dissemination on the website) started and correctly concluded in the 87% of the runs, with an average duration of 16 h from the job submission. This result is particularly satisfactory since no dedicated resources and/or specific priority has been given to the operational chain. Moreover, as can be observed in Fig. 6, it was never necessary to re-initialise the system, thus implying a continuity and a consistency in the products time series.

Secondly, two different models (the OPA Tracer Model and the BFM) were successfully coupled to give rise to the OPATM-BFM code, that has been built up through an intensive parallel optimisation of the OPATM-BFM transport model. The off-line strategy chosen to couple physics and biogeochemistry resulted very useful since it gives now the possibility to use different OGCMs to force the biogeochemical model. This means that every improvement in the physical model is directly reflected into the biogeochemical compartment. In perspective, backup physical forcings may be used in case of missing INGV data, ensuring higher reliability to the system.

Considering the scientific point of view, the pre-operational system represents an assemblage of codes (i.e. the OPA, MFS and BFM models) that were only verified individually. The analysis of the present results has hence allowed an assessment of the system as a whole, exploiting previous scientific achievements obtained by each component and applied to the Mediterranean Sea.

In particular, basin-aggregated chlorophyll surface data produced by the OPATM-BFM in the period between April 2007 and September 2008 have been compared with MODIS satellite data supplied by ISAC CNR. The more significant outcomes from this comparison are here outlined:

- the model basically reproduces the seasonal variability of the surface chlorophyll in the Mediterranean basin, characterized by lower concentrations in the summer and higher during the late winter, showing a Spearman correlation with satellite data equal to 0.7;

- in summer the OPATM-BFM median and variability is in good agreement with MODIS data, while during September–February semester the model tends to overestimate the satellite evaluation;

- the onset of the chlorophyll winter growth over the entire Mediterranean basin takes place earlier in the simulation than in the satellite data;

- at a sub-basin scale, the range of variability of the surface chlorophyll is well reproduced by the model better in the North-western Mediterranean Sea rather than in the eastern basin, the latter being characterized by a significant overestimation of the satellite data;

– the model variability does not change throughout the analysed period for both the sub-basins, whilst the satellite data show an increase of variability during spring, especially in the North-western Mediterranean where is related to spring bloom events;

– the model forecasts the dynamics (timing, location and intensity) of chlorophyll bloom related events during the simulation period in the Gulf of Lions consistently with the satellite observations.

A full assessment of the system performances is planned in the near future, since at least two years of model outputs and satellite observations can provide time-series for sound statistical indicators.

To improve the model results, more information, such as time-dependent extinction coefficient obtained from satellite measurements and/or a data assimilation scheme for the biogeochemical compartment, are going to be introduced into the system, as already done for the Eastern Mediterranean Sea (Triantafyllou et al., 2007). This is planned to be implemented in the following development into a fully operational system, as required in MyOcean project.

In particular the improvements of the model will focus on the following aspects:

1. integration of a time-dependent extinction coefficient provided by satellite measurements to improve the current solution based on a longitudinal, climatological extinction coefficient (Crispi et al., 2002);

2. implementation of the data assimilation for the surface chlorophyll, which will provide the possibility to enrich the model with the satellite observed data;

3. porting of the entire system on a new facility hosted at CINECA together with the implementation of a strict quality control that will also contribute to standardize the whole procedure.

The system here presented is the result of the efforts carried out during MERSEA-IP, and will be further developed within MyOcean program according to the points mentioned above.

Acknowledgement. This work was partially co-founded by MERSEA–IP FP6 European project (http://www.mersea.eu.org/) and by the Italian VECTOR program (http://vector-conisma.geo.unimib.it/).

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OSD

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Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

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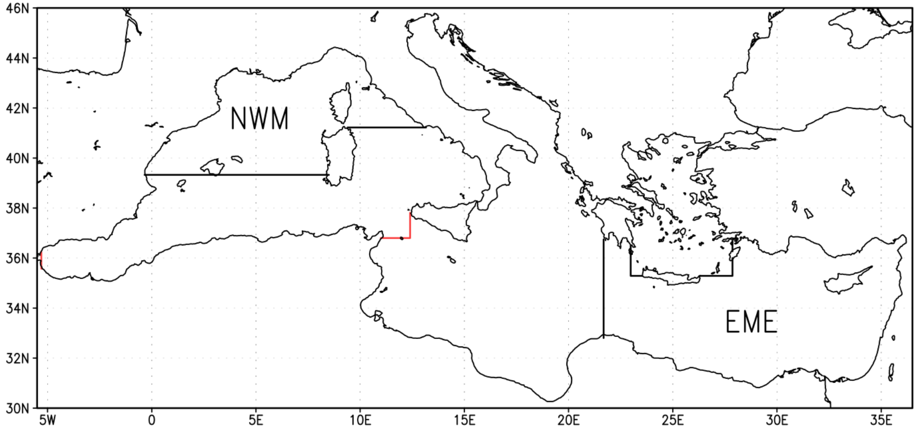

Fig. 1. Map of the Mediterranean Sea with two selected areas of investigation NWM=North-western Mediterranean and EME=Eastern Mediterranean; transects at the Gibraltar and Sicily Straits are depicted in red.

OSD

6, 1223–1259, 2009

Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

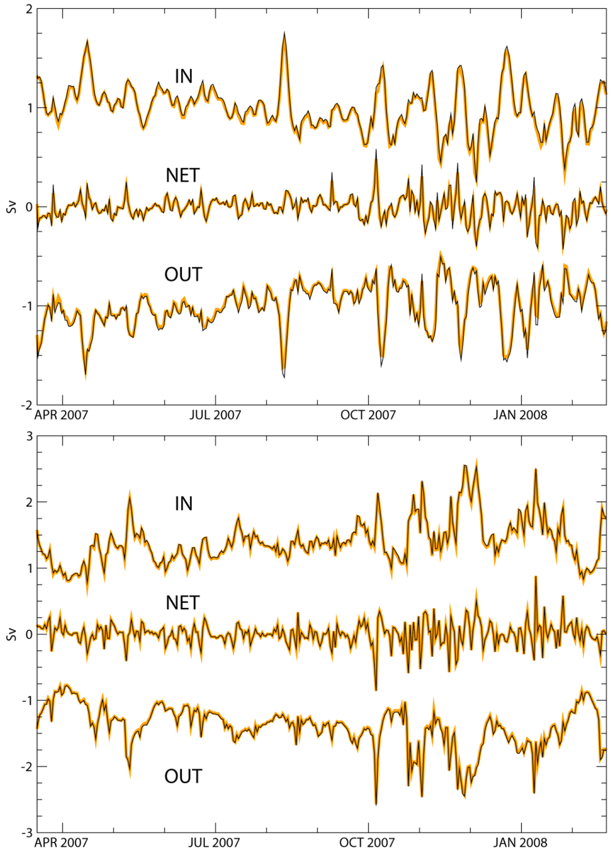

Fig. 2. Water mass inflow, outflow and net flow for the Gibraltar Strait section (top) and the Sicily Strait section (bottom) before (black) and after the interpolation (orange). The Straits sections are plotted in Fig. 1.

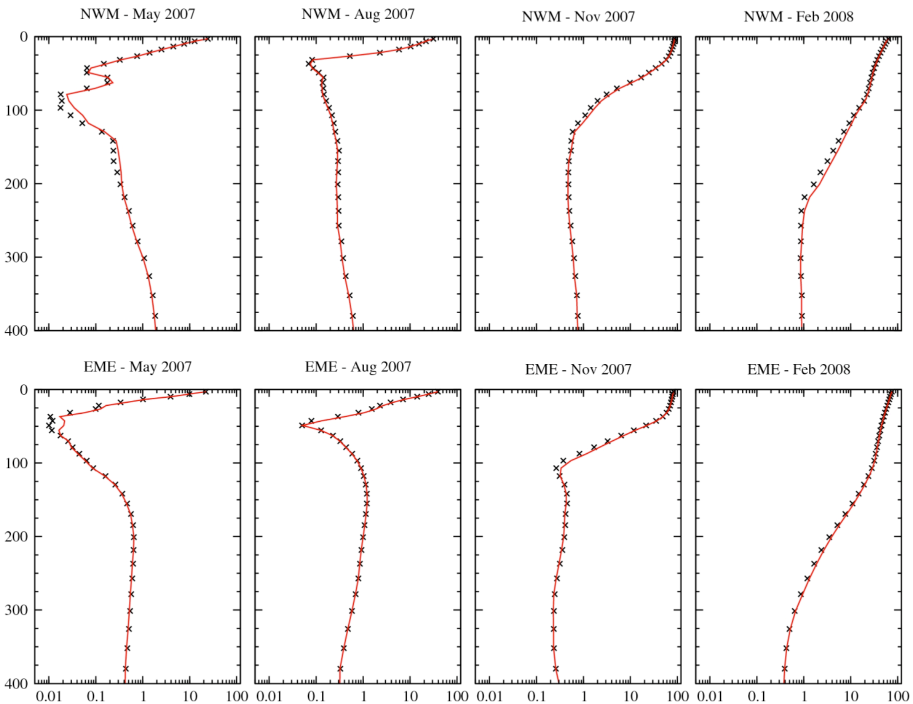

Fig. 3. Mean monthly vertical profiles of vertical eddy diffusivity coefficient k_v (m^2/s), areal-averaged over sub-basins NWM and EME for the fine grid (1/16°; crosses) and for the coarse grid (1/8°; red line).

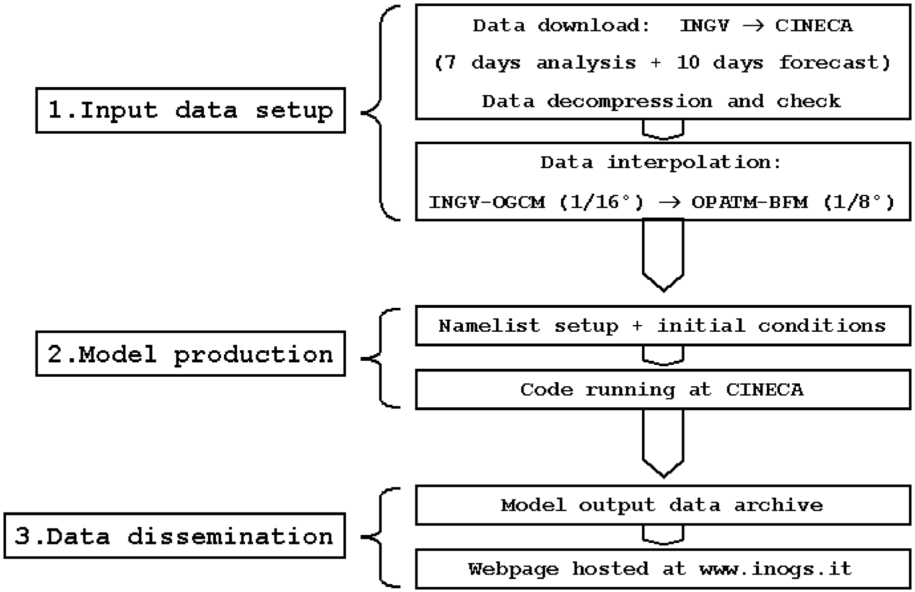

Fig. 4. Flow diagram of the pre-operational infrastructure system.

OSD
6, 1223–1259, 2009

Pre-operational short-term forecasts for the Mediterranean Sea biogeochemistry

P. Lazzari et al.

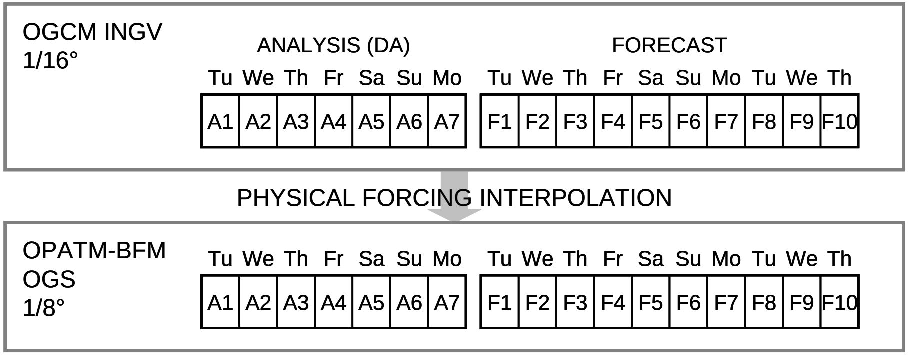

Fig. 5. Layout of the interpolation phase with reference to the weekly run; DA means "Data Assimilation" to indicate that the OGCM analyses are produced with the SOFA scheme.

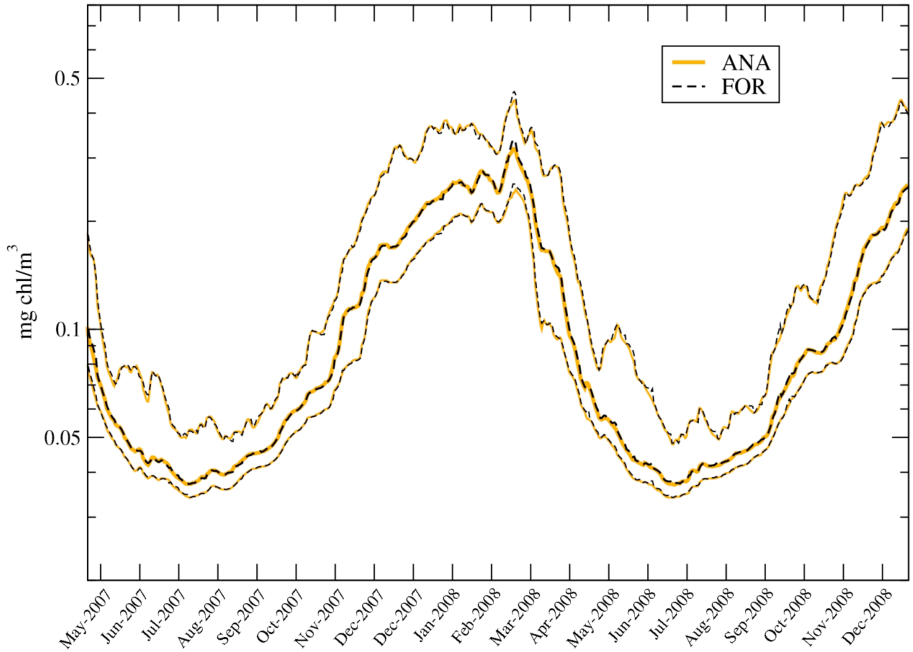

Fig. 6. Temporal evolution of the daily surface chlorophyll concentration spatially estimated over the Mediterranean Sea, obtained using the forecast (black dashed line) and the analysis (orange solid line): median (thick line), 25th and 75th percentile (thin lines).

OSD
6, 1223–1259, 2009

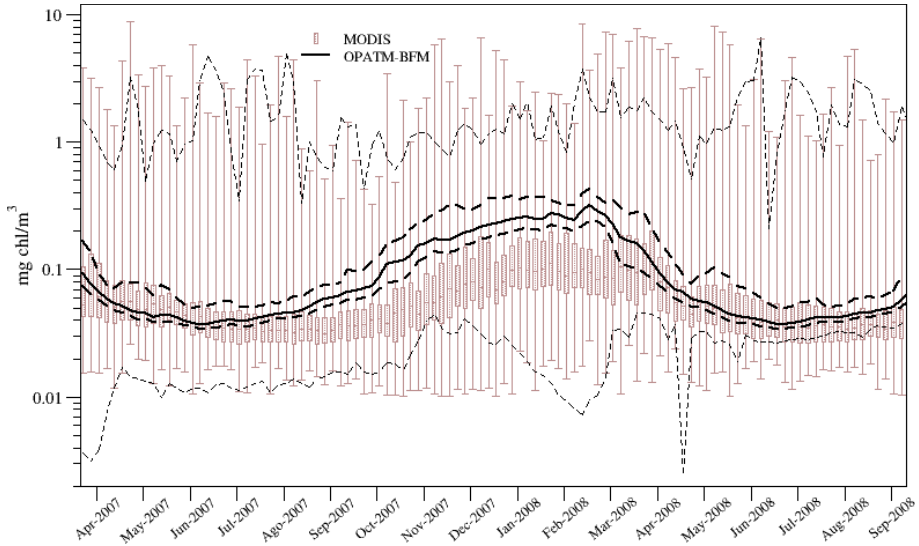

Fig. 7. Temporal evolution of the 5-d mean surface chlorophyll concentration for the Mediterranean Sea: biogeochemical model results (median, solid line; 25th and 75th percentiles, thick dashed line; minima and maxima, thin dashed line) and MODIS satellite data (box and whisker plot).

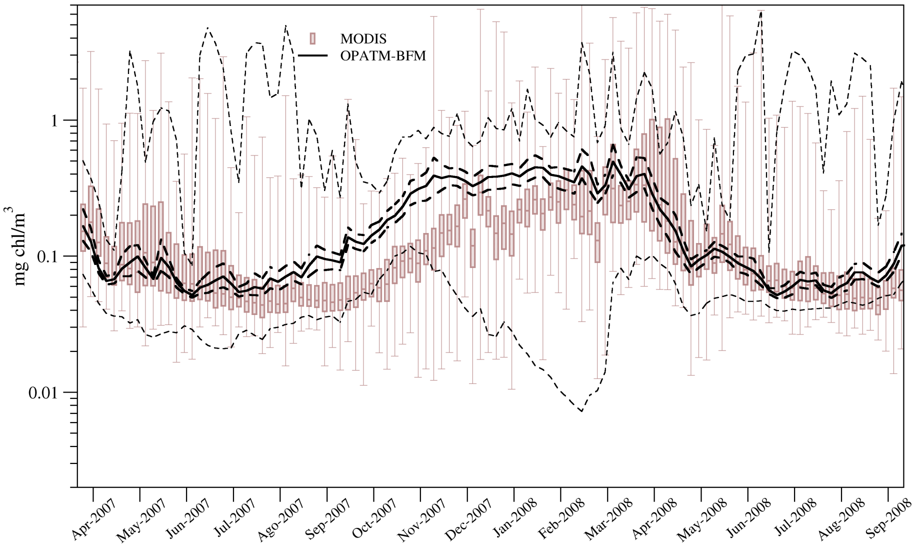

Fig. 8. Temporal evolution of the 5-d mean surface chlorophyll concentration for the North-western Mediterranean Sea: biogeochemical model results (median, solid line; 25th and 75th percentiles, thick dashed line; minima and maxima, thin dashed line) and MODIS satellite data (box and whisker plot).

OSD
6, 1223–1259, 2009

Title Page
Abstract | Introduction
Conclusions | References
Tables | Figures
◀| |▶
◀ ▶
Back | Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion

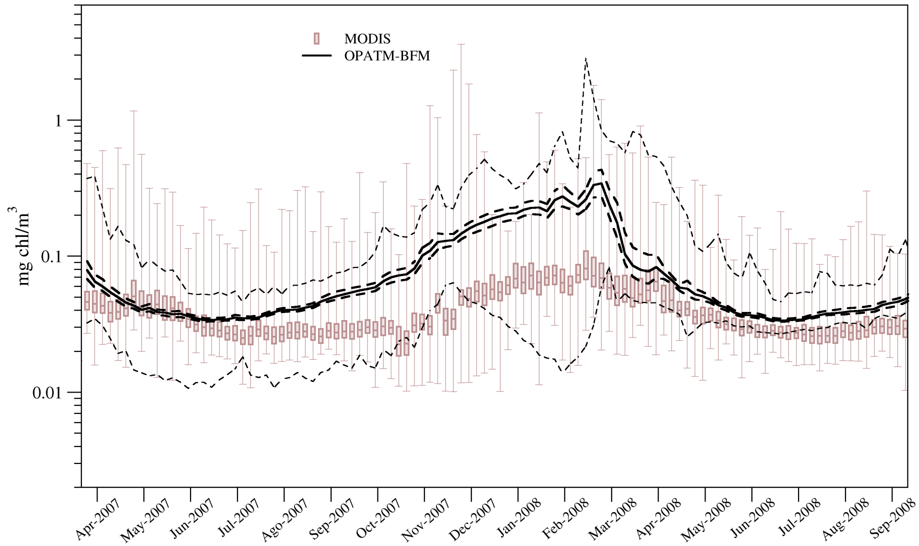

Fig. 9. Temporal evolution of the 5-d mean surface chlorophyll concentration for the Eastern Mediterranean Sea: biogeochemical model results (median, solid line; 25th and 75th percentiles, thick dashed line; minima and maxima, thin dashed line) and MODIS satellite data (box and whisker plot).

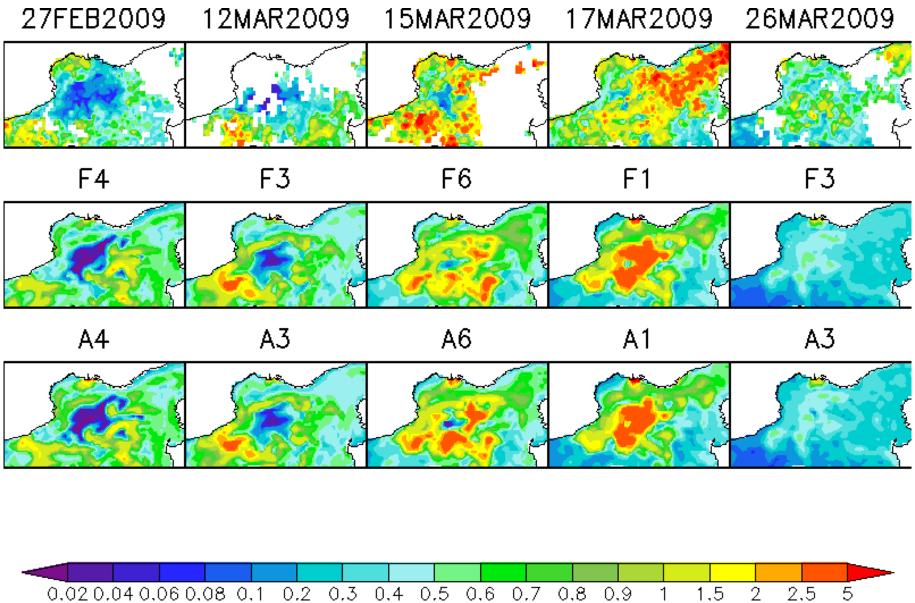

Fig. 10. Surface chlorophyll concentration (mg chl/m^3) observed between February and March 2009 in the Gulf of Lions: MODIS-Aqua satellite (top), OPATM-BFM model forecasts (centre) and analyses (bottom). The labels F# and A# refer to Fig. 5.

OSD
6, 1223–1259, 2009

Title Page
Abstract Introduction
Conclusions References
Tables Figures
◀| |▶
◀ ▶
Back Close
Full Screen / Esc
Printer-friendly Version
Interactive Discussion