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TOWARD A DATA ASSIMILATION SYSTEM FOR NEMO

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Abstract

In this note, we discuss the project that has been conceived and the first achievement steps that have been carried out to set up a data assimilation system associated to NEMO. Of specific interest here are applications to operational oceanography. This data assimilation system is schematically made of three subcomponents: Interface Components, Built-in Components and External Components. Several elements of this NEMO data assimilation system have already been developed by various groups in France and in Europe and several of them could be introduced in the system (the linear Tangent and Adjoint Model, TAM, is one of the most important of them as far as variational assimilation is concerned), some others will require specific developments. Finally, we introduce the SEABASS reference configuration that is proposed to be the NEMO data assimilation demonstrator and the experimentation and training platform for data assimilation activities with NEMO. These various thoughts take advantage of the advances and discussions that have been carried out by the NEMOASSIM working group.

Introduction

Other contributions of this issue discuss how the NEMO modeling platform can be used to simulate the time evolution of the ocean circulation including its variability from global to regional scales. Due to the non-linearity of the equations governing the ocean dynamics, a wide range of such temporal and spatial scales interact together in such a way that the ocean evolution is partly chaotic and beyond some limit, unpredictable. Therefore, the routine monitoring and forecasting of oceanic variables, which is the essential goal of Operational Oceanography, must be treated as a series of inverse problems that require observed data at regular intervals to re-initialize the model state “close” to the observed ocean using all available data combined with the latest model predictions. In this respect, operational ocean monitoring is similar to numerical weather forecasting.

The terms “Data Assimilation” (DA) designate the range of objective methods enabling optimal combination of observations, model simulation and error statistics, in order to reduce as much as possible the uncertainty of ocean state estimations involved in short-term predictions or more or less long-term reanalyses. Very significant progress has been accomplished in ocean data assimilation during the past 20 years in the framework of a variety of pre-operational projects, such as the French SIMAN/QADRAN program in the nineties (*e.g.* Blayo et al., 1994), the DIADEM, TOPAZ (Brusdal et al., 2003), ENACT (Davey et al., 2006) and MERSEA European projects (Brasseur et al., 2005), and more recently the GMES MyOCEAN and on-going MyOCEAN2 and SANGOMA projects. The choice made in Europe to routinely monitor the ocean down to the meso-scales has strongly guided the first stages of the assimilation strategy in place today in most operational centres. At international level, the effort of the nations involved in the development of DA for Operational Oceanography were coordinated in the framework of GODAE (Cummings et al., 2009), demonstrating the relevance of the concept which is further developed in the framework of the on-going GODAE Oceanview.

Briefly speaking, two different categories of algorithms can be distinguished to solve the DA inverse problems: the optimal control approach, most often based on the variational adjoint method (Le Dimet and Talagrand, 1986) and the stochastic methods mostly derived from the Kalman filter concept. In its 4D-Var formulation, the variational method requires the adjoint of the linear tangent model to compute the gradient of the cost function to be minimized, and in that case can therefore be designated as a « model-dependent » DA method. By contrast, stochastic methods such as the Ensemble Kalman filter introduced by Evensen (1994) or the SEEK filter introduced by Pham et al. (1998) can be considered as « model-independent » DA methods which intensively use the direct model code to propagate ensemble statistics, while the update of these ensemble statistics requires additional « model-independent » algebraic operations. The EU SANGOMA project has been set up during the period 2012-2015 to advance stochastic assimilation methods, focussing on non-linear and non-Gaussian assimilation schemes to be used in the next operational systems of the GMES Marine Core Services.

Due to the fast evolution of ocean models during the past 20 years, thanks mainly to computer power increases, the flexibility of « model-independent » DA methods has been an asset to follow the successive updates of ocean model versions without much recoding. Today, the convergence of some of the oceanographic community in Europe toward the NEMO modeling platform provides the opportunity to revisit the overall assimilation strategy, since a more stable and smoother evolution of the model platform can be expected in the future. This is in essence the primary motivation of the project described in the present paper.

Despite some earlier attempts, no assimilation system had ever been formally included in the NEMO system so far. However, a number of DA frameworks already use NEMO as model component: e. g. SESAM (Brankart et al., 2001), SAM (Drillet et al., 2008), OPAVAR/NEMOVAR (Weaver et al., 2003, Mogensen et al., 2009), OceanVar (Dobricic and Pinardi, 2008) and many papers have been published discussing data assimilation results within OPA/NEMO. Since some common components are required by every system, there was therefore some duplication of efforts. In order to provide a more structured offer to a large number of users, CNRS proposed in 2009 to set up the so-called NEMOASSIM working group. This group gathers experts involved in the development of such systems (members of CERFACS, CNRS, ECMWF, INGV/CMCC, INRIA, MERCATOR and MetOffice), and members of the NEMO system team. This leads to sketch a strategy for implementation of an assimilation component associated to the NEMO code system and thereby make assimilation tools for NEMO more readily available to the user community.

In this note, we present the current status and perspectives of what could be the different components of a NEMO data assimilation system, which are categorized into Interface Components such as OBS, ASM components which make the link between observations and model-structured information, "Built-In" Components, such as TAM that is the linear tangent and adjoint models of NEMO, which are intrinsically linked to the direct NEMO code, and External Components to be included into NEMO DA system (4DVAR minimizer, square-root or ensemble analysis kernels, singular value decomposition), which are technically independent from NEMO, but nonetheless essential to build a stand-alone assimilation system. All these components (Interface Components, Built-in Components and Externals Components) are thus needed together to implement the NEMO DA system. Then, SEABASS, an academic NEMO configuration will be proposed as NEMO benchmark basis and demonstrator for DA. A number of perspectives will be discussed regarding the future of the NEMO DA system as a conclusion to this note.

NEMO Data Assimilation: Interface Components

The interface components are the modules that are NEMO-dependent, and which connect NEMO to external information independent from the model output.

The first two components to be included in the standard release of NEMO (from version 3.3 onward) were the *observation operator* (OBS) and the *application of the analysis increment* (ASM) since they represent the common interfaces needed to most assimilation schemes relevant to systems like NEMO. Indeed, the fundamental input to any assimilation kernel is the vector of differences between the observations and the reference state. This vector is usually known as the *innovation vector*, and is a direct product of OBS. On the other hand, the fundamental output of any assimilation kernel is a vector of corrections to the background state on the model grid (known as the *analysis increment*). Typically, it consists of corrections to the model current state but may also include corrections to other fields such as the surface forcing fields, model tendencies, or system parameters. The analysis increment is used to initialize or correct the model trajectory, and this is done through the ASM component.

The main purpose of observation operators is to transform model variables on grid points into quantities which can be directly compared with observations. For example, for in situ observations this can simply be interpolation from the model grid to observation points, but more complicated operators involving non-linear transformations of model variables to produce the observable quantity are also possible. Observation operators are mostly independent of the assimilation kernel. Moreover they are also valuable as a diagnostic tool for evaluation of model performance, since they provide the possibility of comparing model variables with observations. The choice proposed by the NEMOASSIM working group was to include, as a first version, the OBS module coming from NEMOVAR. It came in the NEMO 3.3 reference version as a contribution from the MetOffice (which is also a member of the NEMOVAR consortium) along with full documentation (Lea et al., 2012a).

There are several issues to deal with when developing such operator, namely what input file format should be available, how the output will be handled over any assimilation or diagnostic tool and how and where the observation operators are called. For the latter, two choices are available: either it is done off-line, once the model has finished its time integration, but that would potentially require a tremendous amount of extra I/O, or it can also be done on-line, for an extra computing time during the model integration, and that is the adopted solution in NEMO. In the current version, OBS is able to read data such as profiles of temperature and salinity from CORIOLIS or ENACT/ENSEMBLE database, GRHSTT or Reynolds sea surface temperature, AVISO sea level anomaly, sea ice concentration, and TAO/PIRATA/RAMA velocity, both in their original format and in the NEMOVAR feedback format. In the future it is likely that only the latter (with some improvement if needed) will be available in order to avoid maintaining many possible formats. A set of converting tools to produce feedback formatted observation files is already available in the NEMO reference version. The feedback format is also used as the output of the OBS module where the model equivalent to observation at the same time and place is also present, along with all associated information (position, time, QC flags, observation type and instrument, etc). This format represents the interface on the model side, it is then up to the user to build the interface between feedback files and the desired assimilation scheme or diagnostic package.

In most of the assimilation methods relevant to NEMO, the trajectory is controlled by introducing a correction to the model state. This correction, or *increment* is produced by the *analysis step* on variables linked to a control vector. The increment updates the model trajectory either directly, or in a gradual manner over a time period around the analysis date. This latter approach, usually referred to as the *Incremental Analysis Updates* (IAU) methodology (Bloom et al., 1996), tends to reduce shock in the model restart stage and to minimize spurious adjustment processes. From a technical point of view, this latter concept of a correction introduced progressively during the model run is not closely linked to the assimilation methods and could also be seen or interpreted as a use of forcing terms. In practice, these forcing terms correspond to 2D and/or 3D fields (*e.g.* temperature, salinity, or currents) and are applied directly as additional terms in the equations of the NEMO code (Ourmières et al., 2006).

As for the OBS module, the first version of ASM was imported from NEMOVAR as a Met Office contribution (Lea et al., 2012b). Both these choices were driven by the fact that the NEMOVAR code is sufficiently compatible with the NEMO code (same coding convention and practices and limited modification required to the standard reference).

Several possible further developments and improvements to the interfaces (OBS and ASM) are considered today. For instance, for the ASM module, new specificities will be introduced such as new fields (*e.g.* ice concentration), new IAU weight functions and memory usage optimisation. It would also be appreciated that ASM could manage several increments at the same time (as it is done in SAM). The supervision of their development is under the responsibility of the MetOffice.

Regarding the OBS module, its evolution goes through adding new types of observations. Special care should be devoted to ensure that OBS remains flexible enough to easily include both simple or sophisticated new operators.

NEMO Data Assimilation: Built-In Component

The other current key element of the NEMO DA system is NEMOTAM (stands for NEMO Tangent and Adjoint Model) or simply TAM. The development of tangent and adjoint models is an important step in addressing variational DA problems. In such methods, one minimizes a cost function that is a measure of the model-data misfit, and the adjoint variables are used to build the gradient for descent algorithms. Similarly the tangent model is used in the context of the incremental algorithms to linearize the cost function around a background control. During the ANR–funded project VODA, specific effort was dedicated to the development of the TAM for the ocean engine component of NEMO.

The only needed interface between the direct model and the TAM is the handling of the non-linear trajectory (required for differentiating around). So, once available, the inclusion of the TAM within the NEMO framework is straightforward. A version of TAM was released along with NEMO 3.2.2 and made available to the users on the NEMO website, although it was not fully part of the standard release due to lack of resources. With the support of CNRS, recent efforts have been dedicated to this point that will allow TAM to be soon part of the standard release as of NEMO 3.4 (Bouttier et al., 2012).

Assimilation-wise Tangent-linear and Adjoint Models are mainly used for variational assimilation applications. However they are also powerful tools for the analysis of physical processes. They can indeed be used for sensitivity analysis, parameter identification and for the computation of characteristic vectors (singular vectors, Lyapunov vectors, etc), which in their turn can be used for defining reduced order assimilation schemes.

Sensitivity analysis for instance is the study of how model outputs vary with changes in model inputs. The sensitivity information is given by the adjoint model, which provides the gradient of the outputs w.r.t. the inputs. One can find an example of application of such methods in the study conducted by Vidard et al. (2010) on the GLORYS ¼° global ocean reanalysis. The initial objective was to estimate the influences of geographical areas to reduce the forecast error using an adjoint method to compute sensitivities. They conducted a preliminary study by considering the misfit to observations as a proxy of the forecast error and sought to determine the sensitivity of this misfit to changes in the initial condition and/or in the forcing fields. Without going into the details of this study, one can see an example of sensitivity to initial temperature (surface and 100m) as shown in the two bottom panels of Figure 1. In this example it is clear that the SST misfit (top left) is highly sensitive to changes in surface temperature (bottom left) where the initial mixed layer depth (top right) is low. The opposite conclusion can be drawn from the sensitivity to the initial temperature at 100m (bottom right). This is obviously not a surprise, and is more useful here for the assessment of the model (more precisely of the tuning of vertical mixing) rather than to the original goal of assimilation system improvement.

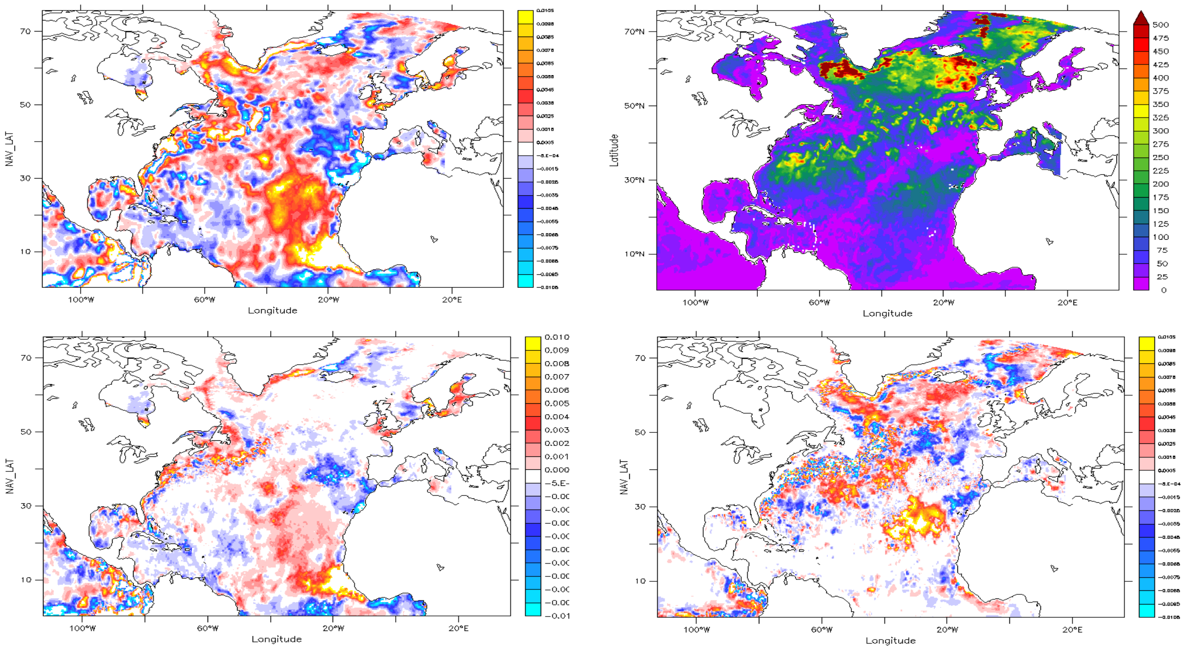

Figure 1: Top: misfit between forecast and observed SST (left) and mixed layer depth (right). Bottom: sensitivity to one-week lead-time SST error with respect to variations in initial surface (left) and 100m (right) temperature.

TAM and associated minimization tools have originally been developed for DA purposes. However, as mentioned above, they could be used for improving the understanding on the model behaviour as well. For example, they can be used to diagnose the differences between model simulations and ocean measurements and to provide valuable information on the robustness of numerical schemes. They can also be used to improve the balance in initial conditions, particularly for shelf-seas models or to assess the structures of the fastest growing instabilities in any flow.

For the future, it is expected that a number of further developments should be added. Several NEMO functionalities (for example AGRIF or Open Boundary Conditions), are not available yet in the current development of TAM. They will be under consideration for next versions of TAM. Estimation of error statistics is a key product of data assimilation and is not readily (and simply) available in variational schemes. There are some potentialities from the hybridization of variational and stochastic methods to bring some solutions. This should be studied further in the future. In addition, one could think that diagnostic tools should be made available in a coordinated way to the users of the NEMO data assimilation system. Note that many of such tools have already been developed in various groups. Built-in components would include physical diagnostic tools whereas specific methodological diagnostics should be in the following external components.

NEMO Data Assimilation: External Components

The NEMO data assimilation interfaces described before has been developed seeking generality and hopefully should be usable easily by any modular-enough assimilation engine. These interfaces have already been used by at least two major complex DA systems: NEMOVAR and SESAM (precursor of Mercator-SAM2). Although they are not part of the NEMO system per se, they are distributed under the same Cecill licence and can therefore be used in conjunction with NEMO.

These two External Components are quite different in their concept; therefore it is a good illustration of the generic aspect of the interfaces. On the one hand NEMOVAR is based on optimal control techniques where the model trajectory is kept close to the observation through the minimization of an objective function, using a descent algorithm. It uses the so-called incremental formulation where the minimization of the full problem is approximated by a succession of simpler problems, assuming that the evolution of the increment follows the tangent linear model. The algorithm is composed of sequences of two-stage processes: an integration of the non-linear direct model that computes the misfit to observations and possibly outputs the non-linear trajectory (outer iteration) and a minimization of the linearized problem (inner loop). The non-linear trajectory is then updated applying the computed increment during a new outer iteration possibly followed by another inner loop, and so on and so forth. In NEMOVAR, outer iterations and inner loops are separate executables. The outer loop is a standard NEMO model integration making use of OBS (resp. ASM) output (resp. input) files to communicate with the inner loop, while the inner loop is a specific program including the multiplication by the error covariance matrices, the computation of the cost function and its gradient thanks to a tangent-linear and adjoint models integrations and several minimization drivers. Note that NEMOVAR can also perform a 3D-FGAT-type assimilation where the evolution of the increment is assumed stationary in the inner loop, avoiding the need for the tangent and adjoint models integrations.

On the other hand, SESAM is a toolbox of assimilation modules originally developed to implement the SEEK filter algorithm (a reduced rank Kalman filter developed by Pham et al., 1998). In sequential methods, the assimilation algorithm consists of two successive operations: a forecast step to propagate in time the initial probability distribution for the state of the system and an analysis step to update this distribution using available observations. The forecast step is performed using the NEMO model, either by propagating the initial covariance using a linearized model operator (as in the original SEEK algorithm) or by producing an ensemble of model forecasts starting from a sample of the initial probability distribution. The analysis step is implemented in SESAM using the SEEK observational update algorithm, which is especially efficient with large observation vectors and low rank covariance matrices. Moreover, the original algorithm is now extended to work efficiently with localization of the forecast error covariance matrix, non-diagonal observation error covariance matrix and adaptive forecast and observation error statistics. It is still a linear algorithm, but extensions exist in SESAM (providing that an ensemble forecast is available) to account for non-Gaussian distributions using anamorphosis or a truncated Gaussian assumption. From a practical point of view, there is a clear separation between the forecast step, only involving NEMO model integrations, and the analysis step, implemented in the SESAM software. The overall system can thus be written as a master program (a shell script for instance) cycling forecast and analysis steps with quite simple interfaces between them.

For some scientific applications, especially for academic process configurations, it is sufficient to use simple error covariance matrix definitions. The so called B matrix required by 4D-VAR DA can thus be defined more simply than going through NEMOVAR: a simple tool should be developed for this. In the same way, a simplified version of the error observation definition routine (the so-called R) is under consideration.

CNRS manpower could be devoted together with other partners, to work toward the integration of these external components within the overall NEMO DA system.

SEABASS: a NEMO reference configuration for data assimilation

In the same way than the NEMO code has some reference demonstrating configuration (such as ORCA2, GYRE, etc …), it is proposed here to set up a reference assimilating configuration that can be used as a first demonstrator of several assimilation methodologies applied to NEMO. In this first stage, such a configuration has to be flexible, easy to manipulate and to maintain. Physically, it has to represent some key ocean dynamical processes. Moreover, its numerical cost must be reasonable.

An academic ocean basin double-gyre configuration is proposed. The rectangular domain of this configuration, now called Sea Box for Assimilation (SEABASS) extends from 24°N to 44°N and over 30° in longitude. Any horizontal resolution can be simply specified. For a 1/4° horizontal resolution, the grid contains only 121 points in longitude and 81 points in latitude. The ocean is sliced into 11 verticals levels, from surface to 4000 meters, described with a z-coordinate. The domain is closed and has a flat bottom. Lateral boundaries conditions are frictionless and bottom boundary condition exerts a linear friction. The circulation is only forced by a zonal wind. Lateral dissipation is performed on dynamics and tracers with a biharmonic diffusion operator. The salinity is constant over the whole domain and the initial stratification is produced using an analytical temperature profile. Details can be found in Cosme et al. (2010), for example.

Actually, this type of configuration has a long story that comes from ancient QG models implemented earlier to mimic the Gulf Stream system (e. g. Holland & Lin, 1975) and serve as a common basis through years to exemplify dynamical processes typical of the mid latitude like the Gulf Stream system with an unstable central jet, presenting meanders and eddies, as illustrated on Figure 2. Even very simplified, it is statistically meaningful regarding the eddy activity and the non-linearity amplitude of the actual Gulf Stream system. Clearly, the horizontal resolution of SEABASS configuration can be simply modified. As seen on Figure 2, which shows instantaneous relative vorticity at surface for three different horizontal resolutions (1/4°, 1/12° and 1/24°), increases in resolution allow stronger evidence of mesoscales and smaller scales activities.

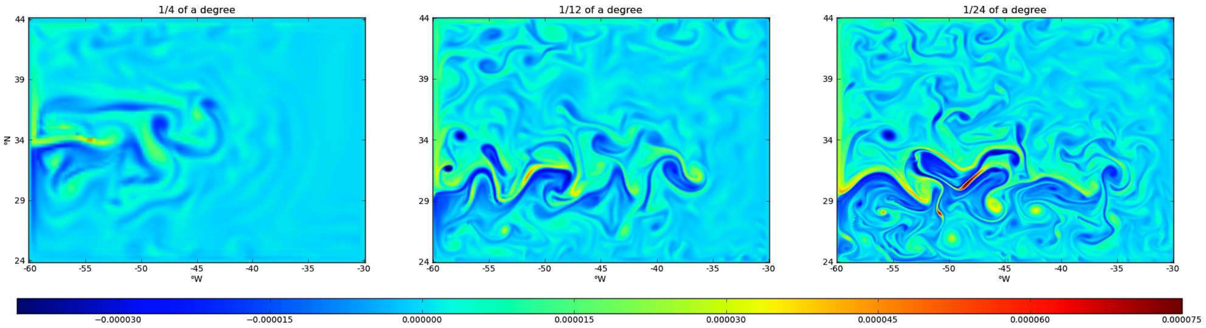

Figure 2: Instantaneous relative vorticity fields from SEABASS configuration, taken at different horizontal resolutions (from left to the right 1/4°, 1/12°, 1/24°)

SEABASS is a compromise between simplicity and a good representation of non-linear dynamical processes, increasing with its horizontal resolution. From a practical point of view, this configuration is easy to maintain across NEMO evolutions. This simplicity ensures that results obtained with different DA systems will probably be robust to most possible numerical evolutions of the NEMO code. In addition for variational DA, this configuration is fully differentiable, which ensures that Tangent and Adjoint Models do not contain approximations of the direct model. Several DA methods have also already been studied and tested on this configuration: SEEK filter and smoother, variational DA methods, nudging, Back-and-Forth nudging, ...

The ambition for SEABASS within NEMO is to have this simple model configuration together with the above DA methodologies and the associated tools and interfaces freely available to users.

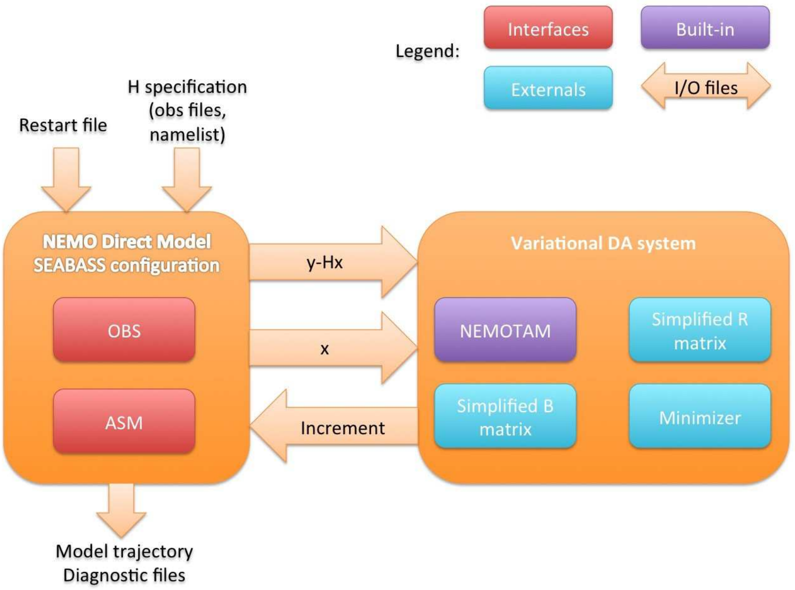

Figure 3a

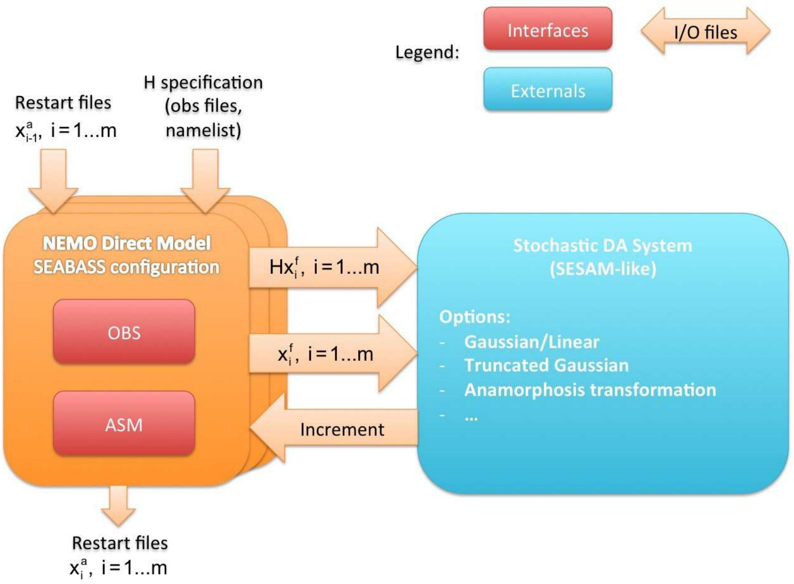

Figure 3b

Figure 3: Sketch of a data assimilation system for the SEABASS demonstrator: a) for a variational DA system, b) for a stochastic DA system

Figure 3 intends to show in a schematic representation how the NEMO data assimilation system presented here could be set up with the present SEABASS demonstrator in the case of a variational DA system (Figure 3a) and of a stochastic DA system(Figure 3b). Note that in this simplified SEABASS test case, some external components have been added: a minimizer, simplified error covariance matrices (B and R) and a stochastic analysis tool.

Conclusion

The goal of this paper was to set up some proposals to rationalize the developments related to data assimilation in NEMO and with the aim of building progressively a flexible data assimilation component designed for the NEMO system. In addition and most importantly, there is the willingness to make all of these freely available to all interested users.

There is a real diversity of data assimilation methods, addressing different scientific and operational challenges. In the future, the accumulated experience in inverse methods and the growing amount of computing resources will even accentuate the use of these different data assimilation methods for multiple applications: operational forecasting, parameter estimation, sensitivity analysis, design of new parameterizations… New observations from space or in-situ will also be a strong incentive for these developments. This will result in a number of new challenges, among which some can probably be anticipated.

From a methodological point of view, it appears clearly that Ensemble approaches encounter increasing interest, either for operational oceanography, for research studies, or for climate prediction. These Ensemble approaches can be either purely stochastic, as EnKF and its derivatives, or hybrid methods, as En-4DVAR under present development in several meteorological operational centres (Buehner et al., 2010).

Another important aspect of future data assimilation systems will be their capacity to take into account totally new types of observations and/or a dramatically higher flux of information. This will be the case with the advent of high resolution altimetry satellites such as with the NASA-CNES SWOT satellite mission project that should be launched around 2019. Relatively new sensors such as gliders also offer prospects that have not been carefully explored. Also, one can question the optimality of the use of existing sensors in assimilating mode, e. g. ocean colour satellite data. The increasing flux of information of SWOT type for example may raise new methodological issues for data assimilation, e.g. in the direction of image data assimilation or of multi-incremental approaches.

In the future the scope of ocean applications making use of data assimilation will broaden. For example, biogeochemical models bring their own specificities to data assimilation. They are generally highly non-linear and statistically not well conditioned (e. g. non-Gaussianity) and include a number of poorly known parameters. In this context, data assimilation tools may not only be used to perform state estimation but also to calibrate those parameters and validate model outputs. The expertise gained on these topics with NEMO will be a valuable asset when going toward more integrated Earth systems, coupling the ocean to components (atmosphere, ice, hydrosphere, …). In this prospect, the NEMO data assimilation environment should be adaptive enough to help the users to properly cope with these present and future scientific and operational issues.

Acknowledgement

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