Nemovar

22/4/2007

1 The NemoVar Project

The objective of this project is to develop NemoVar a multi-incremental variational data assimilation platform for multiple ocean configurations with NEMO. The project will build on variational assimilation developments made within the framework of the ORCA2 configuration and the OPA8.2 source code. The variational assimilation system that has been developed for OPA8.2 is called OPAVAR. It is currently used or has been used by various research groups in France and abroad

A swift transition to NEMO was seen as vital for the future of variational assimilation with OPA for both research and operational applications. An important example is the application of variational assimilation to global configurations with resolution finer than that of ORCA2, which introduces important computational issues (parallelization, memory, efficiency of numerical algorithms) that would be difficult to resolve within the current OPAVAR framework based on OPA8.2. The transition from OPAVAR to NEMOVAR, as well as the application of NEMOVAR to higher resolution global and regional configurations are part of the priorities of the project.

The variational assimilation problem solved by OPAVAR is defined very generally as the minimization of a cost function of the form

$$J[\mathbf{v}] = \frac{1}{2}[\mathbf{v} - \mathbf{v}^b]^T[\mathbf{v} - \mathbf{v}^b] + \frac{1}{2}[G(U(\mathbf{v})) - \mathbf{y}^o]^T\mathbf{R}^{-1}[G(U(\mathbf{v})) - \mathbf{y}^o] \tag{1}$$

where $\mathbf{v}$ is the control (analysis) vector, $\mathbf{v}^b$ is the background estimate of the control vector, $\mathbf{y}^o$ is the vector of observations, $\mathbf{R}$ is an estimate of the observation error covariance matrix, U is a (possibly) nonlinear operator that maps the control vector onto the model state (initial condition) space ($\mathbf{x} = U(\mathbf{v})$)[1] , and G is a nonlinear operator that maps from model state space onto the space of the observation vector (this includes the integration of the model from initial time to the observation times, as well as the interpolation onto the observation points). The background-error covariance matrix of the control vector is assumed to be the identity matrix ($\mathbf{B}(\mathbf{v}) = I$) as evident by the use of the canonical inner product for the background term in (1). In other words, background errors for $\mathbf{v}^b$ are assumed to be uncorrelated and to have unit variance. There are two advantages that result

[1] By interpreting $\mathbf{x}$ to be the initial conditions, the model and external forcing fields are tacitly assumed to be perfect. This assumption can be relaxed in the above formulation by considering $\mathbf{x}$ to contain model-error or external forcing terms in addition to the initial conditions.

from this formulation where the background term takes on a very simple form. First, it generally improves the convergence properties of the minimization when the problem is solved with a conjugate gradient algorithm. For quadratic cost functions, this is often explained by a reduction in the condition number of the Hessian (Golub and Van Loan 1996). Second, all constraints in the assimilation problem are now imposed through the nonlinear observation operators G and U , including multivariate and smoothness constraints that are used in conventional model-space (matrix) formulations of the background-error covariance model. In particular, this opens the way for incorporating potentially more realistic (nonlinear) multivariate balance relationships in the analysis problem. Details on techniques for constructing the transformation U (and its inverse U^{-1}) can be found in Weaver et al. (2006). OPAVAR employs a variant of the incremental algorithm (Courtier et al. 1994) for approximately minimizing the nonquadratic cost function (1). In particular, the algorithm is defined by the iterative minimization of a sequence, $k = 1, ..., K\_o$, of quadratic cost functions

$$\begin{aligned} J^k[\delta \mathbf{v}^k] &= \frac{1}{2}\left[\delta \mathbf{v}^k - \mathbf{d}^{b,k-1}\right]^T \left[\delta \mathbf{v}^k - \mathbf{d}^{b,k-1}\right] \\ &+ \frac{1}{2}\left[\mathbf{G}^{k-1}\mathbf{U}^{k-1}\delta \mathbf{v}^k - \mathbf{d}^{o,k-1}\right]^T \mathbf{R}^{-1}\left[\mathbf{G}^{k-1}\mathbf{U}^{k-1}\delta \mathbf{v}^k - \mathbf{d}^{o,k-1}\right] \end{aligned} \tag{2}$$

where

$$\mathbf{d}^{b,k-1} = \mathbf{v}^b - \mathbf{v}^{k-1}, \tag{3}$$

$$\mathbf{d}^{o,k-1} = \mathbf{y}^o - G(U(\mathbf{v}^{k-1})), \tag{4}$$

$\mathbf{v}^{k-1}$ is a reference state, $\delta \mathbf{v}^k$ is an increment defined by $\mathbf{v}^k = \mathbf{v}^{k-1} + \delta \mathbf{v}^k$, and $\mathbf{G}^{k-1}$ and $\mathbf{U}^{k-1}$ are linearized operators defined such that $G(U(\mathbf{v}^{k-1} + \mathbf{v}^k)) \approx G(U(\mathbf{v}^{k-1})) + \mathbf{G}^{k-1}\mathbf{U}^{k-1}\mathbf{v}^k$ (when this equation is satisfied exactly, (2) is identical to (1)). The superscript $k-1$ indicates that $\mathbf{G}^{k-1}$ is the result of linearizing G about $\mathbf{v}^{k-1}$. The sequence $k = 1, ..., K\_o$ are called outer iterations while the minimization iterations performed within each outer loop are called inner iterations. Equations (3) and (4) are the effective "background" and "observation" vectors for the inner loop minimization. In practice, it is customary to set $\mathbf{v}^0 = \mathbf{v}^b$ and to choose $\mathbf{v}^{k-1}$, for $k = 2, ..., K_o$, to be the solution obtained at the end of the previous outer loop. The minimum of (2) after the K_o-th outer iteration defines the analysis increment, $\mathbf{v}^a = \mathbf{v}^{K_o}$.

2 Nemovar workshop

NEMOVAR-LEFE Workshop

Thursday 22[nd] *of March*

9.00–9.15 Arthur Vidard: Presentation

9.15–9.45 Kristian Mogensen: Current status of NEMOVAR

9.45–10.15 Hicham Tber: Current status of NEMOTAM

10.15–10.45 pause

10.45–11.00 Sophie Ricci: Assimilation of SST

11.00–10.30 Nicolas Daget: Ensemble methods for computing background error statistics

11.30–12.00 Florian Sévellec: Optimal surface salinity perturbations influencing the ocean circulation

12.00–13.30 lunch

13.30–13.45 Monika Krysta: A hybrid approach to data assimilation

13.45–14.15 Bruno Ferron: Premières expériences jumelles d'assimilation de profils hydrologiques et d'altimétrie avec OPA-var dans une configuration 1/3° "eddy-permitting"

14.15– ... Discussions and future plans

3 Organisation of the Project

There are two tribes within the nemovar partners : the Operationals (and their accomplices) and the Academics. The formers need a stable and resilient system that is well tested and reasonably expensive. They want to focus on one (or two) given configuration(s) and need to develop a lot of paraphernalia (acquisition of data and forcing, archiving of data, automatic cycling, etc.). In fewer words, the Operationals want to develop a 3DVar, Global 1°, with all the operational machinery, as soon as possible. On the other hand the Academics want to test their new (or not so new) ideas on advanced assimilation schemes and on multiple configuration (multiple limited areas and multiple resolutions, and sometime at the same time). To a certain extent they don't need a resilient and computationally efficient system. Regarding organisation and priorities it makes sense that core developers are more focused on the Operationals needs because rushing to produce a working system will make the 'resilient & efficient' aspect difficult to achieve. However we have to keep in mind that the Academics should be able to start playing with it as soon as there is a stable-ish version (they do not need to wait for the operational ready system).

3.1 Developers and Users

As for other projects, NemoVar should be divided into Developers who will be working on the development version and the Users who will use the latest (or not) release. Users will, if needed, develop code/tools for their own needs (e.g. adapt to a specific configuration)and then feed them back to the developer if they think they can be useful for the community.

The developers can themselves be divided into 3 subcategories :

- The Core Developers, who are developing the software that is specific to NemoVar (i.e. the inner loop). It was pointed out that we want to keep the system flexible in those parts where scientific diversity is desired (e.g., covariance modelling).

  Participants: CERFACS, ECMWF and MOISE.

- The model developers (outer loop): It would be logical to include the outer loop assimilation developments in the NEMO reference code: the standardization of observation operators and assimilation interface for NEMO is of importance. Observation operators are useful for other assimilation schemes and the observation operators can be used for diagnostics to compare any model run (forced or coupled) with observations.

  The Observation operators and the ability to use the increment produced by the inner loop will be handed over to the OPA system team (ESOPA) to be included in the direct model source code. Both modules are general and can be used with any assimilation scheme and/or for diagnostics.

  Participants: ESOPA, ECMWF (K. Mogensen[2])

- The TAM developer. Tangent and Adjoint models can be used for other applications than data assimilation and therefore the TAM developers group is separated from the

[2] link with Core Developers

Core Developers group. TL/AD can (should) be developed and tested independently of 4D-Var (at least initially). Moreover a close interaction with NEMO developers is needed here to define Tapenade-friendly coding practices and select the most common options that need "adjointing"

Participants: TROPICS, MOISE, LPO, ESOPA (R. Benshila[3])

What about MERCATOR/E. Rémy and UK-Met-Office/M. Martin ? How do they fit in ?

3.2 Workplan

Originally the workplan was divided in 5 phases

- Phase 1: Split the existing OPAVAR Fortran code into separate executables for inner and outer loops. Completed

  In OPAVAR, the incremental algorithm has been implemented as a single FORTRAN executable. This has been identified as a major inconvenience, notably for the transition to NEMO. A much more flexible approach is to control the execution of the outer and inner loop calculations at the UNIX script level, and to exchange information between each loop via binary restart files. Decoupling the outer and inner loops in this way would give us considerable flexibility in choosing 1) the model configuration to be used in the outer loop to compute the observation-minus-model misfit; and 2) the type of assimilation method to be used in the inner loop to compute the analysis increment.

- Phase 2: Develop an MPP implementation of the observation operators in the outer loop using NEMO. being finalised, will be handed over to ESOPA soon ?

  This phase, which involves the outer loop only, requires incorporating into NEMO all components involved in the computation of the observation-minus-model misfit vector. These components include the observation processing (reading, sorting, grid search,...), the observation operators (1D and 2D interpolation methods), and I/O observation diagnostics (innovation, residual, quality control information). This infrastructure was developed for OPAVAR for profile and altimeter observations, except for the capacity to work with MPI which is a new development needed for NEMOVAR. Apart from its obvious importance for data assimilation, Phase 2 will result in a valuable stand-alone diagnostic module for ocean model validation in forced-only integrations. In fact, the algorithm is still valid for forced-only intergrations by setting the total number of outer iterations to zero ($K = 0$). For this special case, the model-observation misfit information would be computed (with respect to the model background) but there would be no attempt to correct the model initial conditions (or other parameters) to reduce the misfit.

- Phase 3: Develop a hybrid system with NEMO in the outer loop and OPAVAR in the inner loop. being finalized, a first working version is being tested

  The objective of Phase 3 is to replace OPA8.2 with NEMO in the computation of the observation-minus-model misfit vector, while retaining the existing OPAVAR code for computing the increment in the inner loop. While this phase is designed primarily for intermediate testing, it will give us

[3] link with ESOPA

access to a preliminary variational assimilation system for NEMO, with both 3D-Var and 4D-Var capabilities. Additional data assimilation inter- faces will need to be implemented in NEMO to read and apply the analysis increment generated in the inner loop. These interfaces exist in OPAVAR and will be standardized in NEMO following recommendations from the NEMO Working Group (see Phase 2). The increment can either be applied directly to the model initial conditions, as is typically done in 4D-Var, or can be forced in gradually using IAU (Bloom et al. 1996), as is typically done in 3D-Var. Both possibilities need to be accounted for, as well as the possibility of using different IAU weights (e.g., constant or saw-tooth-like). For simplicity, work in Phase 3 will involve the ORCA2 configuration in both the outer loop and inner loops. The possibility of using higher resolution configurations will be addressed in the next phase.

- Phase 4: Develop an MPP implementation of the 3D-VAR with NEMO in both inner and outer loops. Has just started, alpha version expected by the end of the year or early 2008

  The work involved in Phase 4 will be substantial, requiring a major rewrite of the inner loop of OPAVAR. Special consideration will be given to improving the modularity of the different operators used in the inner loop, the use of dynamic memory and massively parallel processors, and ensuring that ongoing scientific developments to the OPAVAR system (satellite data assimilation, minimization, background-error modelling,...) are accounted for in the new NEMOVAR structure. The possibility of using multiple global configurations will be accounted for in this phase, including the use of different resolution in the outer and inner loops.

- Phase 5: Develop an MPP implementation of the full 4D-VAR with NEMO in both inner and outer loops. Work in progress see section 4

  Progress in this phase will mainly depend on progress in developing MPI parallel tangent-linear and adjoint models which is being coordinated through a complementary LEFE proposal as discussed in the Introduction. It is worth emphasizing, however, that the work outlined in Phases 1 to 4 is a prerequiste to having an effective and affordable implementation of 4D-Var with high resolution global versions of NEMO. One aspect of 4D-Var that will be considered in this proposal is the implementation of a MPI parallel I/O module for the model state trajectory variables that are needed by the tangent-linear and adjoint operators. Identification of the nonlinear terms needed to be stored and retrieved for the tangent-linear/adjoint integrations can be done before the actual codes are fully developed.

Once a Phase 4 prototype is ready, user may be able to start playing with it. For the time being most of them can continue with OPAVAR. The FGAT formulation allows us to treat 3D-Var as a special case of 4D-Var (The Tangent linear model is approx by the Identity) Everything else in 4D-Var is the same as in 3D-Var! Therefore it should be relatively easy to "plug" NEMOTAM into NEMOVAR-3DVar to get NEMOVAR-4DVar once both components are ready. It means as well that Users can start their own developments with the 3D-Var without waiting for the 4D-Var

3.3 Improving the visibility and strategic plan

A common diagnostic is that we need more visibility. To that purpose, several paths have been identified :

- The project needs to build up a large proposal to ANR or FP7/idea
- Distribute officially OPAVAR (with minimalistic support)
- Set up a web site for the project (A&A agreed to coordinate, hosted ?). This website has to show
  - A global description of the project
  - The Nemovar Partners (see section 3.4) and their objective
  - The workplan
  - The distribution of the latest release of OPAVAR-ORCA2 sources along with a ready-to-go set up and/or a small tutorial.
  - ?

Note that a wiki has already been installed for developer communications
`http://www.cerfacs.fr/globc/nemovar/index.php/Main_Page`

It was noticed that the opportunity to get extra financial support is relatively reduced from the Operationals side: they provide priceless workforce but focus on their interests. There are more opportunities from the Academics side (even though it is probably a good strategy to target operational applications, but let's call it prospective operational applications). We need an additional person to work on the Tangent and Adjoint Models to get something compatible with NemoVar (see the NEMOTAM meeting report) a possibility is to submit an ANR proposal early 2008 asking for financial support to hire someone for this task. The drawback of this path is that this financial support would start in 2009. We are currently trying to find a way to fill this gap. Discussions about what to include in this ANR proposal should start in September to avoid a last minute rush.

3.4 Partners

This part needs to be developped. Each partner could write a small paragraph describing what they intend to do. Or I get it from the lefe proposal

- CERFACS/ECMWF + Collaboration MOISE
  - Operational System. (global 1° (2, 0.5 ?), first 3D-Var and at medium/long term 4D-Var)
  - Assimilation of SSH, SST and SSS
  - Multi-incremental system
  - improving **B**
- NEMOTAM subgroup (ESOPA/MOISE/TROPICS)
- PONGO (LEGI/MOISE)
  - Higer res (1/4+) 4D-Var

  - Hybrid Filter/Var
  - weak constraint 4D-Var
  - reduced domain and nested grid
- LPO
  - Higer res (1/3+) 4D-Var, North atlantic
  - Sensitivity analysis
- External Users (MERCATOR?, UK-MetOffice?)
  - Same as CERFACS/ECMWF but potentially Higer resolution and limited area model
- Other ?
  - Reanalysis ?