data assimilation

University of Reading

ESA

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1 Introduction

1.1 Background

On 10-12 September 2012 an international workshop was held at the University of Reading, Reading, U.K. on the topic of data assimilation for coupled environmental models (especially coupled atmosphere-ocean models). The workshop formed part of a contract from the European Space Agency (ESA) to carry out research by scientists of the National Centre for Earth Observation (NCEO) at the University of Reading, the University of Edinburgh and the European Centre for Medium-range Weather Forecasts (ECMWF). The research aims to develop methods for estimating the state of the atmosphere and ocean in a consistent manner by simultaneously combining satellite measurements of both systems with computer models. These new methods are predicted to make significant improvements in operational weather and climate forecasting and will prepare the ground for improved use of satellite-based datasets within ESA's Climate Change Initiative.

A major goal of the project is to investigate the impact of incorporating near-surface oceanic and atmospheric data, such as sea surface temperature, surface wind and wave data, supplied by the ESA satellites, into the ECMWF system. However there are many scientific and computational challenges to be overcome, especially since the ocean and atmosphere change on very different spatial and temporal scales. The workshop invited international scientists working in this field, with the following aims:

- to review the current status of data assimilation for coupled models;
- to set out the requirements for coupled data assimilation over the coming decade;
- to identify the challenges to be overcome;
- to prioritise research work in this area.

1.2 Workshop overview

The workshop was attended by 43 participants from Europe, U.S.A., Australia and Japan, both from operational forecasting centres and academic environments (see Appendix A for workshop agenda and Appendix B for the list of participants). The first 1.5 days of the workshop consisted of scientific presentations from 17 of the participants, reviewing the current status of the science of coupled data assimilation and the current research and development plans at the different centres represented.

Delegates then split into three working groups for the afternoon of the second day and the morning of the third day. Each group was asked to discuss in detail a specific scientific aspect of the coupled data assimilation problem, with the aim of producing a set of recommendations for future research. In particular, the following topics were allocated to the working groups:

- WG1: Dealing with different time and space scales.

- WG2: Better use of near-surface observations.
- WG3: Model errors and biases.

The more detailed brief given to the groups is copied in Appendix C of this report.

Results of the working group discussions were related to all delegates in a brief plenary session at the end of the first breakout session and in a longer plenary at the end of the workshop. Reports on the discussions from the different working groups and the emerging recommendations, taking into account the comments from the plenary sessions, are presented in the next sections.

2 Working Group 1 Report: Dealing with different time and space scales.

Members: *Matthew Martin (Chair), Polly Smith (Rapporteur), Patrick Laloyaux (Rapporteur), Oscar Alves, Fenwick Cooper, Amos Lawless, Kristian Mogensen, Drew Peterson, Nozomi Suguira, Yannick Trémolet, Anthony Weaver.*

This section summarises discussions and recommendations arising from working group 1. The group began with an introductory discussion, looking at the question of which problems we are trying to address (e.g. NWP, seasonal, decadal, reanalysis) and identifying the dominant time and space scales for the different systems involved. It was agreed that the focus of the discussion should be on coupling of the atmosphere and ocean; sea-ice, waves and land components are issues for future consideration. The group then moved on to consider the current position in terms of existing data assimilation systems, and their strengths and weaknesses. This was followed by discussion of a list of key research questions posed by the chair. Finally, potential ways forward were agreed and collected together to form the list of recommendations given at the end of this section.

2.1 Time and space scales

The NWP, seasonal, decadal, and reanalysis problems are inter-related but are often currently addressed using different approaches. The group were of the opinion that a single approach to coupled data assimilation for all time-scales would be useful to explore, although differences may remain for historical periods when the data are sparse. Processes occur on many space and time scales and there is variation both within and between systems. In terms of physics, the dominant time scales were identified as 6-12 hours for the atmosphere, of the order of a day for the upper ocean, and several days for the mesoscale ocean (and much longer for the deep ocean). The question was raised as to whether we should only be concerned with capturing the dominant scales. The general consensus was that there would be a range of time scales involved whatever the application but that the importance of each would depend on the purpose of the assimilation, e.g. whether the aim is NWP or we wish to capture phenomena such as the MJO in which case representation of the diurnal cycle is important. It was noted that time scales for data assimilation will also depend on the number and frequency of observations available. For reanalysis, there tend to be far fewer observations available before the satellite era and so a longer assimilation time window may be appropriate.

A similar conclusion was made for space scales: these vary depending on the resolution of the model and observations, the degree of smoothing required etc. However, for the dominant time-scales identified in the previous paragraph, the spatial scales could be characterised as 100-1000km for the atmosphere and ocean near-surface, and 10s of kms for the mesoscale ocean. These various scales highlight the significant challenge that coupled atmosphere-ocean data assimilation presents.

Coupling frequency was identified as an important issue in terms of time and space scales as this needs to be frequent compared to the length of the assimilation window and will affect the observations and scales resolved. It was questioned whether sub-daily time scales are required. Again, it was felt that this is likely to depend on the features we are trying to capture/analyse although it is likely that this will be required for most applications.

In terms of the scales resolved/represented by current observations, it was agreed that not all required scales are currently resolved; precipitation and mesoscale ocean scales were given as examples. It was noted that even if we could observe smaller spatial scales there would still be the issue of representativity errors. It was noted that the time of observations is also important and that we need to ensure longer timescales are correctly represented when using a short assimilation window.

A particular issue is that some ocean observation types are not available until several days after they are collected (e.g. altimeter sea surface height data). Observation processing and calibration procedures mean that there is a significant delay between the time of an observation and it being made available to forecast agencies. For coupled ocean-atmosphere data assimilation the timeliness of ocean observations needs to be brought into line with the timeliness of atmospheric observations. A figure of ~3 hours was suggested; however, it was acknowledged that this was a major challenge for some observing systems.

2.2 Existing algorithms and their strengths and weaknesses

Data assimilation is currently applied separately in the ocean and atmosphere using a variety of approaches. In terms of complexity/sophistication of algorithms, atmospheric data assimilation systems are currently ahead of their ocean counterparts, mainly due to the larger resources available for NWP development and operations. For the atmosphere, operational centres tend to use 4D-Var and hybrid 4DVar/ensemble methods; for the ocean the approach tends to be 3D-Var or ensemble methods.

The atmosphere and ocean assimilation time-windows currently used by operational centres are very different. For example, the ECMWF uses a 12-hour assimilation window for the atmosphere and a 5-10 day window for the ocean, whereas for the UK Met Office the time-windows are 6 hours and 1 day for the atmosphere and ocean respectively. It was agreed that there is a need for consistency of approach for coupled methods and that ocean data assimilation systems need to be brought up to the same level as atmospheric systems. In addition, it was felt that a move towards 4DVar/ensemble hybrid type systems would offer greater flexibility to the coupling problem.

It was commented that for 4D-Var we need to be able to write tangent linear and adjoint models and the linear approximation needs to hold for the duration of the time-window; sea-ice and land processes are very non-linear and the validity of the linear assumption may significantly limit the length of time-window. It is also questionable as to whether there would be much benefit from running a 4D-Var on the ocean over the short time-windows currently used for the atmosphere. Even a 24-hour time window may not provide much benefit in the ocean, particularly the mesoscale, although upper ocean processes which vary diurnally may benefit. It was agreed that this is something that would need to be investigated further.

2.3 Main research questions

2.3.1 Which methods should be used for coupled data assimilation?

The group considered the question of weakly coupled (where the background is generated using the coupled model but the data assimilation systems for the ocean and atmosphere are run separately) vs. strongly coupled data assimilation (where the inner loops of the data assimilation are also coupled, including the use of coupled background error covariances and a coupled observation operator), and the possibilities for something in between the two. The general consensus was that a weakly coupled system would offer more flexibility for the initial development than a fully coupled system, although the latter would ultimately be desirable. Key disadvantages of a fully coupled system were cost and complexity. Realistically, we can currently only start to develop a weakly coupled operational system with research into more fully coupled aspects being done in parallel.

Yannick Tremolet proposed a variational framework for coupled data assimilation that could offer a way of moving more easily between weakly and fully coupled systems. The method involves combining the cost functions for the atmosphere and ocean in the same minimisation, and adding an additional coupling term to control any errors in the coupling fields,

$$J(x^{atm}, x^{ocn}) = J_b^{atm} + J_o^{atm} + J_b^{ocn} + J_o^{ocn} + J_{cpl}$$

The advantages of this approach are that it only requires a single minimization and would allow for different time scales to be used for the atmosphere and ocean. It assumes that there are no background error cross-correlations between the atmosphere and ocean. The observation operator in the observation cost terms could use either separate ocean/atmosphere models (where linear and adjoint models exist) or the coupled model when its linear and adjoint are available. This formulation would require some of the fully coupled infrastructure to be put in place initially, and may make the inclusion of more fully coupled aspects easier. The idea was received with interest and it was suggested that it should perhaps be investigated further in a simplified system.

It was agreed that the initial aim should be to use the same assimilation time window for both the atmosphere and ocean (although the above framework may allow more flexibility). It was asked whether atmospheric systems are flexible enough to extend to ocean time scales. For coupled atmosphere-ocean NWP only the near sea surface is important and here timescales are similar to the atmosphere. It was suggested that, due to improvements in models, observations and error covariance models, an assimilation window of 1-day would not be unreasonable for the atmosphere. Longer term, a 5-day atmosphere-ocean assimilation window may be possible, assuming weak constraint 4DVar algorithms are available for the atmosphere (as is the case at ECMWF).

The group felt that it was important that operational centres move towards using weakly coupled systems as soon as possible in order for the benefits of the approach to be demonstrated.

2.3.2 What would an ideal fully coupled data assimilation system look like?

The group thought that weak constraint 4D-Var with hybrid ensemble flow-dependent error covariances would enable the required flexibility in terms of time and space scales, and would enable the system to make the most of the available observations.

2.3.3 Do we need to represent observation error correlations?

The answer to this question was yes, but with the caveat that observation error correlations are typically ignored in most current systems as including them is a complex task. In particular, SST is fundamental to ocean-atmosphere coupling and needs to be treated properly. Chris Merchant's talk demonstrated that spatial SST error correlations are significant and so efforts should be made to explore this further.

It was noted that data thinning methods such as super-obbing can relieve some of the problems with observation error correlations. It was commented that experiments to include observation error correlations in the ECMWF atmospheric system encountered difficulties with the inversion of the R matrix due to poor conditioning. Little research has been carried out into the use of observation error correlations in ocean assimilation systems.

The group agreed that the inclusion of observation error correlations is desirable and potentially beneficial but that a suitable, efficient approach to approximating their structure is yet to be found.

2.3.4 Do we need flow dependent covariances?

It was agreed that a hybrid approach would offer the most flexibility by allowing the possibility of both static and flow dependent elements, as described in Craig Bishop's talk. The estimation of the coupled covariances was put forward as an area for future research.

2.3.5 Is there a need for covariance localisation in time/space/scale/variable?

The group agreed that localisation would be an issue within hybrid covariance models as applied to the coupled problem. Oscar Alves' and Craig Bishop's talks gave some idea of the complicated (and often large-scale) structures in the coupled error covariances. Progress may be made by using ideas of localisation in spectral space, and vertical localisation issues would need to be investigated. New research on this topic is essential if hybrid techniques are to be used to model coupled error covariances.

2.3.6 Simplified models for assessing different approaches - how realistic should these models be?

A key issue was how much of the physics should be included in models used for idealised studies. The importance of diabatic processes within coupled systems was highlighted but it was acknowledged that the necessary level of complexity of a model will depend on the aims of the research. For example, the aim of the current idealised coupled data assimilation studies being carried out at the University of Reading is not to try to model the full system but to gain a greater theoretical understanding of the coupling problem and to develop and test various coupling strategies using realistic timescales. It is important to recognise that there are limitations to what can be achieved within the timescales of a typical research project (~2-3 years). Even relatively simple models require a certain amount of time and effort to set up; over-complexity can introduce unnecessary complications and hinder new developments.

It was agreed that there is a need to increase the collaboration/interaction between the academic and operational communities to ensure that new research is relevant to operational issues/concerns. The academic perspective was that it would be useful to have a hierarchy of simplified coupled models available that could be used to aid new research; sources of funding for this would need to be explored. It would also be useful if operational centres could make some staff time available to provide support and advice to the academic community.

2.3.7 Initialisation shock

The chair asked the group for ideas on identifying and mitigating against initialisation shock. The usual method used to identify such shocks in individual systems is to look for the generation of gravity waves. However, it is unclear whether these are likely to be generated when imbalances between ocean/atmosphere fields are present, and whether the coupled model adjustments will be detrimental to the forecast. Ultimately the extent to which initialisation shock is an issue will depend on the properties of an individual system and this area will need further investigation once the weakly coupled DA systems are set-up.

2.3.8 Other comments

There was a feeling amongst the group that the main drive for new research was coming mainly from the ocean data assimilation community and that greater interest needed to be encouraged from the atmospheric community.

2.4 Summary of recommendations

Observation agencies

- Make ocean observations available at much closer to real time (ideally within ~3 hours of measurement time).

Operational forecasting agencies

- Bring ocean data assimilation systems up to the same level as atmospheric systems so that there is consistency between the two and move towards hybrid systems for greater flexibility.
- Increase interest from the atmospheric data assimilation community.
- Move towards weakly coupled data assimilation systems as soon as possible so that the benefits can be demonstrated.

- Make (a small amount of) staff time available for supporting academic community.

New research areas

- Investigate different forms of coupling in simplified systems; in particular, possible hybrid formulations.
- Investigate how feasible it is to linearise the important processes in the boundary layer.
- Look at how to do control variable (balance) transforms for coupled systems (including cross variable relationships).
- Look at how to estimate coupled covariances.
- Investigate localisation in the coupled system (within a hybrid approach).
- Do we need different data assimilation systems for longer range (~3-year) forecasting vs. short-range forecasting and, if so, why?

Useful community actions

- A hierarchy of simplified coupled models should be developed, and made available, to support research.
- Demonstrate and advertise benefits/ impact of coupled data assimilation.
- Hold regular scientific sessions on coupled data assimilation at large conferences to promote sharing of ideas.
- Ensure that research problems are relevant to the operational community, but also allow for investigation of more novel approaches.

3 Working Group 2: Better use of observations

Members: *Peter Janssen (Chair), David Mulholland (Rapporteur), Ross Bannister (Rapporteur), Eric de Boisseson, Yosuke Fujii, Keith Haines, Christopher Merchant, Steve Penny, Robin Wedd*

3.1 Which current and future observations will most benefit coupled assimilation and how can we best use these?

The working group discussed a variety of observations that can yield information about the interface between the atmosphere and the ocean, which can provide information for both systems. Coupled data assimilation (in all its flavours) is expected to allow an improved interpretation of these observations, leading to a more accurate analysis of the complete geophysical picture.

Of satellite observations, the retrieval of sea surface temperature (SST) is perhaps the most important to the coupled system. SST retrievals currently use instruments AVHRR and AATSR. Atmospheric profiles obtained from reanalyses are used in the retrieval process, and so developments in reanalyses at the operational centres, and the use of 'profiles of the day' rather than climatological profiles, will benefit SST retrievals, particularly when dual-view instruments are not available. Coupled models resolving the diurnal cycle can be combined with observations at different times to give an optimum estimate of the diurnal cycle. This avoids misinterpreting all of the difference between observations made at different times of the day as a relative error. ESA's Sentinel-3 (planned for launch in 2013) will provide improved spatial coverage for SST retrievals. SST information can be assimilated into the coupled model system as an increment to either the skin SST directly, and/or indirectly as an increment to surface heat flux or the thermocline position. The use of other observed variables, such as wind, with multivariate statistics, can be used to help inform this decision. A well designed coupled data assimilation system with accurate multivariate error characteristics should perform these tasks automatically.

Observations are currently available (Aquarius, SMOS) for sea surface salinity (SSS) retrievals, but such retrievals may have diurnal cycle-related issues arising from up- and down-track observations being separated by ~12 hours. This could be mitigated using SST information simultaneously.

Scatterometer measurements provide surface wind information (relative to surface currents) via measurements of surface waves, so retrievals can benefit from surface current information obtained from a coupled model. Scatterometer measurements are most difficult to use in conditions of low windspeed, which is when the diurnal cycle in SST is likely to be large. In a coupled data assimilation system, an observed large-amplitude SST diurnal cycle can help infer information about the surface wind speeds.

Sea ice is important in the coupled system due to its albedo effect and the related latent and sensible heat flux contributions to the atmospheric and oceanic energy budgets. There is scope to allow sea ice concentration satellite data to be assimilated with a coupled system.

Of the above, SST and sea ice are considered essential climate variables (ECVs) by ESA's Climate Change Initiative (CCI). Other sources of data available from satellite (and pertinent to coupled data assimilation) include satellite altimeter, gravity, freeboard and ocean colour data.

There was discussion in the group on the production of 'trusted observations', and how these may be defined. A key property of trusted observations is that they should have negligible bias (probably defined to be less than 0.1 K). Such observations are essential, e.g., for isolating model biases. Such observations should not necessarily be restricted to in-situ observations and may be applicable for instance to a sub-set of SST retrievals. For SST, an uncertainty limit of around 0.1°C was suggested as a requirement for a trusted observation. It was noted though that from a data assimilation perspective, the provision of an accurate uncertainty estimate can be more important than a particularly precise observation. As a general point it was agreed that the inclusion of uncertainties along with measurements would greatly increase the usefulness of the data for assimilation purposes.

In situ measurements, from floating buoys, of SST, SSS, wave height and ocean currents remain very important. It is possible to estimate fluxes at the air/sea boundary by in-situ measurements using eddy correlations, but fluxes of heat and momentum – which are the dominant means by which the atmosphere and ocean are coupled together – are likely to be quantities that are most comprehensively obtained from a coupled model, rather than directly from observations.

Observations can benefit from the use of models in quality control – using a model 'first guess' to identify bad observations. There is a case for dedicated groups of experts to work on this task. A naive application of quality control though could lead to accurate and valuable observations of a real feature to be rejected because the model has not predicted it (e.g. small-scale, but large-magnitude SST anomalies, which a model might not be expected to represent) . For genuinely 'bad' observations it would be desirable to share 'black lists' of such observations so that different groups have knowledge of the observations that should be avoided. Another area in which observers can use models to improve the utility of their products (including error characterisation) could be by using ensembles of model reanalyses, when available, as background information for retrievals (e.g. atmospheric profiles in SST retrievals). This will aid in error characterisation, and could lead to the production of ensembles of retrieved values.

Observation simulation experiments should be performed with a coupled data assimilation system to evaluate the benefit of future observations, e.g. from the Sea and Land Surface Temperature Radiometer (SLSTR) on Sentinel-3.

3.2 Which phenomena are likely to benefit from coupled DA?

Phenomena that involve a direct interaction between the ocean and atmosphere, such as ENSO, Madden-Julian Oscillation, hurricanes and typhoons will most obviously benefit. Oceanic phenomena such as the Meridional Overturning Circulation, western boundary currents, tropical instability waves and eddy dynamics will also benefit. A coupled model approach is useful for studying the diurnal cycle, where local observations may only be available at low temporal frequency.

3.3 How can we estimate and model cross-covariance information?

Cross-covariance information, both spatially and between different interdependent observed variables (e.g. SST and surface winds), was agreed to be another important potential addition to observational datasets. It was suggested that more work needs to be done by the observation and retrieval experts to derive and understand this information. How these cross correlations could be represented in a compact way, such as through a single isotropic length scale or with a latitude dependence, was raised. It was also noted that work may be needed at the operational centres to ensure that this cross-covariance information, when available, could be properly used in the assimilation schemes.

Error covariances can be calculated using coupled model ensemble runs, long historical datasets and innovation diagnostics. Time-lagged covariance relationships between observation errors were also discussed but these may be difficult to handle, especially if they occur over a longer timescale than that of the assimilation window, but this extra information is potentially valuable and should be used by the coupled system if possible. The use of covariances between multiple observed variables can provide important information on how to implement balance relationships, e.g. by distinguishing between baroclinic and barotropic modes in the ocean. Desroziers-type diagnostics may provide very useful information on covariances (Desroziers et al., 2005). Such diagnostics comprise 'observation-minus-background' and 'observation-minus-analysis' covariances. These covariances are calculable and for a suitably large volume of observations can help to diagnose the (more difficult to measure) background and observation error covariances.

3.4 Summary of recommendations

Observation agencies and operational forecasting agencies:

- Observers, and producers of retrieved products should aim to attach accurate error estimates (both bias and random) to all data. Projects that fall under ESA's Climate Change Initiative (CCI) have a requirement to produce error characterisations and so this recommendation reinforces this need.
- The current buoy network should be maintained or expanded, as in-situ measurements provide an important ground truth for satellite observations.
- The possibility of obtaining more subsurface ocean data should be investigated
- Information on observational quality control be shared amongst users.
- Ensembles of analysed atmospheric profiles should be made available to observers for use in satellite retrievals.

New research areas:

- Work should be done by observation and retrieval providers, and assimilation experts (including at operational centres) to improve our ability to estimate and use cross-error covariance information. This includes cross-error covariances for all data used in the assimilation: observations and retrievals (this information should be provided alongside data where possible) and for model forecasts used as a-priori information in coupled data assimilation. This will require an interdisciplinary collaboration, as required by the ESA CCI.

3.5 Reference

Desroziers G., Berre L., Chapnik B., Poli P., Diagnosis of observation, background and analysis-error statistics in observation space Q.J.R.Meteorol.Soc. 131 pp. 3385-3396 (2005)

4 Working group 3: Model errors and biases

Members: *Craig Bishop (Chair), Stefano Migliorini (Rapporteur), Alison Fowler (Rapporteur), Magdalena Alonso Balmaseda, Philip Browne, Katherine Howes, Nobumasa Komori, Orial Kryeziu, Daniel Lea, Nancy Nichols, Roeland Stappers, Yannick Tremolet, Peter Jan van Leeuwen, Laure Zanna, Shaoqing Zhang*

4.1 Introduction

All models of the ocean and atmosphere are imperfect. Coupled ocean-atmosphere models are no exception. By model error, we mean the forecast error that would result over a single time step of the model if the model were initialized with the truth filtered to the spatio-temporal resolution of the model. Three possible sources of model error include: (S1) spatio-temporal scales unresolved by the model changing the trajectory of the resolved scales (S2) inaccurate parameterization of the averaged effect of unresolved scales, and (S3) misrepresentation of aspects of the governing equations; for example, the model may fail to conserve momentum and energy at the model air-sea-wave interface or atmospheric methane may be affecting outgoing long wave radiation in the atmosphere but may be entirely unrepresented in the model.

The connection between these three sources of model error and the statistical mean and covariance of model error is of some interest. While it is clear that, by definition, S1 only contributes to the variance of model error, S2 and S3 are likely to vary with the flow of the day and hence not only contribute to the variance of samples of model error collected over a period of time but they will also contribute to the mean model error.

The mean and the covariance of the model error distribution are required for the optimization of 4-dimensional state estimation techniques (eg Tremolet, 2007). Knowledge of the model error distribution would also be useful to researchers trying to reduce the error of a model. Ideally, data assimilation schemes would use information about the mean and covariance of model error conditioned on the flow of the day. However, if such information were not available then the mean and covariance of model error conditioned on the season and/or latitude would also be of use – if that were easier to obtain. The reality is that estimation of the model error distribution of any given model remains one of the outstanding research challenges in environmental state estimation.

The aim of this section is to summarize our working group's discussions and suggestions.

4.2 Discussion

4.2.1 Quantifying the mean model error in coupled DA

The group began by discussing the previous work into quantifying mean model error for non-coupled models. We identified the following possible approaches:

- Aspects of seasonal averages of model error may be assessed off-line by the averaging of analysis increments over a 1-3 month period (see Rodwell and Palmer, 2007 for a study of model error in climate prediction). This should theoretically be zero if the observation and background errors are unbiased. Of course, this approach is only likely to work in regions where unbiased observations are numerous enough to enable the accurate depiction of the key energy containing eddies.
- Model bias may be estimated per time step within sequential data assimilation by augmentation of the state vector. The choice of bias variable should be consistent with a physically informed description of the source of model error. These ideas have been previously applied to ocean data assimilation, see Bell et al. (2004), Balmaseda et al. (2007), as well as Martin (2001).
- An augmented state vector in data assimilation could also be used for in-line estimation of model parameters.

Inaccurately known model parameters could be a large source of model error. Care is needed to understand the time scales over which the errors in model parameters are important. It is easier to correct parameters in which the errors are seen at short time scales than those that are seen at long time scales. This is due, in part, to the difficulty in separating out the different model error sources.

- Another possible approach could be an extension of the model error forcing approach used at ECMWF for weak-constraint 4D-Var (see Tremolet, 2007). In this work the model bias is estimated alongside the initial state variables. Also discussed in Tremolet (2006) is an approach in which the 4D state is represented in terms of a disjoint sequence of model trajectories and a corresponding sequence of estimates of accumulated model error. Each estimate of the accumulated model error is given by the difference between the end of a trajectory segment and the beginning of the next trajectory segment. A seasonal average of such estimates of model error could also be used as an estimate of seasonal mean model error.
- Quantification of the extent by which the model fails to satisfy known physical conservation properties may also provide clues about mean model error.

It has been found in previous work that what appears to be a bias is actually a problem in some other aspect of the system; for example problems with the balance or initialization shock. To investigate this particular issue we highlighted the following possible areas of research:

- A study to understand how estimated model error varies from one DA system to the next with the same dynamical model. This may make it possible to separate out the effect of initialization shock.
- A study to gain knowledge of the characteristic time scales of initialization shock.

It is unclear how the estimation of model bias will change when the models are coupled as much of the bias may be caused by the forcing from the other system when uncoupled. Another open-ended question was how we could deal with different timescales in which a bias may develop; from a few hours in the atmosphere to a few days in the ocean.

4.2.2 Estimation of model error covariances

A particular problem in previous work on the inclusion of model error in data assimilation is the estimation of the model error covariances, stored in a model error covariance matrix Q. We believe that work is still necessary in this area on simple models. We had the following suggestions:

- Previous work has shown that approximating Q as proportional to the background error covariance matrix is not ideal (see Tremolet, 2007) as it gives corrections within the same state subspace as the background corrections. However, in some systems, this assumption may be better than entirely ignoring model error covariance.
- Could estimate Q from comparison of high resolution and low resolution models.
- Could also calculate Q iteratively using discrete-in-time formulation of weak constraint 4DVAR. Finding the covariance of these over a 1-2 month period provides new (and possibly improved) estimate of model error covariance Q.
- Could look at the covariance of a historical collection of analysis corrections.

In ensemble based data assimilation stochastic physics could be used to impart aspects of model error covariance to the ensemble covariance to represent the model error:

- Stochastic physics representations could be informed comparing high resolution and low resolution simulations.
- An augmented state vector in data assimilation could also be used for in-line estimation of parameters controlling stochastic perturbations.
- One might also develop stochastic parameterization schemes from the pdfs that are often used to construct deterministic parameterization schemes.

4.2.3 Use of model error in forecasting

The group discussed how best to correct for bias/systematic model errors in the forecast. Once an estimate of the bias in a coupled system has been achieved it could be used in the following ways to improve the coupled forecast:

- Turn bias estimate into estimate of bias per time step. This may then be used to correct the forecast, or alternatively the correction could be applied every n-time-steps, where n-time-steps is the time between DA cycles.
- It may be important to allow for seasonal variations and the attenuation of bias with time by the introduction of a memory term (see e.g. Balmaseda et al. (2007)). This hypothesis is related to the fact that, currently, it is difficult to know whether

the biases estimated over a certain time period is relevant for a forecast of arbitrary length over a differing time period. More investigation is needed in this area.

4.2.4 Separating model and observation error bias

As our only independent means of assessing the accuracy of a forecast is an independent observation, it is extremely difficult to determine mean model error if the mean observation error is non-zero. As such, the better we are able to independently characterize observation error characteristics, the better our chance of characterizing the model error statistics.

An accurate estimate of the observation error statistics would be very helpful. Observation error statistics depend on both instrument error and the error of representation. The error of representation depends on the effective spectral truncation of the model. At best, models can represent a truth spectrally truncated to a level that is resolvable by the model grid. The convolution theorem equates spatio-temporal spectral truncation with a spatio-temporal averaging of the truth. Some observations, such as a thermometer, measure the state at a point. Others, such as satellite radiances, represent a spatially weighted integral of atmospheric properties. In either case, the error of representation is the difference between the spatio-temporal average of the truth estimated by the observation and the spatio-temporal average of the truth represented by a model forecast of the observation. A model forecast of the observation is obtained by applying the operator that would map the true unfiltered state to the true value of the observation to the model forecast. In general, it is much more difficult to estimate the covariance of the error of representation than it is to estimate the covariance of the instrument error.

The suggestions arising from our discussion were focused on understanding and reducing the effect of observation error bias in data assimilation and are summarized in the following:

- It would be helpful to hold a field experiment aimed at accurately characterizing the error characteristics of key observation types such as those from satellites. The experiments would involve oversampling model grid boxes with high quality in-situ observations with very low instrument error and remotely sensed observations. In the context of coupled modelling, a helpful focus would be to use a field experiment to better characterize the error characteristics of observations that are affected by characteristics of both the ocean and characteristics of the atmosphere – such as satellite radiances.
- Designers of observing systems should strive to help data assimilation scientists characterize the statistical distribution of instrument errors and the error of representation.
- When using observations to estimate model bias, it may be helpful to limit the observations used for this task to observations likely to have zero mean error and well known observation error covariances.
- We speculated that knowledge of how observation error bias covariances differed from the model error bias covariances might enable one to at least partially

distinguish model error bias from observation error bias. For example, if observation error bias had smaller spatial scale than model error bias (as in the case of radar altimeter observations (Lea et al., 2008)) then this might help distinguish the two types of bias.

- Progress might be made if one could justifiably identify differing predictors for observation and forecast biases.

4.2.5 The different DA methods

We discussed the usefulness of a study comparing the differing DA methods. It would be interesting to try and understand the "structure" of model error covariance with different DA methodologies. For example:

- By running a perturbed parameter ensemble from same initial conditions and compare tendencies and accumulated 6 hr covariances
- Document covariances of differences of tendencies from high resolution model and coarse resolution model and also 6 hr (say) accumulations.
- Measure accuracy of pdfs produced by ensembles with model error representation.

4.2.6 Implications of model error on ensemble design

Stochastic physics should be applied to all members. However it is unclear whether the ensemble members should sample the estimated distribution of model biases.

4.3 Summary of recommendations

Observation agencies:

- Fund campaigns to independently assess observation bias and observation error correlations.
- Make suggestions about what might be good predictors of the bias.
- Provide observation error covariances of retrieved quantities.
- Maintain high quality in-situ observations to test remote-sensing observations. Ocean is under-observed. Improvements in coupled models will be difficult without better observations. Need better observations of the mixed layer, more observations of currents, more observations of the deep ocean – it is full of eddies – and is critical to long term prediction.
- Observational campaigns from time to time to check parameterizations of fluxes of heat, momentum, and moisture – same for ice.
- More accurate drifter locations

Operational forecasting agencies

- A reliable estimation of model error bias is crucial.

- Ultimate aim is to remove time correlation of innovations or account for the time correlation of innovations
  - Try on-line estimation of parameters
  - Pay more attention to archives of corrections that are or should be made available by operational NWP centres.
- Model Error fluctuation statistics
  - Consider on-line estimation of parameters controlling stochastic noise terms
  - Compare models at different resolutions
  - Pay more attention to archives of corrections
- Try to assimilate radiances instead of retrievals – where possible.

New research areas

- Explore estimation of bias parameters and stochastic error parameters in simple and intermediate models
- Innovations can be correlated in time either because there is model error or because the error covariance matrices used in the data assimilation scheme are inaccurate. As such new research aimed at distinguishing between these two causes of the correlation of innovations through time would be helpful.
- Spatial, temporal covariance of bias, for both model and observation error.
- Develop tests for the quality of the model error representations
  - Chi-square test for model error term in weak constraint 4D-VAR
  - Tests of accuracy of flow dependent forecast error variances and covariances
  - See if changes to model change "measure" of model error.
- Strategies for distinguishing bias in innovations due to model error from bias due to spurious imbalance associated with poor background error covariance modelling

Useful community actions

- Tighter connection between operational and research communities.
  - Make archives of corrections more easily available.
- Add archive of corrections and innovations to reanalysis data sets.
- Compare estimates of model error from different systems.

4.4 References

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5 Conclusions

The workshop provided very useful input into the current project being carried out as part of the contract between ESA and the NCEO and ECMWF. With regard to the part of the contract being developed on the ECMWF system it was noted that the workshop participants recommended moving towards a weakly coupled data assimilation system as soon as possible, which fits very well with the work proposed in Tasks 2 and 4 of the contract. At the same time some longer term aims were defined, such as attempting the online estimation of parameters. Although this would not be possible within the current 2-year contract, it supports the research programme on longer time scales.

The workshop was particularly supportive of studies using idealised models and recommended the development of a hierarchy of simple systems. The models being developed as part of the current contract will contribute towards this. As well as being supportive of the current planned studies, the workshop recommended ways that they could be extended. Of particular interest was the suggestion to investigate hybrid formulations of data assimilation. This will be incorporated into the current project if time allows, or otherwise would be a natural follow-on project. There were also many suggestions for new research into techniques for estimating model error and for estimating cross-covariances. There are several related projects at the University of Reading and some of the questions raised at the workshop will be incorporated into these projects over the next few years.

Several community actions were highlighted and these will be the subject of further discussion among project partners and other agencies. In particular, it was proposed that we should be proactive in promoting coupled data assimilation research at international conferences. This recommendation will be taken into account within the outreach activities of the contract. Other suggestions accepted by workshop participants require further work over the coming months to understand their practicalities, such as the possibility of sharing more information on quality control or analysis corrections.

Overall the workshop provided strong support for the current direction of the project, while providing many useful recommendations for subsequent work to help move towards fully coupled data assimilation systems.

A Workshop programme

MONDAY 10 SEPT

Session 1 – Chair Peter Jan van Leeuwen

10.00 Pascal Lecomte (European Space Agency) – Welcome and ESA's interest in data assimilation

10.15 Alan O'Neill (NCEO) – Data assimilation within the NCEO programme

10.30 Keith Haines (U. of Reading) – Objectives of the ESA project

11.30 Amos Lawless (U. of Reading) – Idealised studies in the ESA project

12.00 Peter Janssen (ECMWF) - CERA: A weakly coupled data assimilation system for reanalysis

12.30 Matthew Martin (Met Office) - Plans for Met Office system

Session 2 – Chair Keith Haines

14.15 Oscar Alves (CAWCR) - Coupled DA developments in Australia

14.45 Chris Merchant (Edinburgh) - SST retrieval/ assimilation

15.15 Eric de Boisseson (ECMWF) – Can a coupled model beat observed SST forcing in hindcasts of the MJO?

16.15 Yosuke Fujii (JMA) - Activity toward coupled data assimilation in JMA/MRI

16.45 Nozomi Sugiura (JAMSTEC) - 4D-Var coupled DA

TUESDAY 11 SEPT

Session 3 – Chair Magdalena Balmaseda

9.10 Craig Bishop (NRL) - Plans for COAMPS/ Covariance modelling for coupled DA

9.40 Robin Wedd (BMRC) - Covariances for coupled systems

10.10 Steve Penny (U. of Maryland) – Work on LETKF and variational methods for coupled systems at the University of Maryland

10.40 Introduction to working groups (Amos Lawless)

11.15 Nobu Komori (JAMSTEC) - Development of an ensemble-based data assimilation system with a coupled atmosphere-ocean GC

11.45 Shaoqing Zang (GFDL/ NOAA) - Parameter estimation in coupled models: opportunities and challenges

12.15 Laure Zanna (U. of Oxford) - Stochastic parameterisation in the atmosphere and oceans, and its relevance for the coupled data assimilation problem

14.00 Working group discussions

17:00 Plenary session – Chair Amos Lawless

Brief presentations of main questions and intermediate conclusions from working group discussions.

WEDNESDAY 12 SEPT

9.30 Working group discussions

11.00 Plenary session – Chair Amos Lawless

Report back from working groups on main conclusions and recommendations for future research strategies.

12.30 Lunch & end of workshop

B List of participants

Oscar Alves	CAWCR, Australian Bureau of Meteorology
Magdalena A Balmaseda	ECMWF
Ross Bannister	Reading
Mike Bell	Met Office
Craig Bishop	Naval Research Laboratory, Monterey, California
Philip Browne	Reading
Jonny Day	Reading
Eric de Boisseson	ECMWF
Alison Fowler	Reading
Yosuke Fujii	Japan Meteorological Agency/Meteorological Research Institute
Keith Haines	Reading
Ed Hawkins	Reading
Katherine Howes	Reading
Peter Janssen	ECMWF
Nobumasa Komori	Earth Simulator Center, Japan Agency for Marine-Earth Science and Technology (JAMSTEC)
Orial Kryeziu	Reading
Patrick Laloyaux	ECMWF
Amos Lawless	Reading
Daniel Lea	Met Office
Pascal Lecomte	ESA
Matthew Martin	Met Office
Christopher Merchant	Edinburgh
Stefano Migliorini	Reading
Isabelle Mirouze	Met Office
Kristian Mogensen	ECMWF
David Mulholland	Reading
Nancy Nichols	Reading
Alan O'Neill	NCEO
Steve Penny	Maryland
Drew Peterson	Met Office
Tristan Quaife	Reading
Polly Smith	Reading
Roeland Stappers	Reading
Zof Stott	Assimila
Nozomi Sugiura	Japan Agency for Marine-Earth Science and Technology (JAMSTEC)
Yongming Tang	ECMWF
Yannick Tremolet	ECMWF

Peter Jan van Leeuwen	Reading
Anthony Weaver	CERFACS
Robin Wedd	BMRC
Laure Zanna	Oxford
Shaoqing Zhang	GFDL/NOAA, Princeton University
Hao Zuo	ECMWF

C Briefing note for working groups

WG1: Dealing with different time and space scales. Chair: Matt Martin G03

Possible discussion questions:

- What scales should we analyse?
- How can we design algorithms to treat different scales?
- What are the strengths and weaknesses of weakly & strongly coupled 4D-Var, ensemble and hybrid methods in treating different scales?
- How do we deal with initialization shock?

WG2: Better use of near-surface observations. Chair: Peter Jannsen G04

Possible discussion questions:

- Which current observations will most benefit from coupled assimilation? How can we best use these?
- Which phenomena are likely to benefit from coupled DA?
- How can we estimate and model cross-covariance information?
- What future observations would benefit from coupled approach to assimilation?

WG3: Model errors and biases. Chair: Craig Bishop G05

Possible discussion questions:

- How can we best quantify model errors in coupled systems?
- How should we treat errors in the model and parameters in coupled DA?
- How can we correct for model errors in the forecast?
- How can we estimate model error covariances for coupled DA?
- What are the relative benefits of weakly & strongly coupled 4D-Var, ensemble methods and hybrid methods in treating model error?

Advice and recommendations sought

To help frame the reports of the Breakout sessions it may be useful to consider a break down as follows

- Advice to observation agencies (eg. ESA)
- Advice to operational forecasting agencies
- Advice on new research areas
- Advice on useful community actions