Met Office

UERRA Ensemble Data Assimilation Configuration

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Executive Summary

- A regional En4DVAR will provide a better estimate of uncertainty than a MOGREPS based system.
- Regional En4DVAR is simpler to produce since it can be run separately to the deterministic system.
- Regional En4DVAR may cost twice as much as a global & regional MOGREPS ETKF system.
- Costs may be ameliorated by running the ensemble at half resolution or by preconditioning of 4DVAR.
- 4DEnVAR and En4DEnVAR are not expected to be available in time for production.
- A 4DEnVAR/En4DEnVAR system is not expected to be of better quality than a 4DVAR/MOGREPS system.
- Some aspects of the system usually require data from a global model, but this can be avoided as follows:
  - background error covariances - use regional Covariances and VAR Transforms (CVT) package
  - observation background errors - use operational data
  - satellite radiance biases - use regional variational bias correction tool (VarBc)
  - land surface analysis - use regional land surface data assimilation (SURF)
- A regional En4DVAR seems the best option for a regional ensemble reanalysis. The ensemble mean can be used as the deterministic reanalysis as this should be higher quality than hybrid 4DVAR.
- Fallbacks (due to technical difficulties or cost) include
  - running the ensemble at half resolution with hybrid 4DVAR for the deterministic reanalysis.
  - running a MOGREPS system.
- The costs of each system per day of cycling are expected to be
  - En4DVAR - 800 to 1400 PE days/day
  - 4DVAR/MOGREPS - 677 PE days/day

The UERRA project has received funding from the European Union, Seventh Framework Programme (FP7/2007-2013) under grant agreement no. 607193 .

Description of Work

The UERRA WP2 Description of Work (Unden *et al.* (2013)) states:

Objectives:

- Development and production of a satellite-era (1978-present) high-resolution European ensemble regional reanalysis dataset, based on ensemble-variational data assimilation.
- Adaptation and production of a deterministic HARMONIE reanalysis for 1961-present.
- Downscaling of ensemble and deterministic RA to provide km-scale European-wide reanalysis datasets.
- Development of a homogeneous reanalysis system for the pre-satellite-era using a hybrid local ensemble transform Kalman filter/ensemble nudging approach with RA data production of at least 5 years.
- Ensemble reanalysis uncertainty estimates derived from comparison of the UERRA reanalyses against each other, global (ERA) and regional (HErZ) RA.

The EURO4M project (2010-2014) has provided the core 'deterministic' European regional reanalysis system, assimilating conventional, satellite and hydrological cycle (humidity, cloud, precipitation) observations into the Met Office Unified Model (UM)'s advanced four-dimensional variational (4D-Var) data assimilation (Rawlins *et al.* (2007)). The addition of the UERRA-MOGREPS-EU capability will provide consistent ensemble uncertainty estimates using a 20-50 member, regional configuration of the operational MOGREPS-G system currently implemented at Met Office for global operational probabilistic NWP.

Basic observation database will be from ECMWF MARS (ERA-CLIM), supplemented by high-resolution conventional observations made available for regional reanalysis by partners within UERRA WP1. There will be additional hydrological cycle observations suitable for high-resolution reanalysis, namely disaggregated precipitation accumulations and surface/satellite cloud observations for the period of the reanalysis. The Ensemble Variational (EVDA) derived ensemble regional reanalysis will be evaluated deterministically through

a) Comparison of ensemble mean against independent, unassimilated observations

b) Sanity check on quality of forecast run from ensemble control analysis.

Probabilistic evaluation of the quality of the ensemble reanalysis will be provided via spread-skill matching, rank histograms, and Brier skill scores. Additional evaluation against gridded observation datasets (e.g. E-OBS) and intercomparison with global (ERA-CLIM) and regional reanalysis datasets will be performed within UERRA WP3.

The HARMONIE Data Assimilation system as developed and used within the HIRLAM and ALADIN consortia will be implemented and optimised for the entire European area with surrounding sea areas at as high resolution as is possible (11 km and at least 65 levels). It will be run over a 50 year period, from 1961, and serve as one member of a multi-model reanalysis.

The physiographic properties will be derived or modelled to take the time evolution into account. Interaction with the surface (soil and sea and ice) is very important for the near surface ECVs and requires special attention. The data assimilation will be driven by the global ECMWF ERA-CLIM reanalysis and also use a large scale Jk constraint (Dahlgren, 2011) to add large Atlantic scale information from ECMWF satellite assimilation into the 3DVAR minimisation.

MeteoFrance will use the 2D-analysis system MESCAN, developed during the EURO4M project with SMHI, to provide a surface analysis for temperature, relative humidity, precipitation and wind. MF will downscale the HARMONIE 3DVAR analysis as an input field or background for the 2Dˇ2013analysis sysan ensemble surface analysis will be developed and evaluate on a shorter period (5 years) over Europe with MESCAN using uncertainties from task 2.1 and 2.2 and/or observation network and perturbed observations.tem MESCAN at 5.5 km. If possible additional surface datasets from WP1 will be used.

Good quality data CM-SAF data sets exist for both Geostationary METEOSAT and AVHRR polar platforms. They complements each others over the European area but an optimally gridded data set is needed for climate studies, validation of models and solar energy potential. A 2D pan-European analysis of cloud fraction will be run with the SMHI MESAN for 30 years, at 5.5 km resolution 1982-2013.

A hybrid ensemble data assimilation system will be implemented for the DWD NWP model COSMO. The system will be comprised of a local ensemble transform Kalman filter component currently developed at the DWD and an ensemble nudging component for continuous data assimilation between two Kalman Filter initializations. The ensemble nudging will be based on the current nudging implementation in the COSMO model and make use of the covariance structure given by the ensemble realizations. Perturbed observations will be nudged into the system using an observation data set developed in the project.

An ensemble regional reanalyses using the combined data assimilation system will be carried out for a test period. To show feasibility for the pre-satellite era, a probabilistic dataset will be used to compensate for missing satellite data in this era.

The KF ensemble variational DA will be used with a 6-hour Kalman filter interval and continuous ensemble nudging between two Kalman filter initializations. The target resolution for the ensemble is 12 km ensuring high resolution uncertainty estimates for the European CORDEX domain (covering whole Europe). Boundary conditions will be provided by the ERA-20C or NOAA 20-CR reanalyses.

The produced regional ensemble reanalyses data will be evaluated against independent observations, e.g. unused satellite observations as used in the current HErZ regional reanalysis scheme. Probabilistic evaluation will contain standard matches for ensemble reliability and/or resolution, e.g. spread-skill relation, rank histograms, Brier/CRPS scores. Additional comparisons will be made against the high resolution deterministic HErZ regional reanalysis. Extensive evaluation of the reanalysis ensemble will be performed within UERRA WP3.

Tasks:

The Met Office's principal contribution is in 'Task 2.1':

- Ensemble Variational DA development: Development of a European area version of the Met Office Global Regional Ensemble Prediction System (Bowler *et al.* (2008))
- and a regional version of the Met Office's coupled Ensemble-Variational Data Assimilation (EVDA) algorithm (Clayton *et al.* (2013)).
- Ensemble Variational DA observations: Specific observation preparation for ensemble regional reanalysis, beyond that available from ERA-CLIM and UERRA WP1.
- Ensemble Variational DA production: An ensemble European regional reanalysis for the satellite era (1978-present). Production using Met Office HPC resources at ECMWF.
- Ensemble Variational DA diagnostics: Diagnostics of quality of production, mean and uncertainty estimates.
- Deterministic and probabilistic diagnostics for production.

Milestones:

Milestone	Description	Lead beneficiary	Delivery month	Comment
MS4	Preliminary EVDA dataset available for preliminary evaluation studies	Met Office	Dec 2014	data archived
MS5	EVDA ensemble reanalysis raw dataset	Met Office	Jun 2017	data archived
MS6	HARMONIE reanalysis dataset stream	SMHI	Dec 2016	data archived
MS7	KFENDA Observation dataset	DWD	Sep 2014	ensemble data archived
MS8	KFENDA test homogeneous ensemble reanalysis raw test dataset	DWD	Apr 2017	ensemble data archived

Deliverables:

Number	Description	Beneficiaries	Delivery month	Res*
D2.1	Development of ensemble-variational data assimilation capability and report demonstrating ensemble uncertainty products	Met Office	Sep 2015	50
D2.2	Report of observations and datasets assembled for the ensemble-based vatiational assimilation	Met Office	Dec 2015	30
D2.3	Preliminary report with ensemble diagnostics	Met Office	Jun 2016	50
D2.4	Ensemble diagnostics report and documentation	Met Office	Jun 2017	30
D2.5	Report of results and datasets of two physics HARMONIE runs for spread estimation	SMHI, MeteoFrance	Dec 2014	10, 2
D2.6	Preliminary report of the first period of the RA	SMHI	Jun 2016	36
D2.7	HARMONIE reanalysis report of results and dataset	SMHI	Sep 2017	25
D2.8	MESCAN reanalysis dataset and report 1961-present	MeteoFrance	Sep 2017	40
D2.9	Ensemble surface reanalysis report	MeteoFrance	Jun 2016	10
D2.10	UERRA-MESA-CL 30-year European cloud fraction dataset and report	SMHI	Dec 2015	7

Number	Description	Beneficiaries	Delivery month	Res*
D2.11	Probabilistic observations will be generated for Kalman Filter ensemble DA and a report will be written	Univ. of Bonn	Mar 2015	10
D2.12	The KF ensemble reanalysis (KFENDA) system will be developed and with a report demonstrating reanalysis uncertainty capability	Univ. of Bonn	Sep 2015	20
D2.13	KFENDA ensemble diagnostics report and documentation	Univ. of Bonn	Sep 2017	15
D2.14	RA uncertainty evaluation: EVDA/HARMONIE/KFENDA uncertainty evaluation report	Various	Sep 2017	-

* Resources in person-months. D2.14 resources are not recorded here.

1 Introduction

The 'European Reanalyses and Observations for Monitioring' (EURO4M) project ran between 2010 and 2014, producing observation and reanalysis datasets to monitor the climate over Europe, Klein Tank *et al.* (2014). The project included the first generation of limited area model (LAM) based reanalyses for Europe, including a 12km two year regional reanalysis based on 24km 4DVAR (four-dimensional variational data assimilation), produced by the Met Office, Renshaw *et al.* (2014). Verification of this reanalysis compared to the European Centre for Medium Range Weather Forecasting (ECMWF)'s Interim Reanalysis (ERA-Interim, Dee *et al.* (2011)) demonstrated regional reanalyses' capacity for improving representation of surface variables over that of global models. Comparison with the Swedish Meteorological and Hydrological Institute (SMHI)'s High Resolution Limited Area (HIRLAM) reanalysis demonstrated the benefits of using four-dimensional variational data assimilation (4DVAR) over the less costly three dimensional variational assimilation (3DVAR), Renshaw *et al.* (2014).

Although verification of the EURO4M reanalyses provides a measure of the accuracy of the datasets, end users require detailed, understandable measures of uncertainty. Traditionally uncertainty in numerical weather predicition (NWP) has been provided via ensemble forecasts. The spread of the ensemble of forecasts is a measure of the uncertainty in the ensemble mean, a proxy for a deterministic forecast. The Met Office Global and Regional Ensemble Prediction System (MOGREPS) is based on an extended Kalman filter (ETKF) and is used operationally to produce two day forecasts of uncertainty both globally and for a higher resolution domain covering the UK. An experimental version of MOGREPS is also used to forecast to fifteen days globally. In this system, the regional ensemble is created by applying the forecast model to downscaled perturbations from the global ensemble. The MOGREPS ensemble is centred around the global operational analysis, Bowler *et al.* (2008).

In 'static' 4DVAR the background error covariance matrix, $\mathbf{B}$, is a smoothed homogeneous isotropic approximation based on long period ensemble forecast errors, Inverarity (2014). This approximation allows accurate analyses to be calculated, but contains no flow-dependent information. Since July 2012 the Met Office has instead employed hybrid 4DVAR for global data assimilation. The hybrid system combines the static background error covariance matrix with a localised matrix derived from the MOGREPS ensemble. This system improves on representation of static 4DVAR across most variables, Clayton *et al.* (2013). Since the hybrid 4DVAR system uses MOGREPS perturbations and the MOGREPS ensemble is centred about it, these operational systems are two-way coupled. An ensemble of 4DVAR can be constructed, called En4DVAR, by adding different observation perturbations to each member, Piccolo and Cullen (2014).

The time dimension in 4DVAR requires a perturbation forecast model which is costly to maintain and its structure assumes Gaussian covariance errors. With increasing resolution this assumption becomes less valid. Additionally 4DVAR is not expected to perform efficiently across the large number of processors included in future high performance computers (HPCs), Tremolet (2014). Therefore the Met Office is developing an assimilation system which uses ensemble perturbations at each time-step in the assimilation window, in place of the perturbation forecast model. This system is called 4DEnVAR since it uses ensemble information to represent a forecast of, potentially non-Gaussian, error covariances within a variational assimilation, Liu *et al.* (2008), Lorenc *et al.*

(2014). This system can also be used in ensemble mode and is being developed as a potential replacement for MOGREPS, called En4DEnVAR, Lorenc (2013a).

The principal Met Office contribution to the 'Uncertainties in Ensembles of Regional Reanalyses' (UERRA) project is to produce both an ensemble of regional reanalyses and a deterministic reanalysis over Europe for the period 1978-present, Unden *et al.* (2013). The deterministic system will attempt to improve on the EURO4M Met Office regional reanalysis by including for the first time ensemble data assimilation. The combined regional system will either be based on current Met Office operations, i.e. an ensemble reanalysis (either MOGREPS ETKF or En4DEnVAR) which drives hybrid 4DVAR (or 4DEnVAR), or may employ a regional En4DVAR. A regional ensemble may be achieved by downscaling from a global ensemble or by nesting a regional ensemble within a global ensemble such as the new ECMWF Twentieth Century Reanalysis (ERA-20C, Dee *et al.* (2013)).

The aim of this document is to determine the configuration of the UERRA Met Office reanalysis. Configurations of the deterministic and ensemble reanalyses are discussed in Sections 2 and 3, respectively. These regional systems may also require driving global ensemble and deterministic reanalyses, which are discussed in Sections 4 and 5, respectively. Section 6 summarises expected data storage. The different configurations are costed and summarised in Sections 7 and 8, respectively.

2 Regional Deterministic Reanalysis

2.1 Aim

- To produce a satellite-era (1978-present) European regional reanalysis dataset (deterministic), using ensemble data assimilation to improve representation of surface/weather variables over global reanalyses (ERA-Interim) and the EURO4M Met Office reanalysis (which used static 4DVAR).

2.2 Data Assimilation System

As stated in the introduction, the regional deterministic reanalysis, MO-R, will include ensemble data assimilation. Therefore this system could be based on hybrid 4DVAR (Clayton *et al.* (2013)), 4DEnVAR (Lorenc *et al.* (2014)) or the mean of En4DVAR (Piccolo and Cullen (2014)).

4DEnVAR is being developed for operations since it is expected to perform more efficiently at very high resolution on a future HPC, require less maintainance and have a cheaper computational cost than hybrid 4DVAR, Desroziers *et al.* (2014). These features would be of limited benefit to the UERRA project. The UERRA reanalysis will be produced using ECMWF's new Cray HPC, on which 4DVAR is expected to run efficiently on the EU-22 grid (see Section 2.3). Reduced maintainance costs do not benefit reanalyses since the system is frozen throughout production. Although 4DEnVAR iterations are much cheaper than those of hybrid 4DVAR, more iterations are needed for convergence, Clayton (2012), and reading/writing costs are higher, Gustafsson and Bojarova (2014), making the actual reduced cost unclear. Without substantial development and a large ensemble, 4DEnVAR is not expected to out-perform 4DVAR's accuracy, Lorenc *et al.* (2014) and may not be

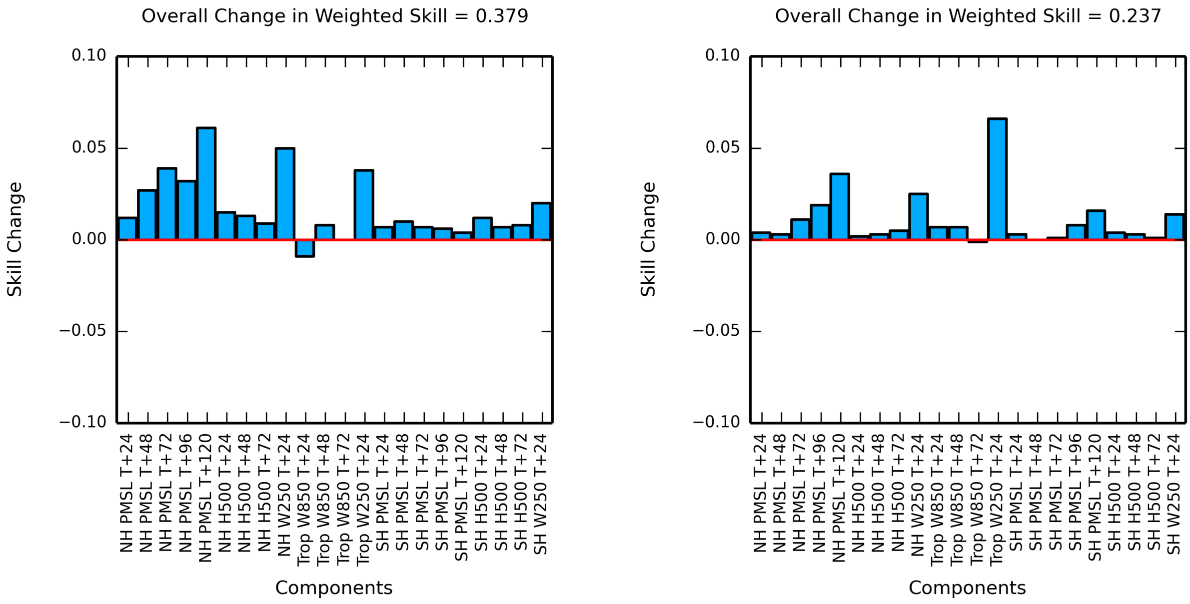

Figure 1: Verification of global hybrid 4DVAR against static 4DVAR, using observations as truth. LHS - June 2010 (two way coupling), RHS - Dec 2009/Jan2010 (one way coupling). These are corrected results from Clayton *et al.* (2013). The trials used N320 (51km) UM and N216 (76km) DA/Ensemble. NH - northern hemisphere, Trop - tropics, SH - southern hemisphere, PMSL - mean sea level pressure, H - geopotential height, W - wind.

available in time for production, Bowler (2014).

By contrast hybrid 4DVAR is a relatively mature system and has been successfully used to produce global operational forecasts for more than three years (from OS27, July 2011). Figure 1 shows verification results prior to it becoming operational. These results show improvement over the static 4DVAR in both winter and, particularly, summer months. Figure 2 displays verification of six hour forecasts, as proxy results for assessing reanalyses, together with those of twenty four hour forecasts. The results shown in this figure suggests that the benefit of the ensemble covariance is primarily seen at relatively long forecast times in most variables. However, precipitation *is* improved at six hours, but not at twenty-four hours. These results will vary for different ensemble covariance localisation distances. Since the highest accuracy is sought across all surface variables, care must be taken when tuning such a system for regional reanalysis.

Trial results from static 4DVAR, hybrid 4DVAR and 4DEnVAR are displayed in Figure 3. Index scores are taken as the weighted sum of skill scores and equitable threat scores (ETS) for twelve hour forecasts at 00Z and 12Z, which are proxy results for assessing analyses. Again these results do not suggest hybrid 4DVAR will perform any better than static 4DVAR for the region. The results in Figure 3 also suggest that the hybrid system performs better than 4DEnVAR for 23 ensemble members. Hybrid results are matched by 4DEnVAR only if eight times as many ensemble members are used, which is unaffordable for reanalysis. The results presented here are similar to Buehner *et al.* (2010), who found that 4DEnVAR performed slightly worse than two flavours of 4DVAR for short forecast times in the northern extra-tropics, and to Gustafsson and Bojarova (2014), who found that 4DEnVAR at 33km resolution performed similarly to 4DVAR at 44km.

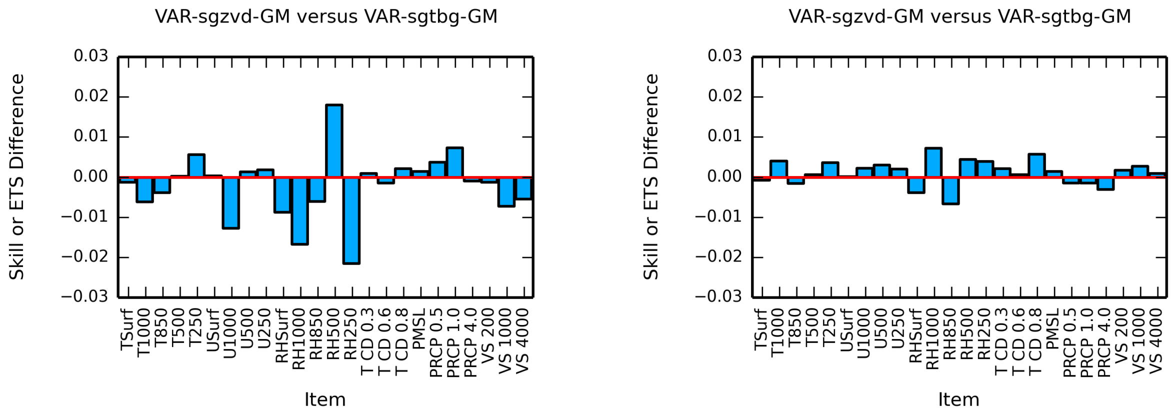

Figure 2: Verification of hybrid 4DVAR against static 4DVAR, using observations as truth for June 2010 (two way coupling) in the northern hemisphere. LHS - six hour forecast, RHS - twenty four hour forecast. These are extended results from the trial presented in Clayton *et al.* (2013). T - temperature, U - wind, RH - relative humidity, T CD - total cloud, PRCP - precipitation, VS - visibility.

Variable	Weight	Skill/ETS
Temperature 100hPa	14	Skill
Temperature 850hPa	6	Skill
Temperature 500hPa	3	Skill
Wind Surface	14	Skill
Wind 500hPa	3	Skill
Relative Humidity 1000hPa	2	Skill
Relative Humidity 850hPa	1	Skill
Relative Humidity 500hPa	1	Skill
Cloud Cover 3/8	4	ETS
Cloud Cover 5/8	4	ETS
Cloud Cover 7/8	4	ETS
PMSL 20	20	Skill
Visibility 200m	8	ETS
Visibility 1km	8	ETS
Visibility 4km	8	ETS
Total	100	

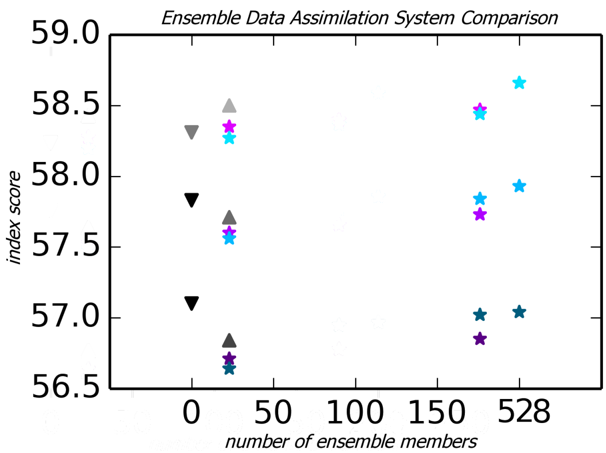

Figure 3: August 2012 trial results for 4DEnVAR including hybrid and static 4DVAR results for comparison, Clayton (2014). The plot shows ensemble size against an index of weighted skill scores/ETS at T+12 over the European domain. Blue (purple) stars show 4DEnVAR configurations using 80% (30%) static, 50% (70%) ensemble covariances. Results are shown for 00Z (lighter colour), 12Z (darker color) and a combination of both. The '528'-member ensemble uses lagged members from the 176 ensemble. The trial used N512 (32km) UM, N320 (51km) ensemble and N216 (76km) assimilation. Index weights are given on the LHS.

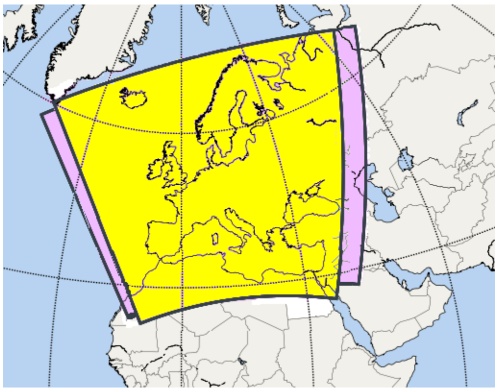

Figure 4: CORDEX EU-11 domain. Rotated pole grid, with pole at (039.25,-162). The corners of the domain are (22.0,-10.1), (24.1,40.0), (61.7,66.1), (57.6,-39.5). The pink region shows the similar EURO4M-MO domain.

Given that scalability and efficiency are not of primary concern to the project, it is clear that hybrid 4DVAR is more appropriate for MO-R data assimilation system than 4DEnVAR since it will produce better results. However, given the results presented here, its benefit over static 4DVAR is expected to be modest. If En4DVAR is used for the regional ensemble reanalysis (MO-RE), see Section 3, then either a deterministic hybrid 4DVAR reanalysis or the mean ensemble reanalysis could be used as MO-R. If the ensemble reanalysis is carried out at full resolution, and the ensemble is well formed, then the ensemble mean analysis should be of higher quality than a similarly set up deterministic reanalysis, Leith (1974).

There is currently no code available for regional version of hybrid-4DVAR (or 4DEnVAR) and development of this capability will require significant work. Development of a limited area hybrid-4DVAR is expected to require 0.2 full time equivalent, Clayton (2014); Lorenc (2014).

2.3 Forecast Model & Resolution

MO-R will use the Coordinated Regional Climate Downscaling Experiment's 0.11° European grid (CORDEX EU-11, Gobiet and Jacob (2012)) as shown in Figure 4. This differs slightly from the Met Office EURO4M domain. The grid is a rotated grid with pole at (039.25,-162) and 0.11 degree spacing. The grid contains 424 $\times$ 412 $=$ 175k points at roughly 12km spacing. Assimilation will probably be carried out using a half resolution grid (212 $\times$ 206 $=$ 45k points at 24km spacing), here called EU-22.

MO-R will use the Unified Model (UM, Davies *et al.* (2005)) to forecast from the start of the assimilation window $(T-3)$ to the analysis time $(T+0)$. The forecast will continue to the end of the next assimilation window $(T+9)$ to produce the background for the next assimilation cycle and to provide hourly forecast fields in between six-hourly analysis fields. Twice a day (00Z and 12Z), the forecast will continue further to produce three-hourly forecast fields for the first twenty four hours (i.e. to $T+24$), Kaiser-Weiss *et al.* (2014).

In 2014 the Met Office upgraded the UM's dynamical core from 'New Dynamics', Davies *et al.* (2005), to 'ENDGAME' (Even Newer Dynamics for General Atmospheric Modelling of the Environment, Wood *et al.* (2014)).

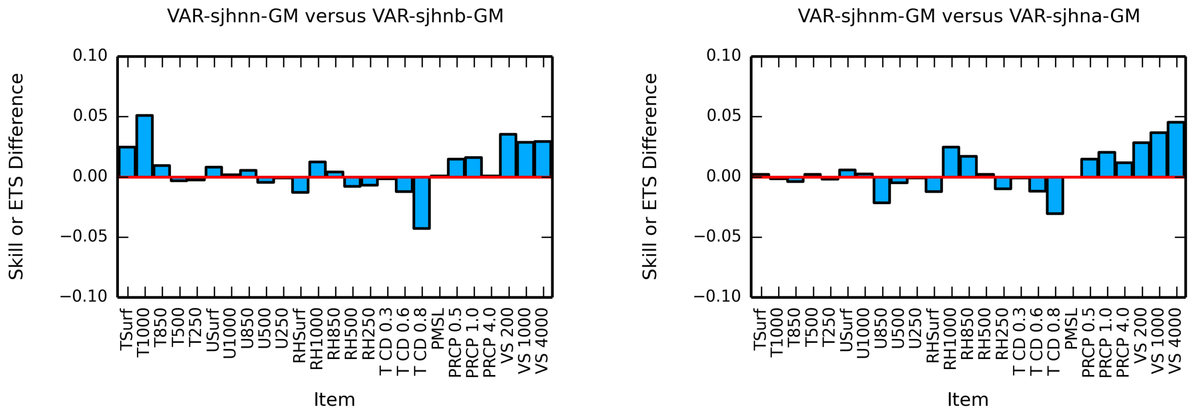

Figure 5: Comparison of 12 hour forecasts of ENDGAME against that of New Dynamics using global forecasts at N512. LHS - November 2012, RHS - July & August 2012. These are results from the Met Office Global Evaluation and Developments' ENDGAME trials, Earnshaw (2013). The suites 'sjhna/b' and 'sjhnn/m' are based on OS32 (GA5) and GA6, respectively.

This upgrade includes improved representation of mass conservation, improved coupling with parameterisations and improved handling of Rossby waves. It is expected that UERRA will use these upgraded dynamics which are available from Global Atmosphere 6.1 onwards. ENDGAME improves representation of orographic effects and has improved stability, but may increase spurious precipitation (Vosper (2013)). Figure 5 compares ENDGAME against the New Dynamics using the EURO4M reanalysis index on 12 hour forecasts. This demonstrates that for resolutions of the order of 30km ENDGAME has a neutral to positive impact on short range forecasts. These results suggest that use of ENDGAME may slightly improve representation of precipitation and visibility, but may slightly degrade representation of cloud.

2.4 Lateral Boundary Conditions & Initialisation

MO-R requires lateral boundary conditions (LBCs) and an initial background from a global model. For EURO4M these were provided by ERA-Interim, which is a high quality reananlysis at 80km resolution, Dee *et al.* (2011). Likewise ERA-Interim or the new ERA-20C, Dee *et al.* (2013), will be used to provide LBCs and an initial background to MO-R unless a global deterministic reanalysis, i.e. MO-G, is produced for UERRA, see Section 5. If MO-G is produced for UERRA, it will be a better source for MO-R's LBCs than the ERA reanalyses since it will be driven by a forecast model consistent with MO-R and is likely to be produced at a higher resolution. Production of MO-G would enable the UERRA reanalysis to be independent of external reanalyses.

To ensure that the regional deterministic system is properly 'spun-up', i.e. the reanalysis is not influenced by the initial background, the system should be run for a limited period before production output is stored. To determine an appropriate spin-up time the differences between a regional model (EURO4M-MO) and its parent global model (ERA-Interim) are considered. Orographic differences may mask the influence of the initial background and so an area of the North Atlantic is chosen for study. As shown by the top row of Figure 6, differences between the two systems are small and variable with no clear spin-up signal. To obtain a clear indication initial background influence, the number of grid points at which the difference between the two systems continues to

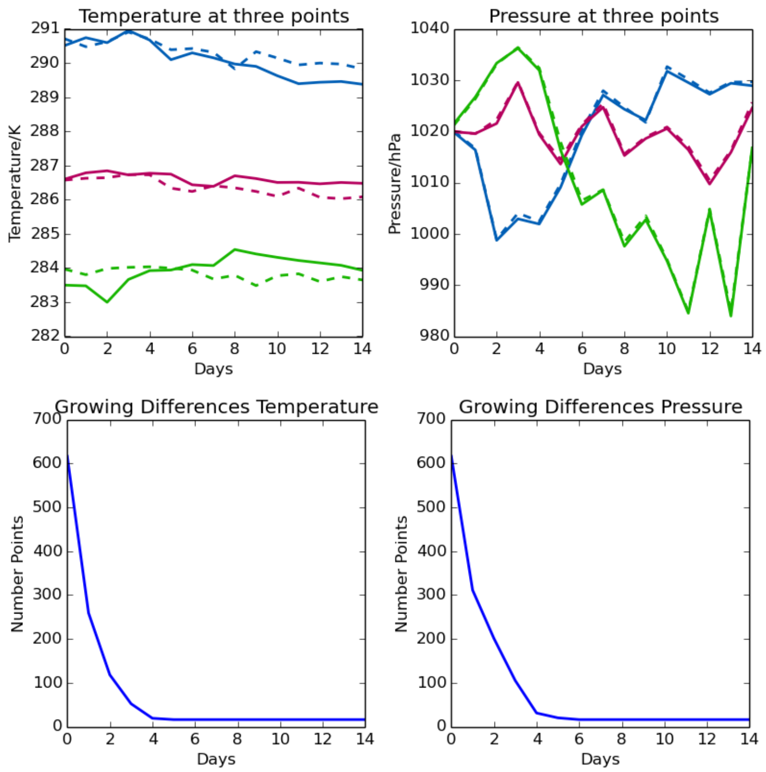

Figure 6: Spin-up in regional deterministic system - displaying differences between a global reanalysis (ERA-Interim) and a regional reanalysis (EURO4M). The top row shows plots of surface temperature (LHS) and pressure (RHS) for three points in the North Atlantic - blue (40.5°,-18.0°), red (49.5°,-15.2°) and green (58.5°,-11.1°). The bottom row shows plots of the number of points within an area of the North Atlantic for which the difference between the regional and global reanalyses is monotonically growing. Again the plots are for surface temperature (LHS) and surface pressure (RHS). The domain used is 31.1° - 60.0° north and -19.4° to -10.4° east, with grid spacing of 0.7°. The number of growing points is calculated at 00Z each day from a reanalysis initialised at 18Z on day '-1'.

grow is considered. A point is considered to have a growing difference if its difference has been greater than or equal to that of the previous day. The reanalyses are sampled at 00Z each day with the regional system initialised on 18Z on day -1. The results are shown in the bottom row of Figure 6 and suggest that a period of a week is sufficient for spin-up to take place.

As with Met Office operational systems, the surface boundary will be given by the land surface data assimilation system (SURF), see Appendix C.7.2, and external sea surface temperatures (SSTs), see Appendix C.7.3. An upper boundary exists at approximately 80km with a zero vertical velocity, Davies *et al.* (2005). If a regional land surface scheme is used within MO-R then it is likely that a significantly longer spin-up period will be necessary. It is usual to allow several years for soil moisture fields to be sufficiently spun-up, Yang *et al.* (2011).

3 Regional Ensemble Reanalysis

3.1 Aim

- To produce a satellite-era (1978-present) European regional ensemble of reanalysis dataset. This will be used to provide estimates of uncertainty and to provide ensemble-based error covariances to the deterministic regional reanalysis.

3.2 Ensemble System

The simplest method of intialising a regional ensemble is to merely downscale the members from a global ensemble, Mo *et al.* (2000); Roberts *et al.* (2014). The forecast model then adds high resolution features to each of the members. An improvement on this method can be achieved by downscaling the perturbations from the global ensemble and centring them about the regional reananlysis (MO-R). This has the benefit that the intial conditions for the forecast model have high resolution detail. This method was used by MOGREPS-R (Bowler *et al.* (2008)) and COSMO-DE (Kuhnlein *et al.* (2013)). Its benefits over simple downscaling are demonstrated in Tennant (2014). The regional ensemble system, MO-RE, could be provided by downscaling perturbations from a global ensemble, using either the MOGREPS ETKF or En4DEnVAR.

Alternately ensemble perturbations may be directly generated within a regional domain as carried out by Wang and Bishop (2003). A direct regional configuration of MOGREPS or En4DEnVAR is not available and development would be beyond the scope of the UERRA project. A direct regional ensemble could be configured, following the model error evaluation project (Piccolo and Cullen (2014)), using En4DVAR.

Reanalysis systems are traditionally based on operational systems, Dee *et al.* (2011); Onogi *et al.* (2007). The maturity of such systems reduces the likelihood of unknown problems with production and allows problems to be diagnosed efficiently since the system is well understood by the operators. Basing the reanalysis on an operational configuration may also provide new insights into these systems. Following this tradition strictly, MO-RE would be based on MOGREPS ETKF since MOGREPS has produced operational ensemble forecasts since 2005, Bowler *et al.* (2008). MOGREPS concentrates on short forecast uncertainty, which is ideal for reanalysis,

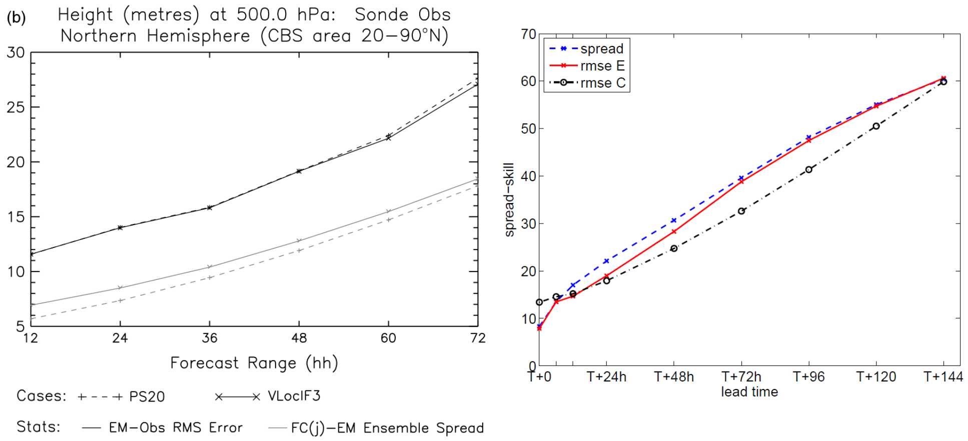

Figure 7: Ensemble forecasts in the northern hemisphere of geopotential height at 500hPa showing ensemble spread and RMSE. LHS - taken from PS20 (dashed) and vertical localisation (solid) trials with spread in grey and RMSE in black. This is Figure 4 of Flowerdew and Bowler (2013). RHS - taken from En4DVAR experiment with spread in red, mean RMSE in blue and control RMSE in black. This is Figure 2 of Piccolo and Cullen (2014).

but is known to be underspread even after inflation, Flowerdew and Bowler (2013). The biggest difficulty in implementing such a system for MO-RE is that it cannot currently be directly applied in the regional domain and so a global ensemble system, MO-GE, would also be required, see Section 4.

En4DEnVAR is currently being developed as a possible replacement for MOGREPS. However, as with MOGREPS, its ensemble is underspread and its implementation for UERRA would require an additional MO-GE system. En4DEnVAR is also immature and is still in development phase. It is unlikely to be sufficiently developed in time for production, Bowler (2014). Therefore of the two perturbation downscaling schemes, MOGREPS ETKF is the most appropriate for MO-RE.

A direct regional ensemble is achieveable via En4DVAR. In this system observations are perturbed for each member by randomly sampling from an assumed observation distribution based on error characteristics usually used for processing and quality control. A separate assimilation is then run for each member. This method should produce a more valid estimate of uncertainty than MOGREPS ETKF since it closely follows the deterministic 4DVAR assimilation. However the cost would be substantial. Prior to UERRA, En4DVAR has been successfully employed to provide estimates of model error. In these experiments, En4DVAR demonstrated a particularly good match between spread and error (RMSE). For northern hempisphere 500hPa geopotential height at T+6 the ensemble spread was slightly larger than the RMSE, Piccolo and Cullen (2014). The equivalent spread from MOGREPS is typically around half the RMSE, Flowerdew and Bowler (2013). An En4DVAR system has been used for operational data assimilation at ECMWF since 2010 Isaksen *et al.* (2010).

Figures 7 and 8 attempt to compare the spread of MOGREPS ETKF with En4DVAR. Although 500hPa geopotential height is not of primary concern to regional reanalysis, these results should give an indication of comparitive performance. Figure 7 demonstrates the relation between spread and error. The primary requirement of MO-RE is that these two measures are a good match at the analysis time. This figure shows that the spread and RMSE of En4DVAR are more closely matched than that of MOGREPS ETKF. Figure 8 displays the quality of

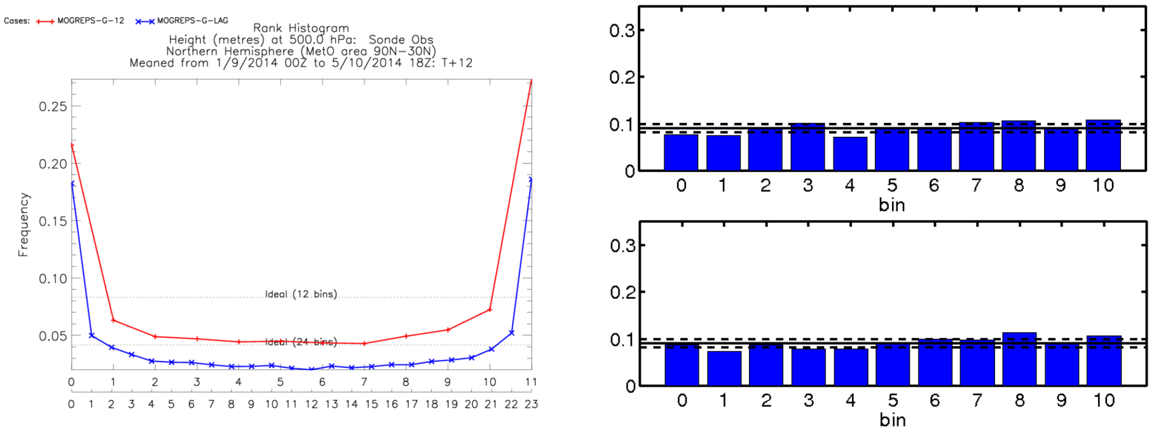

Figure 8: Rank histograms in the northern hemisphere of geopotential height at 500hPa and at T+6. LHS - taken from operational MOGREPS-G verification. RHS - taken from En4DVAR experiment, with close (top) and sparce (bottom) verification points. This is Figure 1 of Piccolo and Cullen (2014).

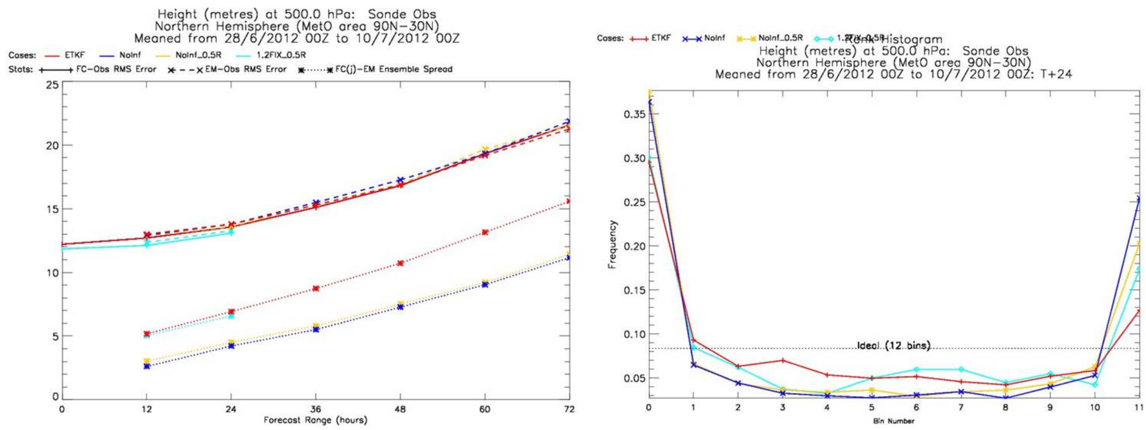

Figure 9: LHS - Northern Hemisphere control error, mean error and spread for MOGREPS and En4DEnVAR in the Northern Hemisphere for increasing forecast time. RHS - Rank Histogram for the Northern Hemisphere at two day forecast time. Red indicates MOGREPS with other colours representing various flavours of En4DEnVAR. These results are taken from development trials of the En4DEnVAR system, Pring *et al.* (2014).

the spread of the two systems, with a flat histogram indicating a perfect spread. This figure shows that while the spread of En4DVAR is reasonable, MOGREPS ETKF is underspread with the truth often lying outside the range of ensemble forecasts. Theses results suggest that En4DVAR will produce a better estimate of uncertainty than MOGREPS ETKF.

Figure 9 compares the spread of MOGREPS with that of various flavours of En4DEnVAR. The left hand plot shows the relationship between error and spread, while the right hand plot shows the rank histograms. These trial results demonstrate that the spread of En4DEnVAR is unlikely to improve much on MOGREPS. Therefore either of these systems will not produce as good an estimate of reanalysis uncertainty as that of En4DVAR.

The ‘mean-pert’ method is suggested by Lorenc (2013b), where the assimilation costs are greatly reduced by minimising for each member against an analysis from an ensemble mean assimilation. This scheme would be useful to reduce the cost of En4DVAR, but the coding required is substantial, Lorenc (2014), and beyond the scope of the project. However any assimilation could provide a guess state, and possibly Hessian preconditioning, to the ensemble assimilation and this has the potential of reducing the cost of the ensemble by half, Payne (2011). This preconditioning may not be useful in the regional model due to the extreme non-linearity of the visibility operatior, Payne (2009).

3.3 Forecast Model & Resolution

The first aim of the ensemble is to represent uncertainty in MO-R. Therefore best results will be achieved if the deterministic forecast grid is used, i.e. EU-11. It is common, however, for ensembles to use a smaller resoltuion than their deterministic counterparts to reduce their cost, Bowler *et al.* (2008), and therefore it is probable that the deterministic assimilation grid, EU-22, could also be used to produce useful ensemble data.

As with MO-R etc, MO-RE will use the UM with the ENDGAME dynamical core, see Section 2.3. However, it is necessary to represent model uncertainty within the ensemble of forecasts. Operationally this is achieved by stochastic physical parameters, Bowler *et al.* (2009). However better results have been achieved by adding random model variable tendencies from an archive of analysis increments to the forecast model, Piccolo and Cullen (2014).

External forcings also contain uncertainty which should be represented in the ensemble forecasts. These forcings include land surface analyses (see Appendix C.7.2) and sea surface temperatures (see Appendix C.7.3). It has been suggested that the uncertainty in aerosol and carbon dioxide should also be represented, Lorenc (2014), but this is likely only to have a small impact on the spread and has not been attempted in previous Met Office ensembles, Piccolo (2014).

Twice a day MO-R will perform twenty-four hour forecasts, however this data is not required for MO-RE. Therefore six hour forecasts will be sufficient to provide reanalysis uncertainty estimates and for cycling the system.

3.4 Lateral Boundary Conditions & Initialisation

Traditionally regional ensembles are nested within a global ensemble which provides boundary conditions. Deterministic boundary conditions are not suitable for a regional ensemble since uncertainty in the larger scales would then be difficult to represent, Zhang *et al.* (2006). Standalone regional ensembles, which do not require a global ensemble, have been attempted by introducing random perturbations at the boundary, Torn *et al.* (2005) or by damping ensemble variation near the boundary so that all members use the deterministic LBCS, Bonavita *et al.* (2010). Since capturing large-scale uncertainty in the Atlantic will be crucial for a useful European ensemble, LBCs from a global ensemble will produce the best results, see Section 4. To correctly represent both large scale uncertainty from the LBCs and smaller scale uncertainty within the domain, it is essential that the same LBC realisation is used by several ensemble members. If every member has a different LBC realisation then the ensemble will not include representation of small scale uncertainty, Piccolo (2014).

If MO-RE uses downscaled perturbations, then no initial spin-up period should be required. The perturbations will be sufficiently spun-up by the MO-GE system, see Section 4. The perturbations will be added to states from

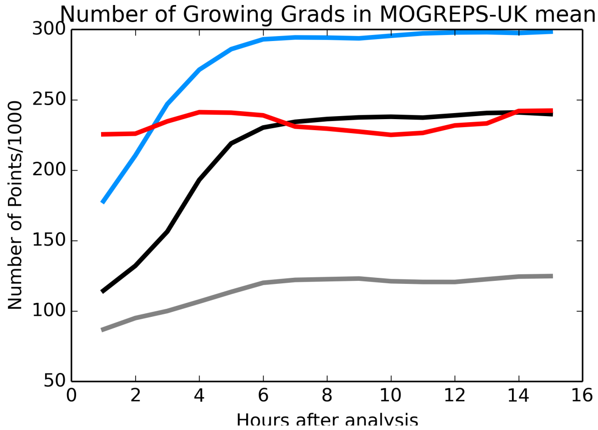

Figure 10: Spin up of MOGREPS-UK mean. Shown is the number of grid points with growing spatial gradients t hours after the start of the forecast. Variables shown are eastward wind (blue), surface pressure (red) and temperature at 850hPa (black) and 500hPa (grey). Data is taken from a single operational cycle of MOGREPS-UK.

MO-R, which will also be sufficiently spun-up, see Section 2.

En4DVAR will require a similar initial spin-up as 4DVAR. Results presented in Section 2 suggest that a period of of a week is sufficient for spin-up to take place.

For operational deterministic forecasts at the Met Office, the low resolution analysis increment (from 4DVAR) is added to the high resolution background (from the previous UM) to initialise the UM. The nominal analysis time is taken three hours from the start of the UM, which is the centre of the assimilation window. During the three hours the UM combines the analysis increment with the background at high resolution in a phyisically consistent manner. There is no difference between this system and any member of En4DVAR and therefore no additonal spin-up time is required within each forecast of such a system. If the fields are not sufficiently spun-up by the nominal analysis time, they also will not be spun-up in the control which the ensemble is following.

The spin-up time is less clear for each forecast of a MO-RE system which uses downscaled perturbations. As a proxy for such a system, the spin-up of the mean of MOGREPS-UK is examined in Figure 10. The metric used is the number of grid points for which the spatial gradient is increasing in magnitude t hours after the forecast. These results suggest that wind and temperature perturbations are at maximum resolution after about six hours and that pressure requires no spin-up period. This figure also demonstrates that the effect of spin-up decreases with height. Since regional reanalysis is most concerned with surface variables it is important that MO-RE is allowed to spin-up before issuing products. The operational regional ensemble (MOGREPS-UK) does not require a period of spin-up since only forecast fields are used for products.

3.5 Coupling

Observations are perturbed in En4DVAR by randomly sampling an assumed observation error distribution. Each member is in principle completely independent from other members and a deterministic control, with the caveat that an archive of analysis increments is required to represent model uncertainty within the UM, Piccolo and

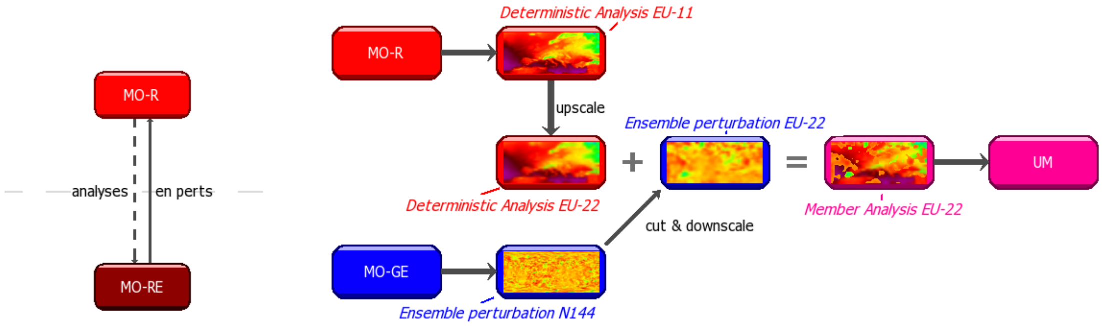

Figure 11: Regional ensemble technical configuration. LHS - Regional deterministic/ensemble coupling. RHS - individual member initialisation.

Cullen (2014). This independence is attractive since it allows a large degree of production flexibility and allows for the ensemble size to be increased after the initial realisations have been produced.

If MO-RE uses the downscaling approach, there is much less flexibility since MO-RE and MO-R will be two-way coupled. The regional deterministic system will provide analyses about which the regional ensemble will be re-centred and its ensemble perturbations will be used as 'errors of the day' for the 'ensemble' background error covariance within hybrid 4DVAR. This coupling is shown in Figure 11 in which the dashed arrow will be ignored if En4DVAR is used. If necessary MO-R can be produced before MO-RE using static 4DVAR as the assimilation system. Likewise if necessary MOGREPS ETKF can be produced before MO-R, driven by downscaled analyses from MO-G or another global reanalysis.

The right hand side of Figure 11 shows individual member initialisation for MOGREPS ETKF. For each member a ensemble perturbation is passed from the global ensemble, MO-GE, the regional domain is cut from the perturbation and downscaled to MO-RE resolution (EU-22). This is then added to the control analysis from MO-R, to form a different analysis for each member. The forecast is then driven from this analysis.

4 Global Ensemble Reanalysis

4.1 Aim & Uncertainties

- **Either** to produce perturbations which can be downscaled to drive a satellite-era (1978-present) European regional ensemble reanalysis.
- **or** to produce lateral boundary conditions for a regional ensemble.

4.2 Data Assimilation System

MO-RE can be produced using either a perturbation downscaling method or a direct regional ensemble, see Section 3.

The perturbation downscaling method requires a global ensemble, MO-GE. This could be produced using either MOGREPS ETKF or En4DEnVAR. As discussed in Section 3, MOGREPS ETKF would be the better choice. MOGREPS is based on the extended transform Kalman filter (ETKF) which is detailed in Appendix J. A similar scheme also drives operational ensemble systems at the national centers for environmental prediction (NCEP), Wei *et al.* (2006).

If the direct regional ensemble is used (En4DVAR), then only perturbed LBCs are required from a global ensemble. To avoid the cost of running MO-GE simply for LBCs, it is suggested that the LBCs are instead taken from ERA-20C. ERA-20C includes an ensemble of ten 4DVAR analyses at 125km resolution and should be available from early 2015, Dee *et al.* (2013). ERA-20C is a climate-style global reanalysis which assimilates only pressure observations. To capture both small and large scale uncertainties, it is necessary for several members of a regional ensemble to share the same LBCs, Piccolo (2014), and therefore ten is a sufficient number of realisations for MO-RE.

4.3 Forecast Model & Resolution

As with other systems, MO-GE would use the UM as a forecast model. Standard UM global grids are listed in Table 1. Since MO-GE will not produce data directly required by the UERRA project, it is necessary to use as cheap a system as possible. N144 (113km) is at a similar resolution to ERA-20C and should be fine enough to produce LBCs representing large-scale uncertainty. However, it is unclear if such a coarse resolution will be suitable for providing perturbations to a 24km regional model. When it was operational, MOGREPS-R had a grid that was approximately twice as fine as it parent, Bowler *et al.* (2008), and therefore, for MO-GE, a compromise is suggested at N216 (76km, approximately three times as coarse as the expected MO-RE grid).

Since MO-GE would only be required for LBCs and analysis perturbations, forecasts are only required to match the six hour cycling pattern of MO-RE.

As with the other configurations the global ensemble would use the ENDGAME dynamical core, see Section 2. As discussed in Section 3 forecast uncertainty could be represented either using the SKEB scheme or by adding randomly selected tendencies from an analysis increment archive. Likewise uncertainty in the land surface analyses and SSTs should be represented, see Appendices C.7.2 and C.7.3, respectively.

4.4 Initialisation

The analysis uncertainty is described by the spread of the initial perturbations. There are many methods to initialise perturbations for ensemble forecasting. These fall into two broad categories: direct, in which perturbations are calculated from error statistics Houtekamer *et al.* (1996); Molteni *et al.* (1996); Toth and Kalnay (1993), and ensemble cycling, in which the system is spun-up from an initial guess Barkmeijer *et al.* (1999). Direct perturbation generation are usually considered inferior to ensemble cycling methods since they rely on predefined

Grid Name	NY	NX	Num Points	∆Lat.	∆Long.	Approx. Spacing	Size of a Grib field
N1024	1537	2048	3.15M	0.12	0.18	16km	9.1M
N768	1153	1536	1.77M	0.16	0.23	21km	5.1M
N512	769	1024	787K	0.23	0.35	32km	2.3M
N320	481	640	308K	0.37	0.56	51km	784K
N216	325	432	140K	0.55	0.83	76km	412K
N144	217	288	62.5K	0.83	1.25	113km	184K
N108	163	216	35.2K	1.10	1.67	151km	104K
N24	37	48	1776	4.86	7.50	674km	5.4K
EU-11	412	424	175K	0.11	0.11	12km	512K
EU-22	206	212	45K	0.22	0.22	24km	129K
EU-44	103	106	11K	0.44	0.44	48km	33K

Table 1: UM global horizontal grids, with UERRA regional grids for comparison.

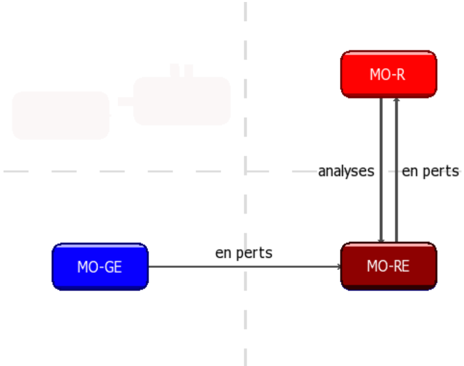

Figure 12: Regional deterministic/ensemble coupling with global ensemble.

or assumed error characteristics, Wei *et al.* (2014). Both MOGREPS and En4DEnVAR use ensemble cycling to generate initial perturbations and therefore both systems require a period of spin-up before the ensemble is useful. Bowler *et al.* (2008) suggest a spin-up period of about a week.

4.5 Coupling

The global ensemble will provide ensemble perturbations to the regional ensemble system if the downscaling perturbations approach is used. This coupling is shown in Figure 12. Since there is only one-way coupling between MO-GE and MO-RE, MO-GE can easily be produced before the regional system. If necessary, it may be possible to produce MO-RE without MO-GE if ensemble perturbations are used from ERA-20C.

5 Global Deterministic Reanalysis

5.1 Aim

- To produce global analyses to drive the global ensemble (if required).
- To produce lateral boundary conditions for the regional deterministic system.

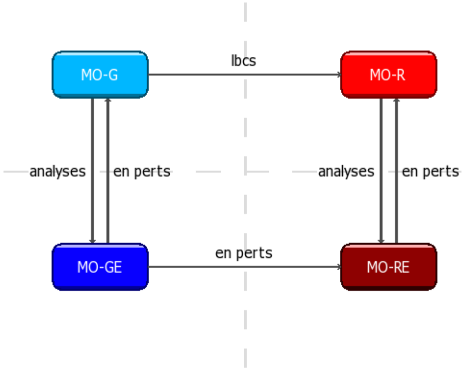

Figure 13: Regional deterministic/ensemble coupling with global deterministic/ensemble coupling.

- To produce observation background error and land surface analyses for the regional deterministic system.
- To calculate satellite radiance biases via VarBC or accumulation of statistics.

If MO-GE is run to produce pertubations and LBCs for MO-RE, then a deterministic global system, MO-G, is also required since a control analysis is required. If MO-G is produced, it is expected to be a better source of deterministic LBCs than ERA-Interim since it will use the same forecast model as MO-R, i.e. the UM. If produced, MO-G will also follow MO-R in using a 4DVAR assimilation system and the UM forecast will use ENDGAME dynamics. Since MO-G is required to drive MO-GE, only forecasts of length sufficient to maintain the six hour cycling system are required. An N216 grid, see Table 1, would be at a similar resolution to ERA-Interim, and therefore suitable to produce LBCs, and is most appropriate to provide control analyses to an N216 MO-GE.

MO-G would be fully coupled to the global ensemble system and will also provide LBCs to the regional deterministic system. This coupling is shown in Figure 13. MO-G could be produced before both MO-GE and MO-R if the assimilation scheme used is static 4DVAR. MO-GE could be produced without MO-G by using global analyses from ERA-Interim. Similarly, MO-R could be produced without MO-G using LBCs from ERA-Interim.

To minimise spinup time, the system will be initialised using data from ERA-Interim (or similar global reanalysis). The necessary time to spin-up from this external analysis is likely to be similar to or less than, that of MO-R, see Section 2.4 and Figure 6, i.e. a week should be sufficient.

MO-G would be useful to calculate several fields and parameters useful for the regional systems:

- Background error covariance
- Observation background error
- Land surface analyses
- Satellite radiance biases via VarBC or accumulated statistics

If MO-G is not run then alternatives are available. There is more discussion on this in Appendices B, C.2, C.7.2 and C.5.

6 Storage

There are two requirements for storage of the data: publically available data and internal experimental data.

6.1 Publically Available Data

For the deterministic regional system it has been agreed in principle to store analysis and hourly fields to T+6. Twice a day three hourly fields to T+24 will also be stored, Kaiser-Weiss *et al.* (2014). Assuming each time set consists of 51 surface fields, 100 pressure level fields and 497 model level fields, this consists of 378 million fields. Using the CORDEX grid a single field is 512KB in grib format so the total storage 194TB for 40 years of fields.

Fields from the regional ensemble system will also be stored for public access. Although these will likely be produced on half-resolution grids, it is likey that the full set of fields will not be stored. A single field is 129KB in grib format and total storage is 968TB for the full set of fields for the full 40 years.

Data from the special experiment where a fixed set of surface stations are used for all UERRA reanalyses (and the remainder retained for verification) may also be stored at ECMWF. Data from satellite sensitivity experiments may also be made publically available.

ODBs from most data types (excluding satellites due to high data volumes) will also be stored at ECMWF for public access.

Public access data will be stored at ECMWF in the MARS archive.

6.2 Experimental Data

For the UERRA project the Met Office may also produce global deterministic and ensemble data. It would be useful to store this data since it would be very valuable to future regional reanalysis projects including IMDAA (Indian Monsoon Data Assimilation and Analysis) and colaborations with other national centers.

The N216 global grid produces fields of size 412KB in grib format will require storage of 95TB, assuming re-Forecasts are not required. An ensemble at this resolution will be 1.88PB.

Component	Resolution	No/day	Cost Calc.	Total/PEs	Cost/day/PEdays	T
MO-R UM to T+9	EU-11	2	64×520	33280	7.6	E
MO-R UM to T+24	EU-11	2	64×1100	69894	16.2	E
MO-R hybrid 4DVAR	EU-22	4	384×340	132040	61.1	A
MO-R OPS	EU-22	4	see Table 9	4171	1.9	D
MO-RE (downscaler) UM reconf	EU-22	20×4	4×35	142.6	1.3	A
MO-RE (regional) 4DVAR	EU-22	20×4	384×340	132040	1222.6	A
MO-RE (regional) 4DVAR	EU-44	20×4	384×53	20352	188.4	R
MO-RE UM to T+9	EU-22	20×4	64×170	10880	100.7	R
MO-GE reconf	N216	20×4	4×46	184	1.7	A
MO-GE OPS	N216	20×4	16×90	1440	13.3	D
MO-GE UM to T+9	N216	20×4	64×350	22400	207.4	D
MO-G UM to T+9	N216	4	64×350	22400	10.4	D
MO-G hybrid 4DVAR	N216	4	384×1400	537600	248.9	A
MO-G OPS	N216	4	see Table 9	19702	9.1	D
MO-G UM reconf.	N320	1	4×110	440	0.1	D
						H
MO-R Total					87	
MO-RE (downscaler) Total					100	
MO-RE (4DVAR EU-22) Total					1400	800
MO-RE (4DVAR EU-44) Total					380	290
MO-GE Total					220	
MO-G Total					270	

Table 2: List of running costs per day of suite components, estimated as follows. E - Averaging over ten cycles of EURO4M, A - Using times from acceptance tests and assuming EU-22≈0.9N108+0.1N216, R - assuming increasing resolution by factor 2 increases cost by factor 6.5 for VAR and by factor 3 for UM. The tabulated costs are estimated using the new dynamics, D - averaging over ten cycles of a development suite. Components with small cost are not shown. P indicates potential cost if preconditioning is used. VAR assimilations are costed using 60 iterations.

7 Running Costs

8 Summary

For the full UERRA reanalysis system three different systems are achieveable:

Downscaler

MO-RE driven by downscaling pertubations from a global MOGREPS ETKF ensemble, with hybrid 4DVAR producing MO-R.

Direct-hybrid

A regional ensemble of 4DVARS for MO-RE, with hybrid 4DVAR producing MO-R.

Direct-only

A regional ensemble of 4DVARS for MO-RE, using the ensemble mean to produce MO-R.

	Downscaler	Direct hybrid	Direct only
MO-R	hybrid 4DVAR	hybrid 4DVAR	ensemble mean
MO-RE	Downscaled perturbations	En4DVAR	En4DVAR
MO-GE	MOGREPS ETKF	none	none
MO-G	hybrid 4DVAR	none	none
Coupling	Ensemble/Deterministic fully coupled	Independent	Single system with independent members
Spread/RMSE	0.5	1.01	1.01
Cost/day/PE/day	677	377 to 1487	800 to 1400
Forecast spin-up	6 hours	3 hours*	3 hours*
Background error covariance	MO-GE	MO-R	MO-R
Observation background error	MO-G	operational data	operational data
Satellite Radiance biases	MO-G	MO-R	MO-R
SURF	MO-G	regional SURF	regional SURF

Table 3: Summary of options for reanalysis set up. * i.e. nominal analysis time

Table 3 summarises the differences between these systems. It is expected that the direct method will produce a higher quality estimate of the uncertainty in the analysis than the downscaler method. The direct method may also cost slightly less than downscaler method if significant cost savings can be achieved at lower resolution. A more valid approach to estimate uncertainties is to perform the ensemble of analyses at the same resolution as the control. This ensemble resolution would also allow the ensemble mean to be used as the deterministic reanalysis. Use of the ensemble mean in this way may reduce costs slightly, but the main benefit is that the system is entirely uncoupled, which creates a simpler, more flexible production. A regional 4DVAR system would still be required to create an archive of analyses needed to perturb the forecast model.

Although the direct method may cost twice as much as the downscaler approach, it is hoped that costs can be reduced by employing Hessian preconditioning. Using the direct only approach no new code is required since a regional hybrid is unnecessary. As can be seen in Table 3, a global model would contribute to a number of aspects of a regional system. It may be necessary even with the direct approach to run a global system for a few short periods.

The approach reccomended here is, therefore, to begin tests using a full resolution En4DVAR, i.e. the direct only method. If costs cannot be significantly reduced with preconditioning then half resolution En4DVAR can be used, together with hybrid 4DVAR to produce a deterministic reanalysis. A suggested development plan is given in Appendix A.

A Suggested Development Plan

- Develop a regional deterministic suite using static 4DVAR at EU-22, using LBCs from ERA-Interim (underway, October 2014).
- Run this suite for a test month (some time in 2008?) and compare verification results against EURO4M
- Run the suite for a several months, archiving the analysis increments for use in testing En4DVAR.
- Add functionality to perturb observations and add random tendencies to the UM to create the En4DVAR suite.
- Run the En4DVAR suite for a month, verifying that the spread matches the error and that the ensemble mean is more accurate than the control.
- Investigate methods for reducing the cost of the ensemble (control analysis as ensemble guess?).
- Check that this does not significantly degrade the ensemble.
- Experiments with different ensemble set-ups could be carried out here e.g. members vs resolution, members per LBC realisation, etc.
- Decide on final configuration (resolution etc), with the option to fall back to the downscaler approach.
- Run the system for two test periods of two months (winter and summer 2008?)
- For production, run the deterministic 4DVAR several years ahead of En4DVAR to create a large archive of analysis increments.
- Begin the production run.

B (Static) Background Error Covariance

Since October 2014 the Met Office has used a parametrisation of the static background error covariances using the Covariances and VAR Transforms (CVT) package. The parametrisation was generated using ensemble differences from MOGREPS with 44 members at N400. CVT can be used to generate background error covariances for regional or global domains and therefore is compatible with any of the options listed in Table 3, Inverarity and Wlasak (2014b). However it is not portable to ECMWF without additional coding work, Inverarity and Wlasak (2014a).

Although the current background error covariances will be useful for the recent past, parametrisations of static background covariances may need to be generated for earlier periods. The characterisation of the background error statistics is expected to have changed dramatically as observation density has increased. However it should be noted that ERA-Interim, which covers a similar period to this project, used a single background covariance throughout, derived from an ensemble of 4DVAR assimilations Dee *et al.* (2011).

C Other System Aspects

C.1 Elements Files

Within the VAR/OPS systems, these files contain lists of observation types to be retrieved and processed. There is one elements file for each observation subtype, see Table 4, containing a list of data and meta-data required to process the observations. A single set of elements files will be used throughout the run, based on those used for EURO4M, but with additional files for those observations new for the UERRA project.

C.2 OPS Background Error

The OPS uses a (global) coarse background error estimate to perform quality control on the observations. Operationally this is calculated every cycle by subtracting the analysis fields from the six hour forecast fields. For the EURO4M project a fixed background error estimate was used - a mean over 240 days of operations - since no global reanalysis was available. If run, MO-G will produce background error estimates on every cycle. If MO-G is not run then a mean of operational data can be used since it is well known that the quality control decisions are insensitive to variations in this background error estimate.

C.3 Scatwind, Sonde, RTTOV & GPSRO Coefficients

The coefficient files for scatwind, sonde, RTTOV and GPSRO contain information for processing the observations. These should be fixed throughout production, but some work is needed to include older observation types.

C.4 Ground GPS biases

These should be fixed throughout production

C.5 Satellite Radiance Biases

Satellite radiance biases are likely to change over the production period. For EURO4M, which covered two years, a pre-production run was carried out which processed satellite radiances, but did not assimilate them. The accumulated statistics were then used to derive biases Renshaw *et al.* (2014). For UERRA, if MO-G is run biases can be calculated during the assimilation via the new variational bias correction tool VarBc Lorenc (2012). If MO-G is not run, it is hoped that a regional version of VarBc can be applied to data from MO-R. Bias correction data from ERA-Interim will also be of use for highlighting sudden shifts in bias.

C.6 Satwind namelists

These provide satellite wind error profiles. The latest operational version should suffice throughout production.

C.7 Surface Boundary

C.7.1 Land use

The land sea mask will be fixed throughout the run and will be appropriate to the global and regional grids.

In operational NWP, land use is assumed not to change, which is sufficient for the relatively short periods covered. This was also the case for the Met Office EURO4M reanalysis. For the UERRA project it will be necessary to vary land use over the forty year period. This could be done using the History Database of the Global Environment (HYDE), Klein Goldewijk *et al.* (2011), or similar land use database.

C.7.2 Land analysis

EURO4M and operational LAMs use reconfigured global fields of soil moisture, temperature and snow cover. The global fields come from a land surface analysis (using SURF). These fields are not available for the production period. If a global system (MO-G) is run, it will include SURF and the resulting analyses will be used by the regional systems MO-R and MO-RE. If an external system is used in place of MO-G it may also provide background fields to drive SURF. Alternatively a regional version of SURF is planned for March 2015 which should be available before the production period.

SURF requires screen-level observations (available throughout) and advanced scatterometer satellite data (ASCAT from 2006). Global SURF also uses the National Environmental Satellite Data and Information Service (NESDIS) snow and ice bulletins. NESDIS bulletins are available daily at 25km resolution from 1997 and weekly at 190km prior to this Ramsay (1998).

Perturbed land analyses are available for use with different ensemble members by running SURF in ensemble mode.

C.7.3 Oceans

Operationally and for EURO4M, SSTs are provided by the Operational Sea Surface Temperature and Sea Ice Analysis (OSTIA, Donlon *et al.* (2012)) at 6km resolution, but are only available from 1985. Although MOGREPS includes a scheme to perturb SSTs from OSTIA for each ensemble member, Tennant and Beare (2014), a better alternative is to use the Hadley Centre's ice and sea surface temperatures - version 2 (HadISST2, Rayner *et al.* (2006)). Although these fields are at 30km resolution, they are available throughout the production period and include an ensemble to represent uncertainty in this forcing. HadISST2 is used in ERA-20C, Dee *et al.* (2013).

C.8 UM Spectral Radiances

The UERRA system will use standard spectral radiance files appropriate to the dynamical core.

C.9 Carbon Dioxide

A constant concentration of carbon dioxide in the atmosphere is assumed for operational NWP. This was also appropriate for the Met Office EURO4M reanalysis since it covered a relatively brief period. However, since carbon concentration varies between 1978 and 2017, a scheme to vary it may be appropriate for the UERRA reanalyses. This could follow the Hadley Centre Earth System model, HadGEM2-ES, Jones *et al.* (2011), which represents the concentration of carbon dioxide via a mass mixing ratio which is constant in the three spatial dimensions and varies with time. Alternatively a more complex scheme could be used.

D Observations

The intended observations to assimilate are given in Tables 4, 5 and 6. Observations intended to use in producing the land surface analysis are given in 7. Some observations that will not be assimilated are given in Table 8. The cost of processing the observations is summarised in Table 4.

E Output Variables

Provisional output variables have been agreed between Deutscher Wetterdienst and the four UERRA producers, the University of Bonn, MeteoFrance, SMHI and the Met Office, Kaiser-Weiss *et al.* (2014).

Following this guidance, expected surface output fields are listed in Table 10, static fields in Table 11, pressure level fields in Table 12 and model level fields in Table 13.

Observation	Subtypes	Variables	Dates	Source	Status
Land SYNOP	Land synoptic observations (LNDSYN), Meteorological airfield reports (METARS), Mobile synoptic observations (MOBSYN), Austrailian point estimates of sea-level pressure (PAOBS), American surface bogus observations (BOGUS)	Surface pressure, temperature, humidity, snow depth, wind	1978-2017	ECMWF	Worked in EURO4M
SYNOP cloud	Land synoptic observations (LNDSYN), Ship synoptic observations (SHPSYN)	cloud	1978-2017	MetDB	Worked in EURO4M, not available at ECMWF
E-Obs	E-Obs	precipitation accumulations	1978-2017	ECMWF	postponed
SHIP	Ship synoptic observations (SHPSYN)	Surface pressure, wind, temperature, humidity	1978-2017	ECMWF	Worked in EURO4M
Buoy	Buoy	Surface pressure, wind, temperature	1979-2017	ECMWF	Worked in EURO4M
Sondes	Radiosondes (TEMP), Wind profilers (WINPRO), Dropsondes (DROPSOND), Wind only sondes (PILOT)	Upper-air wind, temperature, humidity	1978-2017	MetDB	Worked in EURO4M, not decodeable at ECMWF
Aircraft	Aircraft Meteorological Data Relay (AMDARs), Air Report (AIREPs), Tropospheric Airborne Meteorological Data Reporting (TAMDAR), Met Office bogus observations (TCBOGUS), American upper air bogus observations (BOGUS)	Flight-level temperature, wind	1978-2017	ECMWF	Worked in EURO4M
AIRS	Advanced Infared Sounder (AIRS) Local (AIRSL), Warmest Field of View (AIRSWF)	AIRS AIRS AIRS	2003-2017	ECMWF	Worked in EURO4M
ATOVS	Advanced Microwave Sounding Unit-B (AMSUB) Global Operational Vertical Sounder (ATOVSG) Local Operational Vertical Sounder (ATOVSL)	HIRS/AMSU radiances	1998-2017	ECMWF	Worked in EURO4M

Table 4: List of observations (Part 1 of 3).

Observation	Subtypes	Variables	Dates	Source	Status
GPSRO	GPSRO	GPSRO	2006-2017	ECMWF	Worked in EURO4M, but advice needed
Ground GPS	Integrated Water vapour (GPSIWV)	Ground GPS	1999-2017	MetDB	Worked in EURO4M, reprocessed dataset needed for UERRA period
IASI	Global (IASIG) Local (IASIL)	IASI	2007-2017	ECMWF	Worked in EURO4M
satwinds/AMVs	ESA Cloud Motion Winds (ESACMW), ESA High Resolution Wave mode (ESAHRWVW), Geostationary Operational Environmental Satellites (GOESBUFR), Moderate-resolution Imaging Spectroradiometer (MODIS), Meteosat Second Generation satellite winds (MSGWINDS), Satellite Observations (SATOB)	wind wind wind wind wind	1988-2017	MetDB	Worked in EURO4M, not decodable at ECMWF
scatwinds	SeaWinds, WindSat, Advanced Scatterometer (ASCAT), High Resolution Advanced Scatterometer (ASCATHR), ESA High Resolution Wave mode (ESAHRWVW), ESA Scatterometer (ESAUWI)	wind	1992-2017	MetDB	Worked in EURO4M, development needed for UERRA period

Table 5: List of observations (Part 2 of 3).

Observation	Subtypes	Variables	Dates	Source	Status
SEVIRIclear	Meteosat Second Generation clear sky radiances (MSGCSR), Meteosat Second Generation radiances (MSGRAD)	clear sky	1982-2017	ECMWF	Worked in EURO4M
SSMIS	Special Sensor Microwave	Total column water vapour, ocean wind speed	2009-2017	ECMWF operationally	Worked in operations
TOVS	Operational Vertical Sounder	HIRS/MSU radiances	1979-2002	ECMWF	Development needed

Table 6: List of observations (Part 3 of 3).

Observation	Variables	Dates	Source	Status
ASCAT	ASCAT	2006-2017	ECMWF	Worked in EURO4M
Land SYNOP	Screen level temperature, humidity	1978-2017	ECMWF	Worked in EURO4M

Table 7: List of observations expected to be used for soil moisture.

Observation	Variables	Dates
AMSRE	AMSRE	2009-2017
TOMS and SBUV	Ozone	1979-2017
GeoCloud	cloud	2007-2017

Table 8: Some observations that will not be assimilated into UERRA-MO.

Observation	OPS Component	Global		EURO4M	
		Eq	Cost/PEs	Eq	Cost/PEs
Surface	OPS_surface	1 x 57	57	1 x 33	33
E-Obs	OPS_precip			1 x 10	10
Sondes, Aircraft	OPS_aircraftsonde	2 x 98	196	2 x 51	102
AIRS	OPS_AIRS	32 x 228	7296	6 x 301	1806
(A)TOVS	OPS_ATOVS	32 x 163	5216	4 x 133	532
GPSRO	OPS_GPSRO	1 x 117	117	1 x 21	21
Ground GPS	OPS_groundGPS	1 x 60	60	2 x 30	60
IASI	OPS_iasi	8 x 616	4928	5 x 215	1075
satwinds/AMVs	OPS_sat	2 x 147	294	2 x 19	38
scatwinds	OPS_scat	1 x 102	102	1 x 8	8
SEVIRIclear	OPS_SEVIRI	2 x 230	460	5 x 86	430
SSM/I(S)	OPS_SSMIS	8 x 122	976	1 x 56	56
Total			19702		4171

Table 9: OPS components cost - processing for assimilation at EU-22 (EURO4M) and N216 (Global).

No.	Stash	Grib	Variable	W	F	B	S
1.	3236	121/0/0/0/2	Max of Temperature at 1.5m (mx2t6)****	V		y	y
2.	3236	122/0/0/0/3	Min of Temperature at 1.5m (mn2t6)****	V		y	y
3.	3225	165/0/2/2/0	10m Wind U-component (10u)	V	y	y	y
4.	3226	166/0/2/3/0	10m Wind V-component (10v)	V	y	y	y
5.	3463	49/———	Wind Gust (10fg)	V	y		
6.	5201+ 5202	143/0/1/10/0	Convective Precipitation Amount (cp)	V*	y	y	y
7.	5202	239/———	Convective Snow Amount (csf)	V	y	y	y
8.	4201+ 4202	3062/0/1/54/1	LS Precipitation Amount (lsp)	V*		y	y
9.	4202	240/———	LS Snow Amount (lsf)	V			
10.	—-	141/———	Water Equivalent of accumulated snow depth (sd)	V	y		
11.	9217	———-	Total Cloud Amount Max/Rand Overlap	V	y	y	y
12.	16258**	137/———	Total Column Water Vapour (tcwv)	V		y	
13.	16202	156/0/3/5	Geopotential Height (gh)	V	y		y
14.	16222	151/0/3/0	PMSL (msl)	V	y	y	y
15.	409	134/0/3/0	Surface Pressure (sp)	V	y	y	y
16.	5226	228/0/1/52	Total Precipitation Amount (tp)	V	y	y	y
17.	5226	228/0/1/52	Total Precipitation Amount 24hr (tp)	V	y	y	y
18.	—-	178/———	Net SW Radiation Flux -TOA (tsr)*****	V***			
19.	3250	129056/———	Dewpoint at 1.5m (mn2d24grd)	V		y	y
20.	1207	212/———	Incoming SW Radiation Flux -TOA (tisr)*****	V***			y
-	—-	189/0/6/24/1	Sunshine Duration (sund)	N			
21.	3236	167/0/0/0	Temperature at 1.5m (2t)	S	y	y	y
22.	24	235/0/0/17	Surface Temperature (skt)	S	y		
23.	3234	147/0/0/10	Surface Latent Heat Flux (slhf)	S	y	y	y
24.	3217	146/0/0/11	Surface Heat Flux (sshf)	S	y	y	y
25.	31	31/10/2/0	Fraction of Sea Ice In Sea (ci)	S			
26.	3238	139/———	Deep Soil Temperature - 1 (slt1)	S	y	y	y
27.	3238	170/———	Deep Soil Temperature - 2 (slt2)	S	y	y	y
28.	3238	183/———	Deep Soil Temperature - 3 (slt3)	S	y		y
29.	3238	236/———	Deep Soil Temperature - 4 (slt4)	S			
30.	8223	140/———	Soil Moisture Content - 1 (swl1)	S	y		
31.	8223	171/———	Soil Moisture Content - 2 (swl2)	S	y		
32.	8223	184/———	Soil Moisture Content - 3 (swl3)	S	y		
33.	8223	237/———	Soil Moisture Content - 4 (swl4)	S	y		
34	3247	3247	Visibility at 1.5m	S			
35	3245	3247	Relative Humidity at 1.5m	S			
36	3237	3247	Specific Humidity at 1.5m	S	y	y	y
37.	2204	———-	Total Cloud Amount in LW Radiation	R			
38.	1210	———-	Clear-Sky(II) Down Surface SW Flux	R			y
39.	1211	———-	Clear-Sky(II) Up Surface SW Flux	R			y
40.	1201	176/0/4/9/1	Net Surface SW Flux (ssr)*****	R	y	y	y
41.	1235	———-	Total Downward Surface SW Flux	R			
42.	9216	164/———	Total Cloud Amount Rand Overlap (tcc)	U			

Table 10: Expected surface output variables. F, B and S indicate fields that are output by the models of MeteoFrance, the University of Bonn and SMHI, respectively. *Total precipitation is required, but we can't directly output this. **This is a non-standard STASH. ***TOA Net Solar (SW) is required, but we can't directly output this. ****Grib parameter refers to six hour period. *****ECMWF version is an accumulation and not a flux. W indicates why the field is included in the output: V - validation, N - wanted for validation, but impossible to produce, S - standard output parameter, R - radiation fields and U - useful. Bracketed part of variable indicates short variable name at ECMWF.

No.	Stash	Grib	Variable	Why Included	F	B	S
1.	30	172/2/0/0	Land Mask (lsm)	Validation	y	y	y
2.	26	173/2/0/1	Roughness Length (sr)	Validation	y	y	y

Table 11: Expected static output variables. F, B and S indicate fields that are output by the models of MeteoFrance, the University of Bonn and SMHI, respectively.

No.	Stash	Variable	Why Included	F	B	S
1.	16203	Temperature on pressure levels	Validation	y	y	y
2.	15243	U wind on pressure levels	Validation	y	y	y
3.	15244	V wind on pressure levels	Validation	y	y	y
4.	16256	Relative Humidity wrt water	Validation	y		y
5.	16202	Geopotential Height on pressure levels	Validation	y		y

Table 12: Expected pressure level output variables. F, B and S indicate fields that are output by the models of MeteoFrance, the University of Bonn and SMHI, respectively. 7 levels - 1000hPa, 850hPa, 700hPa, 500hPa, 300hPa, 200hPa, 100hPa

No.	Stash	Variable	Why Included	F	B	S
1.	2	U component of wind	Std Param	y	y	y
2.	3	V component of wind	Std Param	y	y	y
3.	4	Potential Temperature	Std Param			
4.	10	Specific Humidity	Std Param	y	y	y
5.	12	Cloud ice content QCF	Std Param	y		y
6.	254	Cloud water content QCL	Std Param	y	y	y
7.	408	Pressure (theta levels)	Std Param	y	y	

Table 13: Expected model level output variables. F, B and S indicate fields that are output by the models of MeteoFrance, the University of Bonn and SMHI, respectively. 5 levels (public) 71 levels (internal).

F hybrid 4DVAR

The VAR assimilation scheme aims to produce an analysis, $\mathbf{x_a}$, which is the most likely state of the atmosphere given the observations, $\mathbf{y}$, and the background, $\mathbf{x_b}$, i.e. the analysis is the state, $\mathbf{x}$, which maximises $P(A|O\cup B)$. Assuming that the observation and background errors are independent and applying Bayes theorem

$$P(A|O \cup B) = \frac{P(O|A)P(B|A)P(A)}{P(B \cup O)} \tag{1}$$

Assuming that $P(A)$ is constant (i.e. each analysis is equally likely) then

$$P(A|O \cup B) \propto P(O|A)P(B|A) \tag{2}$$

The two probabilities on the right hand side are assumed to be Gaussian then

$$\begin{aligned} P(O|A) &= \frac{1}{\sqrt{2\pi}} P_o^{-1/2} e^{-(\mathbf{x}-\mathbf{y})^T P_o^{-1}(\mathbf{x}-\mathbf{y})} \quad \text{and} & (3) \\ P(B|A) &= \frac{1}{\sqrt{2\pi}} P_b^{-1/2} e^{-(\mathbf{x}-\mathbf{x_b})^T P_b^{-1}(\mathbf{x}-\mathbf{x_b})} \Rightarrow & (4) \\ P(A|O \cup B) &\propto e^{-(\mathbf{x}-\mathbf{x_b})^T P_b^{-1}(\mathbf{x}-\mathbf{x_b}) - (\mathbf{x}-\mathbf{y})^T P_o^{-1}(\mathbf{x}-\mathbf{y})} & (5) \end{aligned}$$

where the error covariances for observations and background are P_o and P_b, respectively and the current state, background state and observations are given by $\mathbf{x}$, $\mathbf{x_b}$ and $\mathbf{y}$, respectively. Since $\mathbf{x_a}$ maximises $P(A|O \cup B)$ it will also minimise $-\ln P(A|O \cup B)$, i. e.

$$J(\mathbf{x}) = (\mathbf{x} - \mathbf{x_b})^T P_b^{-1}(\mathbf{x} - \mathbf{x_b}) + (\mathbf{x} - \mathbf{y})^T P_o^{-1}(\mathbf{x} - \mathbf{y}) \tag{6}$$

which is a primitive version of the VAR cost function. Minimising this function leads to the most likely state of the atmosphere. The cost function can be used for 3DVAR, which assumes that all observations within the assimilation window occur at concurrently, and 4DVAR, which uses a forecast model to take observation time into account. The Met Office static 3DVAR cost function may be written as

$$J(\mathbf{x}') = \frac{1}{2}\mathbf{x}'^T B^{-1}\mathbf{x}' + \frac{1}{2}\left(\mathbf{y_b} + \mathbf{H}\mathbf{x}' - \mathbf{y^o}\right)^T R^{-1}\left(\mathbf{y_b} + \mathbf{H}\mathbf{x}' - \mathbf{y^o}\right) + J_c \tag{7}$$

where $\mathbf{x}' = \mathbf{x} - \mathbf{x_b}$ is the increment to the background, B is the estimated background error covariance, $\mathbf{y_b}$ is the background in observation space and $\mathbf{H}$ is a tangent linear approximation to the observation operator, which transforms from model space into observation space. The approximation to the observations error covariance matrix is represented by R and the term J_c is a digital filter which penalises high frequency behaviour which is not representable by the model.

For efficient minimisation, the cost function is transformed into a 'control' space defined by independent model variables. The defining expression for the transform is $\mathbf{x}' = \mathbf{U}\mathbf{v}$ such that $\mathbf{U}\mathbf{U^T} = \mathbf{B}$.

$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}\left(\mathbf{y_b} + \mathbf{H}\mathbf{U}\mathbf{v} - \mathbf{y^o}\right)^T R^{-1}\left(\mathbf{y_b} + \mathbf{H}\mathbf{U}\mathbf{v} - \mathbf{y^o}\right)^T + J_c \tag{8}$$

Similarly the Met Office static 4DVAR cost function may be written as

$$J(\mathbf{x}') = \frac{1}{2}\mathbf{x}'^T B^{-1}\mathbf{x}' + \frac{1}{2}\left(\mathbf{y_b} + \mathbf{H}\mathbf{M}\mathbf{x}' - \mathbf{y^o}\right)^T R^{-1}\left(\mathbf{y_b} + \mathbf{H}\mathbf{M}\mathbf{x}' - \mathbf{y^o}\right)^T + J_c \tag{9}$$

where $\mathbf{M}$ is a tangent linear approximation to the forecast model, which forecasts the model perturbation to the observation time. Again the function is minimised via a transformation into control space.

$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}\left(\mathbf{y_b} + \mathbf{H}\mathbf{M}\mathbf{U}\mathbf{v} - \mathbf{y^o}\right)^T R^{-1}\left(\mathbf{y_b} + \mathbf{H}\mathbf{M}\mathbf{U}\mathbf{v} - \mathbf{y^o}\right)^T + J_c \tag{10}$$

For static 4DVAR the background error covariance, B, is constant. It is contains highly smoothed statistics generated by an ensemble covering a long period, see Section B. For hybrid 4DVAR the background error covariance is a weighted sum of this static covariance and a localised covariance matrix calculated on each cycle from an accompanying ensemble system.

As an aside, DA and ensemble systems are considered one-way coupled if either the DA analysis is used by the ensemble system or the ensemble's error modes are used by the DA system. If both types of coupling occur then the system is two-way coupled.

A normalised vector of ensemble error modes at the analysis time is given by

$$\mathbf{X^b} = \frac{1}{\sqrt{m-1}}\left[\delta\mathbf{x_i^b}\cdots\delta\mathbf{x_m^b}\right] \tag{11}$$

where m is the number of ensemble members, then

$$\mathbf{P_e^b} = \mathbf{X^b}\left(\mathbf{X^b}\right)^T \tag{12}$$

and

$$\mathbf{B_e} = \mathbf{C}\circ\mathbf{X^b}\left(\mathbf{X^b}\right)^T \tag{13}$$

where $\mathbf{C}$ is a localisation matrix applied elements-wise ($\circ$) to the raw ensemble to minimise noise. This is another method for estimating the true background error covariance, $\mathbf{P^b}$. This ensemble-derived estimate can be combined with the static covariance to produce hybrid 4DVAR.

The Met Office hybrid 4DVAR cost function may then be written as

$$J(\mathbf{x}') = \frac{1}{2}\mathbf{x}'^T\left(\beta_s^2\mathbf{B}+\beta_e^2\mathbf{B_e}\right)^{-1}\mathbf{x}' + \frac{1}{2}\left(\mathbf{y_b}+\mathbf{HMx}'-\mathbf{y^o}\right)^T R^{-1}\left(\mathbf{y_b}+\mathbf{HMx}'-\mathbf{y^o}\right)+J_c \tag{14}$$

where β_s and β_e are scalar weights.

G En4DVAR

En4DVAR features an ensemble of assimilations which minimise similar cost functions to (14),

$$J_i(\mathbf{x_i'}) = \frac{1}{2}\mathbf{x_i'}^T\mathbf{B}^{-1}\mathbf{x_i'} + \frac{1}{2}\left(\mathbf{y_{bi}}+\mathbf{HMx_i'}-\mathbf{y_i^o}\right)^T R^{-1}\left(\mathbf{y_{b_i}}+\mathbf{HMx_i'}-\mathbf{y_i^o}\right)+J_c \tag{15}$$

where $\mathbf{x_i'}$ is the analysis increment for ensemble member i, $\mathbf{y_{bi}}$ is the background from the same member in observation space and $\mathbf{y_i^o}$ are perturbed observations such that $\mathbf{y_i^o} = \mathbf{y^o} + \epsilon_i$ where ϵ_i is sampled from an appropriate observation error distribution.

H 4DEnVAR

This scheme is similar to 4DVAR except that instead of using a forecast model to propagate the model state to the observation times, a dynamically consistent set of 3DVARs are solved at each time-step. The analysis increment is a linear combination of ensemble perturbations:

$$\mathbf{x}'_t = \frac{1}{\sqrt{m-1}}\sum_{i=1}^{m}\delta\mathbf{x_i^{bt}}\circ\alpha_\mathbf{i} \tag{16}$$

for each timestep, t, within the assimilation window. The ensemble weights, $\alpha_\mathbf{i}$, vary spatially and by variable, but not with time. Since each ensemble state is a valid, physically consistent atmospheric state, a linear combination will also be valid and physically consistent, but, to ensure the weights vary smoothly, a new term is added to the cost function.

$$J_\alpha = \frac{1}{2}\sum_{i=1}^{m} \alpha_{\mathbf{i}}^{\mathbf{T}} \mathbf{C}^{-1} \alpha_{\mathbf{i}} \tag{17}$$

This term has its own control space defined via $\alpha_{\mathbf{i}} = \mathbf{U}^\alpha \mathbf{v}_{\mathbf{i}}^\alpha$, $\mathbf{U}^\alpha \left(\mathbf{U}^\alpha\right)^T = \mathbf{C}$. These additional control variables are included in the main control vector, $\mathbf{v}$. The cost function is given by

$$\begin{aligned} J(\mathbf{x_0'} \cdots \mathbf{x_T'}) &= \frac{1}{2}\sum_{i=1}^{m} \alpha_{\mathbf{i}}^{\mathbf{T}} \mathbf{C}^{-1} \alpha_{\mathbf{i}} \\ &+ \frac{1}{2}\sum_{t=0}^{T} \mathbf{x_t'}^T \left(\beta_s^2 \mathbf{B} + \beta_e^2 \mathbf{B_{te}}\right)^{-1} \mathbf{x_t'} + \frac{1}{2}\sum_{t=0}^{T} \left(\mathbf{y_b^t} + \mathbf{H}\mathbf{x_t'} - \mathbf{y^{ot}}\right)^T R^{-1} \left(\mathbf{y_b^t} + \mathbf{H}\mathbf{x_t'} - \mathbf{y^{ot}}\right) + J_c \end{aligned} \tag{18}$$

And in control space

$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\mathbf{v} + \frac{1}{2}\sum_{t=0}^{T} \left(\mathbf{y_b^t} + \mathbf{HUv} - \mathbf{y^{ot}}\right)^T R^{-1} \left(\mathbf{y_b} + \mathbf{HUv} - \mathbf{y^{ot}}\right) + J_c \tag{19}$$

Since this method does not require a perturbation forecast model, $\mathbf{M}$, the cost is reduced and the system can be more efficiently shared across multiple processors.

I En4DEnVAR

An ensemble of 4DEnVAR can be achieved by replacing the deterministic background in observation space, $\mathbf{y_b}$, for each member with a background from a previous cycle ensemble member i.e. $\mathbf{y_{bi}}$. For each ensemble member there is then a slightly different cost function

$$\begin{aligned} J(\mathbf{x_{0j}'} \cdots \mathbf{x_{Tj}'}) &= \frac{1}{2}\sum_{i=1}^{m} \alpha_{\mathbf{i}}^{\mathbf{T}} \mathbf{C}^{-1} \alpha_{\mathbf{i}} \\ + \frac{1}{2}\sum_{t=0}^{T} \mathbf{x_{tj}'}^T \left(\beta_s^2 \mathbf{B} + \beta_e^2 \mathbf{B_{te}}\right)^{-1} \mathbf{x_{tj}'} &+ \frac{1}{2}\sum_{t=0}^{T} \left(\mathbf{y_{bj}^t} + \mathbf{H}\mathbf{x_{tj}'} - \mathbf{y^{ot}}\right)^T R^{-1} \left(\mathbf{y_{bj}^t} + \mathbf{H}\mathbf{x_{tj}'} - \mathbf{y^{ot}}\right) + J_c \end{aligned} \tag{20}$$

And in control space

$$J(\mathbf{v_j}) = \frac{1}{2}\mathbf{v_j}^T\mathbf{v_j} + \frac{1}{2}\sum_{t=0}^{T} \left(\mathbf{y_{bj}^t} + \mathbf{HUv_j} - \mathbf{y^{ot}}\right)^T R^{-1} \left(\mathbf{y_{bj}^t} + \mathbf{HUv_j} - \mathbf{y^{ot}}\right) + J_c. \tag{21}$$

This leads to an ensemble whose spread will collapse because it does not represent the uncertainty in the observations. This can be alleviated by relaxing to the prior spread, Flowerdew and Bowler (2013) or by perturbing the observations, Burgers *et al.* (1998), as in Section J.1.1.

J ETKF

J.1 EnKF

The ETKF is an efficient version of the ensemble Kalman filter which is defined as

$$
\begin{aligned}
\bar{\mathbf{x}}^{\mathbf{a}} &= \bar{\mathbf{x}}^{\mathbf{b}} + \mathbf{K}\left(\mathbf{y}^{\mathbf{o}} - H(\bar{\mathbf{x}}^{\mathbf{b}})\right) \qquad \text{where} && (22)\\
\mathbf{K} &= \mathbf{P}^{\mathbf{b}}\mathbf{H}^{\mathbf{T}}\left(\mathbf{H}\mathbf{P}^{\mathbf{b}}\mathbf{H}^{\mathbf{T}} + \mathbf{R}\right)^{-1} \qquad \text{and} && (23)\\
\mathbf{P}^{\mathbf{a}} &= \mathbf{P}^{\mathbf{b}} + \mathbf{K}\left(\mathbf{R} - \mathbf{H}\mathbf{P}^{\mathbf{b}}\mathbf{H}^{T}\right)\mathbf{K}^{T} && (24)\\
&= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{P}^{\mathbf{b}}\left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)^{T} + \mathbf{K}\mathbf{R}\mathbf{K}^{T} && (25)\\
&= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{P}^{\mathbf{b}} - \left(\mathbf{P}^{\mathbf{b}}\mathbf{H}^{T} - \mathbf{K}\left(\mathbf{H}\mathbf{P}\mathbf{H}^{T} + \mathbf{R}\right)\right)\mathbf{K}^{T} && (26)\\
&= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{P}^{\mathbf{b}} && (27)
\end{aligned}
$$

To maintain the $\mathbf{KRK}^T$ term in the analysis covariance given in (25) it is necessary to perturb the observations, Burgers *et al.* (1998), i.e. $y_i^o = y^o + \epsilon_i$ such that $\epsilon\, \tilde{}\, N(O, R)$ else

$$
\mathbf{P}^{\mathbf{a}} = \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{P}^{\mathbf{b}}\left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)^{T} \qquad (28)
$$

J.1.1 DEnKF

An alternate method to maintain the spread takes a Taylor approximation approach:

$$
\begin{aligned}
\mathbf{P}^{\mathbf{a}} &= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{P}^{\mathbf{b}} \Rightarrow && (29)\\
\mathbf{X}^{\mathbf{a}}\left(\mathbf{X}^{\mathbf{a}}\right)^{T} &= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{X}^{\mathbf{b}}\left(\mathbf{X}^{\mathbf{b}}\right)^{T} \Rightarrow && (30)\\
\mathbf{X}^{\mathbf{a}} &= \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)^{1/2}\mathbf{X}^{\mathbf{b}} && (31)\\
\mathbf{X}^{\mathbf{a}} &\approx \left(\mathbf{I} - \frac{1}{2}\mathbf{K}\mathbf{H}\right)\mathbf{X}^{\mathbf{b}} && (32)
\end{aligned}
$$

This is equivalent to relaxing the analysis to the background:

$$
\begin{aligned}
\mathbf{X}^{\mathbf{a}} &\approx \left(\mathbf{I} - \frac{1}{2}\mathbf{K}\mathbf{H}\right)\mathbf{X}^{\mathbf{b}} && (33)\\
&= \frac{1}{2}\left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\mathbf{X}^{\mathbf{b}} + \frac{1}{2}\mathbf{X}^{\mathbf{b}} && (34)
\end{aligned}
$$

This is called the deterministic ensemble Kalman filter or DEnKF.

J.1.2 Serial Inflation

Alternately, if the observations are processed serially such that $\mathbf{HP^bH^T}$ and $\mathbf{R}$ are scalars, we can inflate the Kalman gain matrix by a scalar, α, to account for the lack of spread i.e.

$$\left(\mathbf{I}-\alpha\mathbf{KH}\right)\mathbf{P^b}\left(\mathbf{I}-\alpha\mathbf{KH}\right)^T = \left(\mathbf{I}-\mathbf{KH}\right)\mathbf{P^b} \tag{35}$$

$$-\alpha\mathbf{KHP^b}-\alpha\mathbf{P^bH^TK^T}+\alpha^2\mathbf{KHP^bH^TK^T} = -\mathbf{KHP^b} \tag{36}$$

$$-\alpha\mathbf{KK^T}(\cdots)-\alpha\mathbf{KK^T}(\cdots)+\alpha^2\mathbf{KK^THP^bH^T} = -\mathbf{KK^T}(\cdots) \tag{37}$$

$$\frac{\mathbf{HP^bH^T}}{\mathbf{HP^bH^T}+\mathbf{R}}\alpha^2-2\alpha+1 = 0 \tag{38}$$

$$\text{let}\quad \beta = \frac{1}{\alpha}\Rightarrow \tag{39}$$

$$\frac{\mathbf{HP^bH^T}}{\mathbf{HP^bH^T}+\mathbf{R}}-2\beta+\beta^2 = 0\Rightarrow \tag{40}$$

$$\beta = 1+\sqrt{1-\frac{\mathbf{HP^bH^T}}{\mathbf{HP^bH^T}+\mathbf{R}}} \tag{41}$$

$$\alpha = \left(1+\sqrt{\frac{\mathbf{R}}{\mathbf{HP^bH^T}+\mathbf{R}}}\right)^{-1} \tag{42}$$

J.1.3 ETKF

The extended transform Kalman filter follows the standard EnKF method for updating the ensemble mean, but departs from this scheme in updating individual members. The ETKF is so called because it relies on a linear transform from the ensemble member background perturbations to the analysis perturbations. This is an efficient formulation of the Ensemble Kalman filter and relies on the assumption that the analysis perturbations are linear combinations of background perturbations, i.e. we assume

$$\mathbf{X^a} = \mathbf{X^bT}\qquad\text{then} \tag{43}$$

$$\mathbf{X^bTT^T}\left(\mathbf{X^b}\right)^T = \mathbf{X^b}\left(\mathbf{X^b}\right)^T-\mathbf{X^b}\left(\mathbf{X^b}\right)^T\mathbf{H^T}\left(\mathbf{HX^b}\left(\mathbf{X^b}\right)^\mathbf{T}\mathbf{H^T}+\mathbf{R}\right)^{-1}\mathbf{HX^b}\left(\mathbf{X^b}\right)^T\Rightarrow \tag{44}$$

$$\mathbf{TT^T} = \mathbf{I}-\left(\mathbf{X^b}\right)^T\mathbf{H^T}\left(\mathbf{HX^b}\left(\mathbf{X^b}\right)^\mathbf{T}\mathbf{H^T}+\mathbf{R}\right)^{-1}\mathbf{HX^b}\Rightarrow \tag{45}$$

$$\mathbf{TT^T}\left(\mathbf{X^b}\right)^{-1}\mathbf{H^T}\left(\mathbf{HX^b}\left(\mathbf{X^b}\right)^\mathbf{T}\mathbf{H^T}+\mathbf{R}\right) = \left(\mathbf{X^b}\right)^{-1}\mathbf{H^T}\left(\mathbf{HX^b}\left(\mathbf{X^b}\right)^\mathbf{T}\mathbf{H^T}+\mathbf{R}\right)-\left(\mathbf{X^b}\right)^T\mathbf{H^T}\Rightarrow \tag{46}$$

$$\mathbf{TT^T}\left(\mathbf{X^b}\right)^{-1}\mathbf{H^THX^b}\left(\mathbf{X^b}\right)^T\mathbf{H^T}+\mathbf{TT^T}\left(\mathbf{X^b}\right)^{-1}\mathbf{H^TR} =$$

$$\left(\mathbf{X^b}\right)^{-1}\mathbf{H^THX^b}\left(\mathbf{X^b}\right)^\mathbf{T}\mathbf{H^T}+\left(\mathbf{X^b}\right)^{-1}\mathbf{H^TR}-\left(\mathbf{X^b}\right)^T\mathbf{H^T}\Rightarrow \tag{47}$$

$$\mathbf{TT^T}\left(\mathbf{X^b}\right)^T\mathbf{H^T}+\mathbf{TT^T}\left(\mathbf{X^b}\right)^{-1}\mathbf{H^TR} = \left(\mathbf{X^b}\right)^{-1}\mathbf{H^TR}\Rightarrow \tag{48}$$

$$\mathbf{TT^T}\left(\left(\mathbf{X^b}\right)^T\mathbf{H^TR^{-1}HX^b}+\mathbf{I}\right) = \mathbf{I}\Rightarrow \tag{49}$$

$$\mathbf{TT^T} = \left(\left(\mathbf{X^b}\right)^T\mathbf{H^TR^{-1}HX^b}+\mathbf{I}\right)^{-1} \tag{50}$$

The principal term on the RHS can be decomposed into matrices of its eigenvalues, $\mathbf{\Gamma}$ and eigenvectors $\mathbf{G}$, normalised such that $\mathbf{GG^T}=\mathbf{I}$.

$$\mathbf{G}\mathbf{\Gamma}\mathbf{G}^{\mathbf{T}} = \left(\mathbf{X}^{\mathrm{b}}\right)^{T}\mathbf{H}^{\mathbf{T}}\mathbf{R}^{-\mathbf{1}}\mathbf{H}\mathbf{X}^{\mathrm{b}} \Rightarrow \tag{51}$$

$$\mathbf{T}\mathbf{T}^{\mathbf{T}} = \left(\mathbf{G}\left(\mathbf{\Gamma}+\mathbf{I}\right)\mathbf{G}^{\mathbf{T}}\right)^{-1} \Rightarrow \tag{52}$$

$$\mathbf{T}\mathbf{T}^{\mathbf{T}} = \mathbf{G}\left(\mathbf{\Gamma}+\mathbf{I}\right)^{-1}\mathbf{G}^{\mathbf{T}} \Rightarrow \tag{53}$$

$$\mathbf{T} = \mathbf{G}\left(\mathbf{\Gamma}+\mathbf{I}\right)^{-1/2} \tag{54}$$

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