

Report no. 20/2008 Oceanography ISSN: 1503-8025 Oslo, September 10, 2008

Implementation of the SEIK assimilation scheme into MIPOM

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Number	Subject	Date	Classification	ISSN	
20/2008	Oceanography	September 10, 2008	🛛 Open	1503-8025	
		-	□ Restricted		
Title					
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Authors					
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Client(s)			Client reference		
Abstract					
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MIPOM, the current operational ocean model at met.no. The goal of implementing the SEIK algorithm was to improve the performance of the ocean forecast maximizing the computer efficiency of the data assimilation scheme. A twin experiment has been conducted to look at the impact of the SEIK scheme and to compare its performance with that of the current nudging assimilation method for the operational ocean forecast at met.no. A run with the ROMS model was used as the truth and simulated data were extracted from this run to the SEIK assimilation into MIPOM. Real satellite SST data from OSISAF have also been assimilated in a forecast mode setup. Both experiments show little impact using the global SEIK scheme. The localized SEIK assimilation however, meaning that only data within a limited region are taken into account for each grid point, yielded significant positive impact. The local SEIK also produced more noisy model fields than with no assimilation and global SEIK. We discuss various reasons for this and how it could be resolved.

Keywords

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data assimilation, ocean forecast

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1 Introduction

Data assimilation is a concept encompassing any method for combining observations of variables into numerical models. Various data assimilation techniques have been developed in order to make use of the observations in an optimal way. Data assimilation is today widely used both in atmoshperic and ocean predictions. However, for the ocean the observations are rather limited compared to the case for the atmosphere, and hence the data assimilation schemes applied in ocean models are generally less developed than for atmospheric models. Whereas most atmospheric systems use sophisticated statistical methods as e.g. 4D-Var, many ocean forecast systems still use more simple assimilation shcemes such as nudging and optimal interpolation.

The operational ocean forecast system at the Norwegian Meteorological Institute currently uses a simple data assimilation scheme called nudging. In this report we will describe an attempt of implementing a more statistically correct method in the forecast system. The forecast system consists of daily forecasts of ice and ocean parameters for the Arctic and Nordic seas. Satellite observations of sea surface temperature (SST) and sea ice concentration (SIC) provided by the OSISAF (Ocean and Sea Ice Application Facility) project are being assimilated into the coupled ice-ocean model using the nudging scheme described in Albretsen et al. (2005). Although this assimilation scheme significantly improves the forecast compared to a situation without any data assimilation, a more statistical correct method, yielding a multivariate analysis update from the data assimilation is expected to further improve these forecasts. The reason for this is that in a nudging scheme, only the assimilated variable is being corrected whereas all the other model variables are adjusted within the model itself. Moreover, errors in the observations are not taken into account in such a scheme which could yield unreal spurious effects in the model. In a multivariate assimilation scheme however, all the variables in a defined state vector is being updated at each analysis time, even if only one of the variables have observations. The other variables are updated according to an error covariance matrix, that gives an estimate of how the various model variables are cross-correlated. One could say that the best assimilation scheme is hence the one that best estimates the model error covariance matrix.

A multivariate scheme seems very attractive, but one has to keep in mind that it is also more expensive in computer power compared to simpler schemes such as nudging. The choice of the optimal assimilation scheme is therefore guided by two main factors: 1) it must yield improved forecasts, and 2) it must be sufficiently computer efficient with today's available computing power, allowing daily forecast runs with large scale ocean models. In this project we have implemented one type of multivariate scheme and compared it with the existing nudging.

There are two main families of multivariate assimilation schemes, variational methods and Kalman filter methods. In this report we will only describe Kalman filter methods. These algorithms are sequential, meaning that they only assimilate observations made in the past until the time of analysis. Kalman filter schemes have attracted increased interest during the last years since they provide a good utilization of the observations due to their dynamical approach to estimate the error covariance matrix of the estimated model state. To be able to handle the huge computational cost of the Kalman filter when applied to a large-scale ocean model, several approximating algorithms have been developed, such as the Ensemble Kalman Filter (EnKF, Evensen 1994, 2003), various square-root filters (Tippett et al. 2003), the Singular Evolutive Extended Kalman filter (SEEK, Pham 1998) and the Singular Evolutive Integrated Kalman filter (SEIK, Pham 1998). Nerger et al. (2005, 2006) showed that assimilation with the SEIK filter bears advantages over both the EnKF and the SEEK filters. Based on this study we have implemented SEIK into the MIPOM ocean model using the Parallel Data Assimilation Framework (PDAF) provided by L. Nerger. This ensures an optimal usage of the parallel computer processors.

In order to assess the impact of SEIK assimilation several experiments have been conducted. The first experiment used a simplified version of SEIK with a fixed error covariance matrix. For the full SEIK implementation a theoretical twin experiment has been set up for one of the MIPOM model domains. In this experiment, output fields from a different model run over the same region were used to simulate the observations to be assimilated into the ocean model. In addition to this experiment, real satellite data has also been assimilated into a simulated operational setup.

The report is organized in the following way: Section 2 describes the model system and configuration, followed by a presentation of the Kalman filter in 3, the SEIK assimilation scheme and the implementation of this in section 4. In section 5 the experience with fixed covariance matrix is presented. The experiments with the evolving error covariance are described in section 6 (theoretical twin experiment) and in section 7 (assimilation of real data). Finally, a discussion of the results and future challenges is given in section 8.

2 The ocean forecast model

The ocean model MI-POM (met.no's version of POM, Engedahl 1995,Engedahl 2001) is currently the operational forecast model at met.no. This is a version of the sigma coordinate model POM (Princeton Ocean Model, Blumberg 1987). The model uses 21 sigma levels, with increased resolution in the upper ocean. At the open boundaries a Flow Relaxation Scheme (Martinsen 1987) applies climatological data (see Martinsen 1992, Engedahl 1995), consisting of monthly means of sea surface elevation, currents, salinity and temperature. The model is also relaxed toward climatological salinity and temperature at depths greater than about 1000 m and to climatological sea surface salinity. The atmospheric forcing is provided by the operational model at the European Centre for Medium-Range Weather Forecasts (ECMWF). The ECMWF data are available every 6 hour with a resolution of approximately 1° by 1°, and then provided to the models by interpolating to the model grid.

3 The Kalman filter

The data assimilation problem amounts to finding an optimal estimate of the system state for a certain time interval, given a dynamical model and observations at some discrete times. Let us consider a physical system which is represented in discrete form by its true state \mathbf{x}^t of dimension *n*. Because the model only approximates the true physics of the system, \mathbf{x}^t is a random vector whose time propagation is given by the stochastic-dynamic time discretized

model equation

$$\mathbf{x}_{\mathbf{i}}^{\mathbf{t}} = M_{i,i-1}[\mathbf{x}_{\mathbf{i-1}}^{\mathbf{t}}] + \eta_i \tag{1}$$

Here $M_{i,i-1}$ is a, possibly non-linear, operator describing the state propagation between the two consecutive time steps i-1 and i. The vector η_i is the model error, which is assumed to be a stochastic perturbation with zero mean and covariance \mathbf{Q}_i . At discrete times $\{t_k\}$, observations are available as a vector \mathbf{y}_k^0 of dimension m_k . The true state \mathbf{x}^t at time $\{t_k\}$ is assumed to be related to the observation vector by the forward measurement operator H_k as

$$\mathbf{y}_{\mathbf{k}}^{\mathbf{o}} = H_k[\mathbf{x}_{\mathbf{k}}^{\mathbf{t}}] + \varepsilon_k \tag{2}$$

where $H_k[\mathbf{x}_k^t]$ describes what observations would be measured given the state \mathbf{x}_k^t . The vector ε_k is the observation error. It consists of the measurement error due to imperfect measurements and representation error caused, e.g., by the discretisation of the dynamics. ε_k is a random vector which is assumed to be of zero mean and covariance matrix \mathbf{R}_k and uncorrelated with the model error η_k .

The state sequence $\{\mathbf{x}_i^t\}$ is a stochastic process which is fully described by its probability density function (PDF) $p(\mathbf{x}_i^t)$. Accordingly, the filtering problem is solved by the conditional PDF $p(\mathbf{x}_i^t)|\mathbf{Y}_k^0$ of the true state given the observations $\mathbf{Y}_k^0 = \{\mathbf{y}_{0}^0, ..., \mathbf{y}_k^0\}$ up to time t_k . In practice it is not feasible to compute this density explicitly for large-scale models. Therefore one typically relies on the calculation of some statistical moments of the PDF such as the mean and the covariance matrix.

3.1 The Extended Kalman filter

For linear dynamic and measurement models, the KF is the minimum variance and maximum likelihood estimator if the initial PDF $p(\mathbf{x}_0^t)$ and the model error and observation error processes are Gaussian. The Extended Kalman filter (EKF) is a first-order extension to the KF to non-linear models. It is obtained by linearizing the dynamic and measurement operators around the most recent state estimate. A detailed approach to EKF is described in Jazwinski (1970).

4 The SEIK filter

The Singular Evolutive Interpolated Kalman (SEIK) filter (Pham et al., 1998) is a so-called error subspace Kalman filter (KF). As all KFs, it assimilates the available observations in a sequential manner. In a forecast phase the model is integrated up to the time when observations are available. A new model state is then computed during the analysis phase, on the basis of the predicted model state and the observations with weights computed from the error estimates of both the observations and the model state estimate. Subsequently a new forecast phase is performed. KF algorithms are of multivariate nature. In the case that observations of only one type of physical field are available, other fields of the numerical model are updated in the analysis phase via cross-correlations contained in the error covariance matrix.



Figure 1: A schematic view of a sequential ensemble-based assimilation method like SEIK. The error bars around the model integration curve represent the ensemble spread. The green point is the observed value which is compared with the ensemble mean (red point). The blue point is the analysis update.

For a classical KF and the extended KF (see Jazwinski, 1970) the requirements of storage and computation time are prohibitive due to the explicit treatment of the state error covariance matrix. One approach to handle this problem is to approximate the covariance matrix by a matrix of low rank, so that the analysis step operates in a low-dimensional subspace of the true error space. Another approach is to run an ensemble of several perturbed model states so that the ensemble spread represents the error covariance matrix. For a detailed review of the SEIK filter and a comparison with the other well-known Kalman filter methods Ensemble Kalman filter (EnKF) and the Singular Evolutive Extended filter (SEEK) see Nerger et al., (2005).

The SEIK filter can be interpreted as an ensemble-based Kalman filter using a preconditioned ensemble and a very efficient scheme to incorporate the observational information during the analysis phase of the filter. The algorithm computes the update of the state estimate in the estimated error sub-space which is represented by the ensemble of model states. Figure 1 gives a schematic view of the sequential method with ensembles. At each analysis time, an updates is carried out on the mean of all the ensemble model states. Then a new ensemble is being generated before the next model integration phase.

In the SEIK filter the low-rank approximation of the initial covariance matrix \vec{P}_0 is typically done by a singular value decomposition of \mathbf{P}_0 which only retains a small number r of leading eigen-values and corresponding eigenmodes. \mathbf{P}_0 is approximated in a decomposed form as $\mathbf{VUV}^{T} \simeq \mathbf{P}_0$ where \mathbf{U} is a diagonal rxr matrix holding the leading eigenvalues. The matrix \mathbf{V} holds in its r columns the corresponding eigenmodes. For the forecast phase a random ensemble $\{x^i, i = 1, ...N\}$ of minimum size $\{N = r + 1\}$ is generated which has the properties that it exactly represents the state estimate \mathbf{x}_0 and the approximated covariance matrix. This ensemble can be obtained by minimum order exact sampling (Pham 2001).

The KF analysis equations are applied to update the ensemble mean state and the matrix U. The equations are formulated to treat the covariance matrix in the decomposed form VUV^{T} . Subsequently to the analysis phase, the state ensemble is transformed in a re-initialization phase to represent the updated state estimate and the corresponding error covariance matrix.

A recent study by Nerger et al. (2006) showed that a localization method for the SEIK filter showed advantages over the standard global analysis. In the local SEIK, the state update is only computed on the basis of observations that lie within a specified distance from a grid point of the model domain. This increases the number of degrees of freedom for the analysis and can provide superior estimates of the model state. The region around each grid point is weighted so that the points closest to the grid point gets the largest weight. The weight decreases with the distance according to either an exponential decrease or by the 5th-order function described in Gaspari & Cohn (1999), equation 4.10.

4.1 Implementation of SEIK into MIPOM

The Parallel Data Assimilation Framework (PDAF) from Nerger (2005) was used for the implementation of SEIK into MIPOM. This framework allows one to run both ocean model and assimilation scheme on parallel computer nodes in order to maximize the computer efficiency. The MPI (message passing interface) parallelisation is used both for MIPOM and SEIK. The implementation has the following structure (as shown in Fig.2). First the ocean model and the SEIK filter are being initialized. An ensemble of model states is generated based on the initial error covariance matrix. Then there is the model integration phase with the model time loop and an ensemble loop around this so that the model integration is run as many times as there are ensemble members. The model integration runs in time until an observation is being read. Then all the ensemble members are gathered to a mean value which is compared with the observed value. This is the analysis update phase. The ensemble mean is being updated according to the observations and the SEIK gain matrix. This is followed by a resampling of the model ensembles using the updated covariance matrix, before a new model integration phase for each ensemble member begins.

The SEIK filter runs independently from the MIPOM model and the two can run on the same or different processors. There are three calls to the SEIK filter in the MIPOM main program. The first call is for the initialization which is outside the model time loop. Then for each ensemble member in the time loop there is a call to SEIK in order to get the model state from the actual ensemble member. In the end, before each observation is read, there is a call that transfers the current model state to SEIK for the analysis update.

In addition to this, an input file with assimilation parameters is read into the MIPOM main program. This input file contains the path to the files with the observations, the error on the observations (which until now is a constant number), the ensemble size and the size of the influence region for the observations. Ideally in and assimilation scheme, the model values should be interpolated to the location of the observation. Here however, we used the model value at the nearest grid point to the location of the observations both in the horizontal and in the vertical. This simplification was made since both the model and SEIK run on parallel processors. A full interpolation will require a much larger work in the parallel computing



Figure 2: A schematic view of the SEIK implementation into the ocean model

process.

5 Experiment with fixed covariance matrix

A first experiment was conducted with fixed error covariance matrix during the whole model run. Keeping this matrix fixed simplifies the implementation and the computer resources needed. This matrix was determined from a model run over three years by defining the mean and the deviations from the mean for each grid point and each variable in the state vector. Since the cross-correlation are season dependent, one matrix was defined for each month.

The MIPOM model area used in this experiment covers the North Sea, the Skagerrak and the Kattegat at 4km resolution. The assimilated data were SST-data from the OSISAF (Ocean and Sea Ice Facility) project (http://saf.met.no, Fig.11). These SST-fields were 10km half-daily composites, meaning a value from the ECMWf operational analysis were read in the regions where no satellite data were available, e.g. due ti clouds. The state vector in this experiment consisted of sea surface height, velocities U and V, salinity and temperature. The experiment was run for one month, July 2004.

The results from this experiment showed no improvement compared to the results from nudging of the same data set. Fig. 3 shows the SST field averaged root mean square error compared with the assimilated OSISAF data. An independent set of measurements from the cruise between Hirtshals in Denmark and Torungen in Norway¹(1) was used to validate the model results. Figure 4 shows the cross-section of temperature differences between the measurements and the model run on July 9 2004 for the SEIK assimilation and the nudging. These comparisons also show no improvements from the SEIK assimilation with fixed covariance matrix. The model run closest to the observations seems to be the one with nudging of SST-data. Since the fixed covariance matrix version of SEIK yielded no positive impact, a full SEIK with evolving error covariance were carried out as described below.

6 Twin experiment with full SEIK

A twin experiment was conducted to assess the impact of the MIPOM+SEIK assimilation scheme with an evolving error covariance matrix. Both the global and the local version of SEIK were run. The defined 'true' run was a model run with ROMS (Rutger Ocean Model System) for a one month period, July 2004. Model fields of sea surface temperature (SST) and 10 temperature profiles were extracted to simulate satellite SST data and typical in situ measurements. These simulated data were assimilated into a MIPOM model run every 12th hour during the one month period. The spinup time was 18 months and atmospheric forcing was obtained from the ECMWF for both ROMS and MIPOM run.

The MIPOM model area used in this experiment was the same as above, covering the North Sea, the Skagerrak and the Kattegat at a 4km resolution. The grid points are identical for MIPOM and ROMS in this setup. The state vector consisted of sea surface height, velocities

¹The Torungen-Hirtshals section data was kindly made available to us by the Institute of Marine Research, Flødevigen, Arendal.



Figure 3: The bias, mean and root mean square error between the OSISAF data and the averaged SST-field from the model run with no assimilation, nudging and SEIK with fixed covariance matrix.



Figure 4: Cross-sections of the distance Hirtshals to Torungen showing the difference in temperature between the observations and the model run without assimilation (left), with nudging (middle) and SEIK assimilation with fixed covariance matrix (right).

U and V, salinity and temperature. The initial error covariance matrix was the same as the one used in the experiment described above with a fixed error covariance.

The 5 following experiments were conducted with this model setup and assimilation with global and local SEIK: 1) No assimilation into MIPOM; 2) Global SEIK assimilation of SST, 3) as experiment 2 plus 10 temperature profiles, 4) Local SEIK assimilation of SST, 5) as experiment 4 pluss 10 temperature profiles. A sixth experiment was carried out where the SST data were simply nudged into the model.

Various sizes of ensemble and influence regions were tried out but the results described here were obtained with an ensemble size of 50 for both global and local SEIK. For the local SEIK the influence region was 80x80km² and the Gaspar and Cohn 5th order function (Gaspar & Cohn 1999) was chosen as weight function.

6.1 Results

A first validation by eye (Fig.5) already show that the assimilation had significant effect on the temperature fields. The figure displays the difference in the SST-fields ROMS - MIPOM without assimilation, and ROMS - LSEIK assimilation with local SEIK, just after the first analysis update. The assimilation has significantly reduced the difference between the two model runs.

The SST-fields after no assimilation, nudging, global SEIK and local SEIK are shown for comparison in Fig. 6. There are two things to notice in this figure, 1) The run using local SEIK is the one closest to the truth (ROMS) and 2) the local SEIK run also displays the most noisy field.

For a more statistical validation we look at the the root mean square error (rmse) between the ROMS and MIPOM values averaged over the model field. The rmse for SST, temperature



Figure 5: Difference in the SST-fields, *MIPOM – ROMS* (left) and *LSEIK – ROMS* (right) after the first analysis update for local SEIK assimilation.

at 20m and the salinity at 20m is shown as a function of time for all the experiments in Fig. 7, Fig. 8 and Fig. 9.

The displayed rmse values also indicate that the local SEIK assimilation performs better than global SEIK for the temperature fields. The errors are reduced and maintain small over time with local SEIK whereas for global SEIK the errors increase after a few assimilation steps. The global SEIK performs rather well for the first two analysis updates, but then seems to not take into account any observation anymore, hence increasing the rms with time. This feature with global SEIK is a well known problem since this filter type tend to underestimate the model error estimates (Nerger et al. 2005). A so-called forgetting factor ρ (Pham et al.1998), ($0 < \rho \le 1$) is often used to inflate the model errors. The forgetting factor increases the error estimates in the error covariance matrix and hence guarantees a minimum amount of estimated error. This can stabilize the filter process as SEIK, and other ensemble based Kalman filters, are known to underestimate variances. However, even though $\rho = 0.7$ was applied in this experiment it was clear that the algorithm still underestimated the variances.

For the salinity field the local SEIK has little impact, and towards the end of the run yields larger errors than with no assimilation or nudging (Fig. 9). This is mainly due to the large noise produced in the fields using local SEIK. Various sizes of the influence regions were tried out in order to avoid the noisy fields. Increasing the region gave less noisy fields and the variances became underestimated as for global SEIK. On the other hand, decreasing the size of region means that fewer observations are taken into account and the noise even increased in the field. Making the region smaller and smaller becomes similar to assimilating in situ-like observations. The experiment showed that assimilating 15 temperature profiles in addition to the SST data yields no improvement of the mean rmse. More detailed studies will be carried out to see how in situ observations can be assimilated with SEIK with a positive impact.

Finally, we note that the nudging technique performs well for the assimilated variable (SST) but gives poorer results for the other variables (such as temperature at 20m).

7 SEIK assimilation of OSISAF data in a simulated operational mode

The SEIK assimilation was also tested in a simulated operational mode to see if it could improve the forecast. An experiment with assimilation of real SST data was carried out for a MIPOM model region covering the Arctic oceans at 20km horizontal resolution. Operational mode here means that data are assimilated at -24h and -12h before analysis time (0h), prior to a forecast model run of 120 hours (see Fig. 10). This sequence was repeated for 20 days. The assimilated data were 12 hour mean SST fields provided by the OSISAF project.

For comparison, a forecast model run without any assimilation prior to each analysis was also carried out. The SST-data themselves were used for validation which is far from optimal since one should ideally validate against an independent data set. Nevertheless, this validation gives an indication of the effects of assimilation. The mean rmse between the model run and the SST data is shown as a function of forecast time in Fig. 12. The rmse plots indicate that there is a significant reduction in the rmse when data assimilation is applied. As in the previous experiment, the data assimilation also produced more noisy fields than with no assimilation. There are therefore reasons to believe that the rmse could be reduced further with a more optimal assimilation scheme that does not create these noisy fields.

8 Conclusion and further remarks

The SEIK assimilation scheme has been implemented into the MIPOM ocean model. This is the first time the SEIK has been implemented into a POMS-type model. The MIPOM+SEIK with fixed error covariance matrix has been tested in an experiment assimilating OSISAF SSTdata and the full SEIK setup with evolved error covariance has been tested both in a theoretical twin experiment and with real OSISAF satellite data of SST. These experiments yield overall positive results in the sense that the SEIK assimilation improves the model performance, and for local SEIK it does so to a greater extent than the current nudging assimilation scheme. However, the SEIK assimilation also tends to perturb some of the model fields. Noisy pathces of high gradients can be seen in both the temperature and the salinity fields. This is particularly the case when assimilating in situ data. Attempts with various sizes of the influence regions showed that an infinite size gave the same results as the global SEIK, and hence did not reveal any noisy regions, which is what one expects. However, we were not able to determine an optimal size that removed the noisy parts without underestimating the model variances.

Unfortunately there are very few implementations of SEIK so far, and none in this type of model. It is therefore a challenge to determine if the problem is due to the way MIPOM responds to this assimilation scheme, the implementation of the scheme, or the definition of the initial error covariance matrix. One way is to study the evolution of each ensemble member in detail to check how the error covariance matrix is evolving. One could also implement SEIK into another ocean model and perform the same experiment. If the problem is the way MIPOM responds to the SEIK analysis update, it means that the model fields get some kind of shock because the correction is too strong and immediate at the analysis time. One could think that a more incremental update would improve this, avoiding giving the model a shock in a certain direction but rather letting the model gradually learn the computed correction. The SEIK method would then compute the total correction at the analysis time. A follow-up on all three of these points is planned.

9 Acknowledgment

The work was financed by the Norwegian Research Council through the projects no.152880/120 and no.176096/S30. I would like to thank Dr. Lars Nerger for providing the SEIK PDAF algorithm and for helping in the implementation of this. My appreciations also goes to Jon Albretsen for useful help and many discussions. Thanks alos to Lars Petter Røed for reading through the manuscript.

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Figure 6: SST field after first analysis update. Top left: ROMS (truth). Top right: MIPOM with no assimilation. Bottom left: Assimilation with global SEIK. Bottom right: Assimilation with local SEIK.



Figure 7: rmse in SST as a function of time for the various experiments



Figure 8: rmse in temperature at 20m as a function of time for the various experiments



Figure 9: rmse in salinity at 20m as a function of time for the various experiments



Figure 10: The operational forecast scheme



Figure 11: A typical 12h mean osisaf SST product

10 References



Figure 12: rmse in SST as a function of forecast hour.