DATA ASSIMILATION FOR A MODEL IN ATMOSPHERIC CHEMISTRY AND OCEANOGRAPHY

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Abstract: Three sequential data assimilation schemes (successive corrections, optimal interpolation and analysis correction) are applied to a model in atmospheric chemistry and oceanography. The model simulates the interaction of the various forms of carbon that are stored in three regimes: the atmosphere, the shallow ocean, and the deep ocean. Implementation issues and numerical results from some preliminary investigations are presented.

Keywords: approximate analysis, function approximation, Hermite interpolation, minimization problem, weighting matrice, Kalman filter, data assimilation schemes.

1. INTRODUCTION

The concept of data assimilation normally refers to the process of modifying (or updating) the model state variables of a forecast model with observed information during the time integration of the model. Observations valid at a certain time will influence the model state not only at the observation time but also, in case of a forward data assimilation, at future times within the predictability range. In other words, by using data assimilation the time history of observations will help to improve the initial conditions for numerical forecast model runs.

The basic components of forward data assimilation were introduced operationally already 50 years ago together with barotropic forecast models by Gilchrist and Cressman (1954), and Bergthorsson and Döös (1955). Although many of the assimilation procedures at that time were formulated in an ad hoc manner, they included basic important components like quality control, spatial filtering and spatial interpolation.

The purpose of this study is to describe how three sequential data assimilation schemes (successive corrections, optimal interpolation and analysis correction) are applied to a model in atmospheric chemistry and oceanography. Implementation details and numerical results are also discussed.

2. MATHEMATICAL MODEL

The model developed by Walker (1991) simulates the interaction of the various forms of carbon that are stored in three regimes: the atmosphere, the shallow ocean, and the deep ocean. An informative background article is available at a Web site maintained by the Lighthouse Foundation. See also Martin (2001).

The five principal variables of the model $(p, \sigma_s, \sigma_d, \alpha_s, \alpha_d)$ are all functions of time: p represents the partial pressure of carbon dioxide in the atmosphere, σ_s is the total dissolved carbon concentration in the shallow ocean, σ_d is the total dissolved carbon concentration in the deep ocean, α_s is the alkalinity in the shallow ocean, and α_d represents the alkalinity in the deep ocean.

Three additional quantities (h_s, c_s, p_s) are involved in the equilibrium equations in the shallow ocean: h_s - hydrogen carbonate in the shallow ocean, c_s - carbonate in the shallow ocean, and p_s - partial

pressure of gaseous carbon dioxide in the shallow ocean.

The rate of change of the five principal variables is given by five ordinary differential equations. The exchange between the atmosphere and the shallow ocean involves a constant characteristic transfer time d and a source term $f(t)$.

$$\frac{dp}{dt} = \frac{p_s - p}{d} + \frac{f(t)}{\mu_1}. \tag{1}$$

The equations describing the exchange between the shallow and deep oceans involve v_s and v_d, the volumes of the two regimes.

$$\begin{aligned}
\frac{d\sigma_s}{dt} &= \frac{1}{v_s}\left((\sigma_d - \sigma_s)w - k_1 - \frac{p_s - p}{d}\mu_2\right),\\
\frac{d\sigma_d}{dt} &= \frac{1}{v_d}\left(k_1 - (\sigma_d - \sigma_s)w\right),\\
\frac{d\alpha_s}{dt} &= \frac{1}{v_s}\left((\alpha_d - \alpha_s)w - k_2\right),\\
\frac{d\alpha_d}{dt} &= \frac{1}{v_d}\left(k_2 - (\alpha_d - \alpha_s)w\right).
\end{aligned} \tag{2}$$

The equilibrium between carbon dioxide and the carbonates dissolved in the shallow ocean is described by three nonlinear algebraic equations:

$$\begin{aligned}
h_s &= \frac{\sigma_s - (\sigma_s^2 - k_3\alpha_s(2\sigma_s - \alpha_s))^{1/2}}{k_3},\\
c_s &= \frac{\alpha_s - h_s}{2},\\
p_s &= k_4\frac{h_s^2}{c_s}.
\end{aligned} \tag{3}$$

We used in the numerical simulations the following values for the constants involved in the model equations: $d = 8.64$, $\mu_1 = 4.95\cdot 10^2$, $\mu_2 = 4.95\cdot 10^{-2}$, $v_s = 0.12$, $v_d = 1.23$, $w = 10^{-3}$, $k_1 = 2.19\cdot 10^{-4}$, $k_2 = 6.12\cdot 10^{-5}$, $k_3 = 0.997148$ and $k_4 = 6.79\cdot 10^{-2}$.

The source term $f(t)$ describes the burning of fossil fuels in the modern industrial era. We will use a time interval that starts about a thousand years ago and extends a few thousand years into the future

$$1000 \le t \le 5000. \tag{4}$$

The initial values at the moment of time $t = 1000$ are: $p = 1.00$, $\sigma_s = 2.01$, $\sigma_d = 2.23$, $\alpha_s = 2.20$, $\alpha_d = 2.26$. These values characterize preindustrial equilibrium and remain nearly constant as long as the source term $f \equiv 0$.

The following table describes one scenario for a source term $f(t)$ that models the release of carbon dioxide from burning fossil fuels, especially gasoline. The amounts begin to be significant after 1850, peak near the end of this century, and then decrease until the supply is exhausted.

Table 1. Possible scenario for the source term that models the release of carbon dioxide from burning fossil fuels, especially gasoline.

Year	1000	1850	1950	1980	2000
Rate	0.0	0.0	1.0	4.0	5.0

Year	2050	2080	2100	2120	2150
Rate	8.0	10.0	10.5	10.0	8.0

Year	2225	2300	2500	5000
Rate	3.5	2.0	0.0	0.0

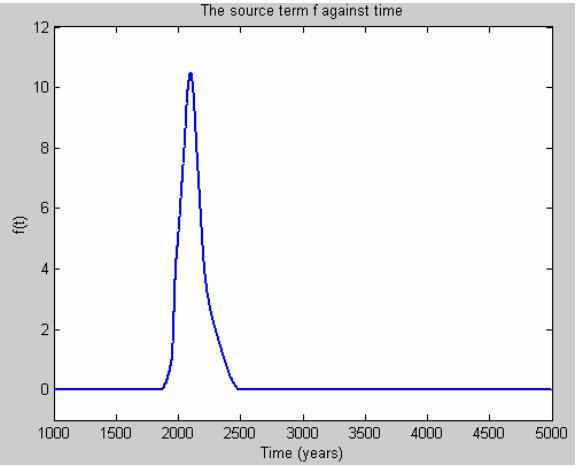


Fig. 1. The plot of the source term f against time. The values in Table 1 were interpolated using piecewise cubic Hermite interpolation method.

The two alkalinity variables of the model (α_s and α_d) are not plottet at all because they are almost constant throughhout this entire simulation. Initially, the carbon in the three regimes is nearly at equilibrium and so the amounts hardly change before 1850. Over the period $1850 \le t \le 2500$, Figure 1 shows the additional carbon produced by burning fossil entering the system.

3. DATA ASSIMILATION SCHEMES

In this section we present three sequential data assimilation schemes: successive corrections, optimal interpolation and analysis correction. The general sequential data assimilation problem can be considered as the minimization of the cost function

$$\begin{aligned}
J = &[y(i) - H(x(i))]^{-1}R^{-1}[y(i) - H(x(i))]\\
&+[x(i) - x_b(i)]^{-1}B^{-1}[x(i) - x_b(i)],
\end{aligned} \tag{5}$$

with respect to $x(i)$. Here $x_b(i)$ is a background state with error covariance matrix B^{-1}, $y(i)$ is a vector of observations with covariance matrix R^{-1}

and H is the (possibly nonlinear) observation operator which converts the model field $x(i)$ into an equivalent model observation value. The solution to the data assimilation problem, which we call the analysis, we write x_a. Each of the data assimilation methods implemented approximates the solution to this minimization problem. Here we do not aim to give a full explanation of the schemes, but just briefly outline how each is implemented. Further details can be found in Martin et al. (1999).

3.1 Successive corrections scheme

The successive corrections method is an iterate algorithm, which can be written as

$$x^{j+1}(i) = x^j(i) + W[y(i) - H(x^j(i))], \qquad (6)$$

where $x^0(i) = x_b(i)$ is the background state, j is the iteration or correction index and W is a weighting matrix. The algorithm is stopped after k corrections, after which the analysis is given by $x_a(i) = x^k(i)$. For the experiments in these programs the weighting matrix is given by $W = 0.5 \times I$, where I is the identity matrix..

3.2 Optimal interpolation scheme

The optimal interpolation analysis is given by

$$x_a(i) = x_b(i) + K[y(i) - H(x_b(i))], \qquad (7)$$

with

$$K = BH^T(HBH^T + R)^{-1}. \qquad (8)$$

If H is a nonlinear operator then it should be linearized around a background state.

3.3 Analysis correction scheme

The analysis correction algorithm is written as

$$x^{j+1}(i) = x^j(i) + WQ[y^j(i) - H(x^j(i))], \qquad (9)$$

$$y^{j+1}(i) = y^j(i) - Q[y^j(i) - H(x^j(i))], \qquad (10)$$

where $y^0(i)$ is the vector of observations, $W = BH^T R^{-1}$, $Q = (HW + I)^{-1}$. If H is a nonlinear operator then its linearization around a background state should be used. The algorithm is stopped after k corrections, after which the analysis is given by $x_a(i) = x^k(i)$.

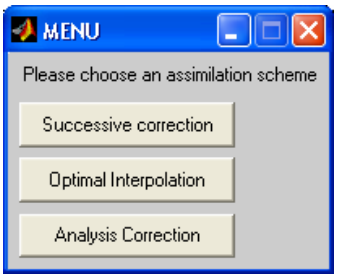
4. IMPLEMENTATION ISSUES AND RESULTS

The source code of the program was performed using Matlab language, version 6.1.

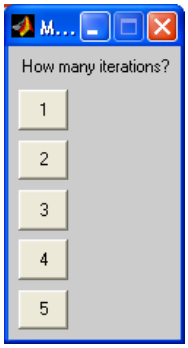
4.1 Input data

Below we describe how the program initiates a dialogue, asking for inputs from the user in the following order:

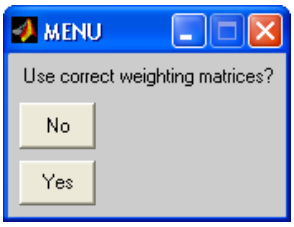
- Please, choose an assimilation scheme:



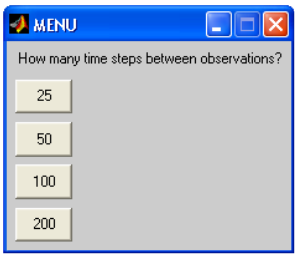
- How many iterations?



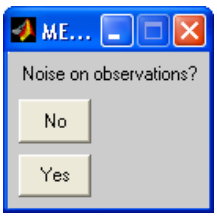
- Use correct weighting matrices?



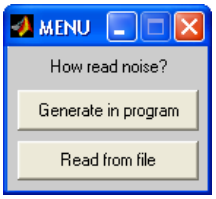
- How many time steps between observations?



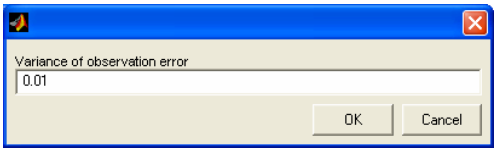
- Noise on observations?



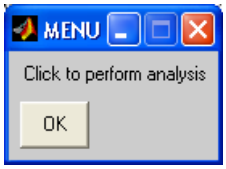
- How read noise?



- Variance of observation error



This allows the user to set the variance of the random noise to be added to the observations.
The user must then click OK on a dialogue box to perform the analysis, which represents the solution of the data assimilation problem.



4.2 Output data

The output from the oscillating system is two figures. Figure 1 shows the solution for the p variable. The truth trajectory is shown by a dashed line, the background trajectory used is shown by a dashed-dotted line and the observations used are shown by circles. The final analysis and forecast from the analysis is shown by a continuous line.

4.3 True and background solution

The true solution can be changed by changing either the parameters of the problem or the initial conditions. The background solution for the model is obtained by running the model from slightly different initial conditions. In this simulation we used the following values: $p = 0.9$, $\sigma_s = 2.1$, $\sigma_d = 2.17$, $\alpha_s = 2.15$ and $\alpha_d = 2.3$.

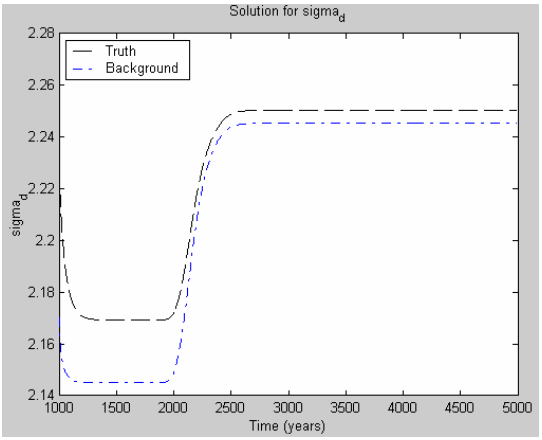


Fig. 2. True and background solution for the component σ_d of the state vector.

An alternative method for generating the background would be to start the model using the true intial conditions with some random noise added.

4.4 Error covariance matrices

The code of the program sets up the observation and background covariance matrices, R and B. These are used in all schemes except the successive correction scheme. If the correct weighting matrices are requested then the true covariances are calculated using the known solution, otherwise these matrices are set to the identity.

4.5 Successive corrections weighting matrix

The weighting matrix W for the successive corrections scheme is set in the code to be 0.5 times the identity matrix.

4.6 Results

The output from the programs is graphical, with figures as follows. Figures 3-5 contain the results of the data ssimilation for the successive correction method. The number of iterations was set to 5, the number of time steps between observations was set to 25, and a random noise with variance equals to 10^{-4} was used.

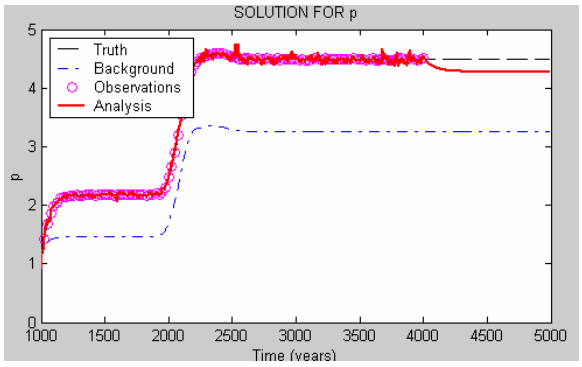


Fig. 3. The data assimilation results for the component p of the model. Analysis scheme: successive correction.

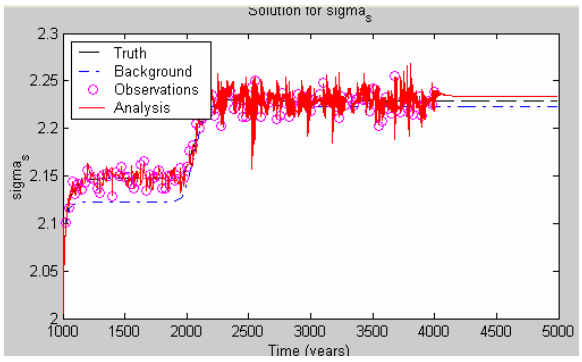


Fig. 4. The data assimilation results for the component σ_s of the model. Analysis scheme: successive correction.

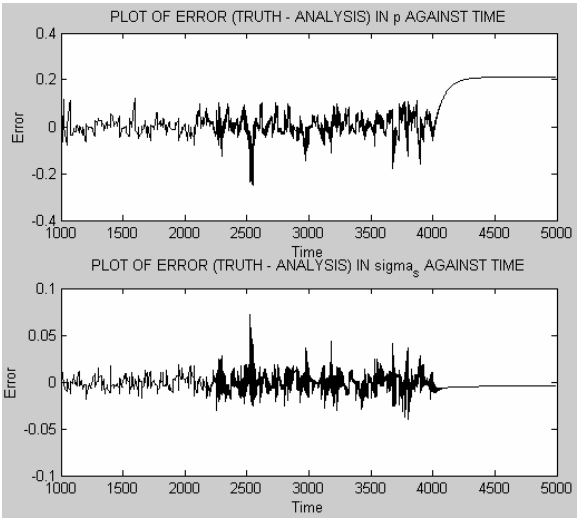


Fig. 5. Plot of error (truth – analysis) against time. Upper plot: error in p. Lower plot: error in σ_s. Analysis scheme: successive correction.

Figures 6-8 present the results of the data ssimilation for the optimal interpolation method using correct weighting matrices. The number of time steps between observations was set to 50, and a random noise with variance equals to 10^{-4} was used.

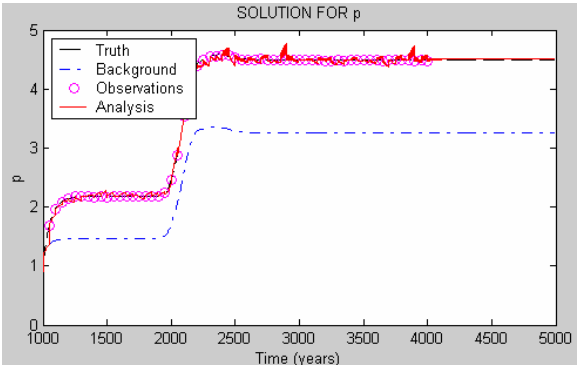


Fig. 6. The data assimilation results for the component p of the model. Analysis scheme: optimal interpolation.

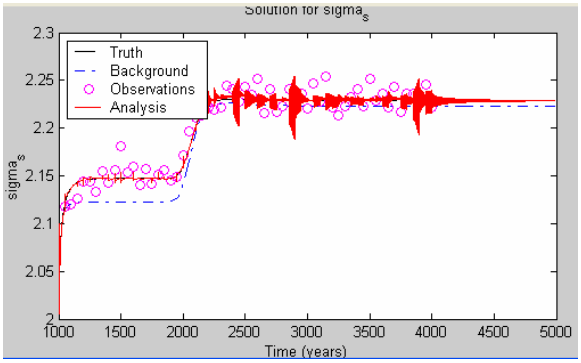


Fig. 7. The data assimilation results for the component σ_s of the model. Analysis scheme: optimal interpolation.

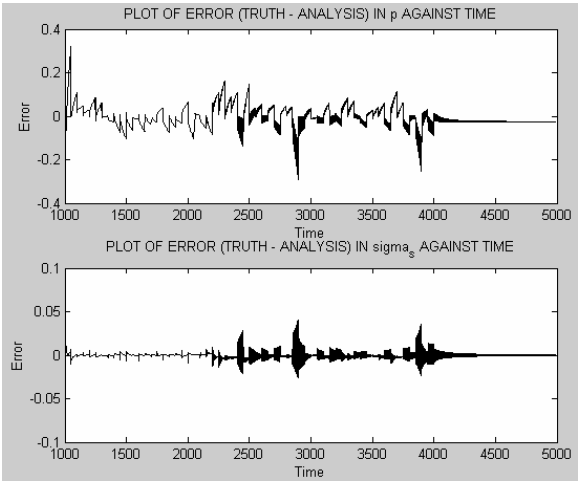


Fig. 8. Plot of error (truth – analysis) against time. Upper plot: error in p. Lower plot: error in σ_s. Analysis scheme: optimal interpolation.

Figures 9-11 contain the results of the data ssimilation for the optimal analysis correction method using correct weighting matrices. The number of time steps between observations was set to 50, and a random noise with variance equals to 10^{-4} was used.

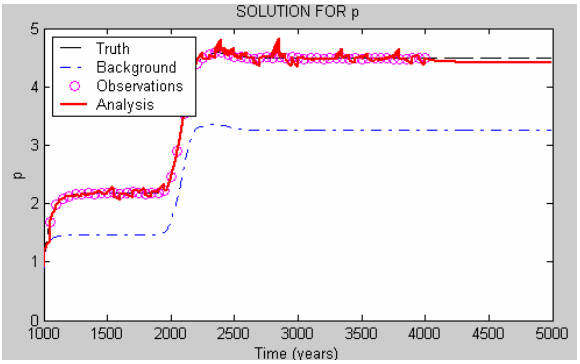


Fig. 9. The data assimilation results for the component p of the model. Analysis scheme: analysis correction.

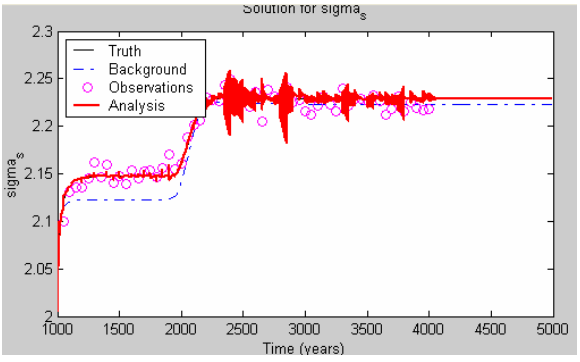


Fig. 10. The data assimilation results for the component σ_s of the model. Analysis scheme: analysis correction.

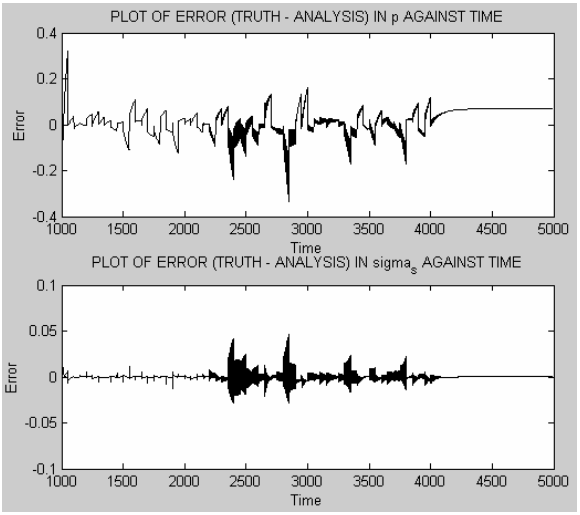


Fig. 11. Plot of error (truth – analysis) against time. Upper plot: error in p. Lower plot: error in σ_s. Analysis scheme: analysis correction.

5. CONCLUSIONS

This study focused on three sequential data assimilation schemes (successive corrections, optimal interpolation and analysis correction), applied to a model in atmospheric chemistry and oceanography. The model simulates the interaction of the various forms of carbon that are stored in three regimes: the atmosphere, the shallow ocean, and the deep ocean.

The equations of the model are mildly stiff, because the various chemical reactions take place on very different time scales. Efficient numerical schemes applied to different stiff ODEs from atmospheric chemistry are described in Zlatev (1995), Verwer and Simpson (1995) and Verwer et al. (1996).

Implementation aspects and numerical results from some preliminary investigations were presented.

There is a recent tendency in data assimilation to find the optimal location of the observations by using the adjoint sensitivity method (see Sandu et al. (2004)), as well as to combine the advantage of the numerical splitting schemes (see Bartholy et al. (2001)), variational methods (Dimitriu (1999), Daescu et al. (2000), Sandu et al. (2004), Dimitriu and Cuciureanu (2005)) and Kalman filter techniques (Chui and Chan (1987), Loon and Heemink (1997) and Segers (2002)).

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