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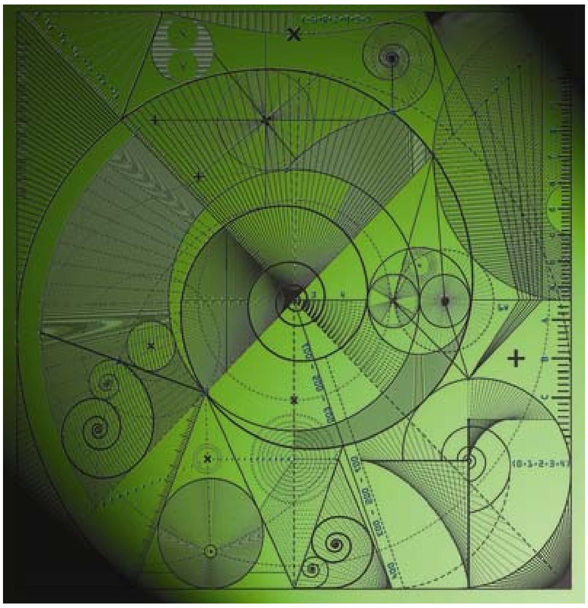

A hybrid data assimilation scheme for model parameter estimation: application to morphodynamic modelling

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Abstract

We present a novel algorithm for joint state-parameter estimation using sequential three dimensional variational data assimilation (3D-Var) and demonstrate its application in the context of morphodynamic modelling using an idealised two parameter 1D sediment transport model. The new scheme combines a static representation of the state background error covariances with a flow dependent approximation of the state-parameter cross covariances. For the case presented here, this involves calculating a local finite difference approximation of the gradient of the model with respect to the parameters. The new method is easy to implement and computationally inexpensive to run. Experimental results are positive with the scheme able to recover the model parameters to a high level of accuracy. We expect that there is potential for successful application of this new methodology to larger, more realistic models with more complex parameterisations.

Keywords: Data assimilation, morphodynamics, parameter estimation, state augmentation

1. Introduction

A numerical model can never completely describe the complex physical processes underlying the behaviour of a real world dynamical system. State of the art computational models are becoming increasingly sophisticated but in practice these models suffer from uncertainty in their initial conditions

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and parameters. Even with perfect initial data, inaccurate representation of model parameters will lead to the growth of model error and therefore affect the ability of our model to accurately predict the true system state.

Parameterizations are typically used in applications where the underlying physics of a process are not fully known or understood, or to model subgrid scale effects that cannot be captured within a particular model resolution. Coastal morphodynamic modelling is one such field; sediment transport models are typically based on empirical formulae that use various parameterizations to characterise the physical properties of the sediment flux [1]. The consequence of this is that model parameters often do not represent directly measurable quantities. Poorly known input parameters are a key source of uncertainty in sediment transport models [1]. A fundamental question in model development is how to estimate these parameters a priori. One option is to use data assimilation.

Data assimilation is a sophisticated mathematical technique for combining observational data with model predictions. Recent examples of the application of data assimilation to coastal modelling are given in [2] and [3]. Most previously published work focuses on either state or parameter estimation. However, by employing the method of state augmentation [4], it is possible to use data assimilation to estimate uncertain model parameters concurrently with the model state. The parameters are appended to the model state vector, the model prediction equations are combined with the parameter evolution equations and the chosen assimilation algorithm is simply applied to this new augmented system in the usual way [5, 6]. The approach has previously been successfully used in the context of model error or bias estimation, e.g. [7, 8, 9], and more recently for parameter estimation in biogeochemical models using the Kalman filter [10].

Here, we combine the technique with a sequential three dimensional variational data assimilation (3D Var) scheme (e.g. [11]). Variational data assimilation is a popular choice for state estimation in large problems; it has many advantages, such as ease of implementation (no model adjoints required), computational robustness and computational efficiency. Under certain statistical assumptions, the 3D Var method approximates the Bayesian maximum a posteriori likelihood estimate of the state and parameters of the system [12].

A key difficulty in the construction of a data assimilation algorithm is specification of the background error covariances. For joint state-parameter estimation, it is the cross-covariances between the parameters and the state that transfer information from the observations to the parameter estimates and therefore play a crucial role in the parameter updating. A good a priori specification of these covariances is therefore vital for accurate parameter updating [13, 14].

By combining ideas from 3D Var and the extended Kalman filter (EKF) we have developed a novel hybrid sequential data assimilation algorithm that provides a flow dependent approximation of the state-parameter cross covariances without explicitly propagating the full system covariance matrix. The technique involves calculating a local finite difference approximation of the gradient of the model with respect to the parameters; it is simple to code and computationally inexpensive. In this paper we give details of this new method and demonstrate its application in the context of morphodynamic modelling using an idealised two parameter 1D sediment transport model. Although the long term goal is to implement a concurrent state-parameter estimation scheme in a full morphodynamic assimilation-forecast system applied to some specific coastal study sites, this simple model provides a framework within which we can develop, test and understand our ideas without the obfuscating features of a more complex system.

This paper is organised as follows. Section 2 introduces the model system equations and gives a brief overview of the data assimilation methods we use in this work. In section 3 we outline our new hybrid approach. Our simple test model is introduced in section 4. The experimental design is described in section 5 together the main results. Finally, in section 6 we summarise the conclusions.

2. Data assimilation

We consider the discrete non-linear time invariant dynamical system model

$$\mathbf{z}_{k+1} = \mathbf{f}(\mathbf{z}_k, \mathbf{p}) \qquad k = 0, 1, \ldots \tag{1}$$

The vector $\mathbf{z}_k \in \mathbb{R}^m$ is known as the state vector and represents the model state at time t_k, $\mathbf{p} \in \mathbb{R}^q$ is a vector of q (uncertain) model parameters, and $\mathbf{f} : \mathbb{R}^m \longrightarrow \mathbb{R}^m$ is a non-linear operator describing the evolution of the state from time t_k to t_{k+1}. We assume that specification of the model state and parameters at time t_k uniquely determine the model state at all future times. We also assume that $\mathbf{f}(\mathbf{z}, \mathbf{p})$ is differentiable with respect to $\mathbf{z}$ and $\mathbf{p}$ for all $\mathbf{z} \in \mathbb{R}^m$ and $\mathbf{p} \in \mathbb{R}^q$.

In the example described in this paper, the model state vector $\mathbf{z}$ is a 1D vector representing bathymetry or bed height, the operator $\mathbf{f}$ represents the equations describing the evolution of the bed-form over time and the vector $\mathbf{p}$ contains parameters arising from the parameterisation of the sediment transport flux. We assume that the system can be represented on a discrete grid and that the system model is 'perfect', i.e. it gives an exact description of the true behaviour of the system on the grid.

In this work, the model parameters are assumed to be constants and so are not altered by the forecast model from one time step to the next. The equation for the evolution of the parameters therefore has the simple form

$$\mathbf{p}_{k+1} = \mathbf{p}_k. \tag{2}$$

The augmented system model is derived by appending the parameters to the model state vector, and combining the evolution equation for the parameters (2) with the model for the evolution of the state (1). This gives the equivalent augmented system model

$$\mathbf{w}_{k+1} = \tilde{\mathbf{f}}(\mathbf{w}_k), \qquad k = 0, 1, \ldots \tag{3}$$

where $\mathbf{w}_k = (\mathbf{z}_k, \mathbf{p}_k)^T \in \mathbb{R}^{m+q}$ is the augmented state vector and $\tilde{\mathbf{f}}(\mathbf{w}_k) = (\mathbf{f}(\mathbf{z}_k, \mathbf{p}_k), \mathbf{p}_k)^T$ with $\tilde{\mathbf{f}} : \mathbb{R}^{m+q} \longrightarrow \mathbb{R}^{m+q}$.

For sequential assimilation, we start with a priori (or background) estimates of the state and parameters $\mathbf{w}_k^b = (\mathbf{z}_k^b, \mathbf{p}_k^b)^T$ at time t_k. We suppose that we have a set of r_k observations to assimilate and that these are related to the model state by the equations

$$\mathbf{y}_k = \mathbf{h}(\mathbf{z}_k) + \boldsymbol{\delta}_k, \qquad k = 0, 1, \ldots \tag{4}$$

Here $\mathbf{y}_k$ is a vector of r_k observations at time t_k, where the number of available observations may vary with time. The operator $\mathbf{h} : \mathbb{R}^m \longrightarrow \mathbb{R}^{r_k}$ is a nonlinear observation operator that maps from model to observation space and the vector $\boldsymbol{\delta}_k \in \mathbb{R}^{r_k}$ represents the observation errors. We can rewrite the equation for the observations (4) in terms of the augmented system as

$$\mathbf{y}_k = \tilde{\mathbf{h}}(\mathbf{w}_k) + \boldsymbol{\delta}_k = \tilde{\mathbf{h}} \begin{pmatrix} \mathbf{z}_k \\ \mathbf{p}_k \end{pmatrix} + \boldsymbol{\delta}_k \overset{\text{def}}{\equiv} \mathbf{h}(\mathbf{z}_k) + \boldsymbol{\delta}_k \qquad k = 0, 1, \ldots \tag{5}$$

where $\tilde{\mathbf{h}} : \mathbb{R}^{m+q} \longrightarrow \mathbb{R}^{r_k}$.

The aim is to combine the measured observations $\mathbf{y}_k$ with the model predictions $\mathbf{w}_k^b$ to produce an updated model state that most accurately describes the true augmented system state $\mathbf{w}_k^t$ at time t_k. This optimal estimate is called the *analysis* and is denoted $\mathbf{w}_k^a$.

The analysis $\mathbf{w}_k^a = (\mathbf{z}_k^a, \mathbf{p}_k^a)^T$ is found by minimising a cost function penalising the misfit between the state, $\mathbf{w}_k$, the observations, $\mathbf{y}_k$ and the background forecast, $\mathbf{w}_k^b$

$$J(\mathbf{w}_k) = (\mathbf{w}_k - \mathbf{w}_k^b)^{\mathbf{T}} \mathbf{B}_k{}^{-1} (\mathbf{w}_k - \mathbf{w}_k^b) + (\mathbf{y}_k - \tilde{\mathbf{h}}_k(\mathbf{w}_k))^T \mathbf{R}_k^{-1} (\mathbf{y}_k - \tilde{\mathbf{h}}_k(\mathbf{w}_k)). \quad (6)$$

The relative weighting of the background and observations in the analysis are determined by their error statistics, expressed as error covariances, $\mathbf{B}_k$ and $\mathbf{R}_k$, respectively.

Prescription of the matrix $\mathbf{B}_k$ is a key challenge. This matrix plays a crucial role in the filtering and spreading of observational data [13, 14, 15]. In the 3D Var method (e.g. [11]), the background covariances are approximated by a fixed matrix (i.e. $\mathbf{B}_k = \mathbf{B}$ for all k) and the nonlinear optimization problem (6) is solved numerically using a gradient iteration algorithm at each time t_k. In the EKF (e.g. [4]), the background covariances are evolved explicitly according to the linearised model dynamics and the analysis is calculated directly.

For joint state-parameter estimation, it is particularly important that the a priori cross-covariances between the parameters and the state are well specified [13, 15]. Since it is not possible to observe the parameters themselves, the parameter estimates depend on the observations of the state variables. It is the state-parameter cross covariances that pass information from the observed variables to update the estimates of the unobserved parameters. Success of the state augmentation approach therefore relies strongly on the relationships between the parameters and state components being well defined. Previous work [15] indicated that whilst the assumption of static covariances made by the 3D Var algorithm is sufficient for state estimation it is insufficient for parameter estimation as it does not provide an adequate representation of the state-parameter cross covariances required by the augmented system. In order to yield reliable estimates of the true parameters these covariances need to evolve with the model. However, updating the background error covariance matrix at every time step is computationally expensive and impractical when the system of interest is of high dimension.

To overcome this problem we have combined ideas from 3D Var and the EKF to produce a new hybrid assimilation scheme that captures the flow dependent nature of the state-parameter cross covariances without explicitly propagating the full system covariance matrix. A simplified version of the EKF forecast step is used to estimate the state-parameter forecast error cross covariances and this is then combined with an empirical, static approximation of the state background error covariances. We outline this new approach in the next section.

3. A hybrid approach

We can partition the background error covariance matrix $\mathbf{B}$ as follows

$$\mathbf{B}_k = \begin{pmatrix} \mathbf{B}_{\mathbf{zz}_k} & \mathbf{B}_{\mathbf{zp}_k} \\ (\mathbf{B}_{\mathbf{zp}_k})^T & \mathbf{B}_{\mathbf{pp}_k} \end{pmatrix}. \tag{7}$$

Here $\mathbf{B}_{\mathbf{zz}_k} \in \mathbb{R}^{m \times m}$ is the background error covariance matrix for the state vector $\mathbf{z}_k$ at time t_k, $\mathbf{B}_{\mathbf{pp}_k} \in \mathbb{R}^{q \times q}$ is the covariance matrix of the errors in the parameter vector $\mathbf{p}_k$ and $\mathbf{B}_{\mathbf{zp}_k} \in \mathbb{R}^{m \times q}$ is the covariance matrix for the cross correlations between the forecast errors in the state and parameter vectors.

In the EKF, the background covariance at t_{k+1} is determined by propagating the analysis covariance forward in time from t_k using a linearisation of the forecast model. We want to avoid updating the whole matrix (7) at every time step. For the state and parameter background error covariances we adopt a 3D Var approach; these matrices are prescribed at the start of the assimilation and held fixed throughout as if the forecast errors were statistically stationary. For the state-parameter cross covariances, we require a flow dependent approximation. If we assume that the state-parameter cross covariances are initially zero, and take a single step of the EKF we find that the state-parameter cross covariance can be approximated as $\mathbf{B}_{\mathbf{zp}_{k+1}} = \mathbf{N}_k \mathbf{P}^a_{\mathbf{pp}_k}$ [14], where $\mathbf{N}_k = \left.\frac{\partial \mathbf{f}(\mathbf{z},\mathbf{p})}{\partial \mathbf{p}}\right|_{\mathbf{z}^a_k, \mathbf{p}^a_k} \in \mathbb{R}^{m \times q}$ is the Jacobian of the forecast model with respect to the parameters and $\mathbf{P}^a_{\mathbf{pp}_k}$ is the parameter analysis error covariance. This leads us to propose the following approximation for the augmented forecast error covariance matrix

$$\mathbf{B}_{k+1} = \begin{pmatrix} \mathbf{B}_{\mathbf{zz}} & \mathbf{N}_k \mathbf{B}_{\mathbf{pp}} \\ \mathbf{B}_{\mathbf{pp}} \mathbf{N}_k^T & \mathbf{B}_{\mathbf{pp}} \end{pmatrix}. \tag{8}$$

In other words, all elements of the augmented background error covariance matrix are kept fixed except the state-parameter cross covariance $\mathbf{B}_{\mathbf{zp}_{k+1}}$

which is updated at each new analysis time by recalculating the Jacobian matrix $\mathbf{N}_k$.

Explicitly calculating the Jacobian of complex functions can be a difficult task, requiring complicated derivatives if done analytically or being computationally costly if done numerically. A simple alternative is to use a local finite difference approximation. Defining $\mathbf{z}_{k+1}^b = \mathbf{f}(\mathbf{z}_k^a, \mathbf{p}_k^a)$ and $\hat{\mathbf{z}}_{k+1}^b = \mathbf{f}(\mathbf{z}_k^a, \hat{\mathbf{p}}_k^a)$, the q columns of $\mathbf{N}_k$ are given by computing

$$\frac{\partial \mathbf{f}(\mathbf{z}_k^a, \mathbf{p}_k^a)}{\partial p_i} \approx \frac{\hat{\mathbf{z}}_{k+1}^b - \mathbf{z}_{k+1}^b}{\delta p_i} \qquad i = 1, \ldots, q, \tag{9}$$

for each parameter p_i. Here $\hat{\mathbf{p}}_k^a$ is the current parameter vector with element p_i replaced with $p_i + \delta p_i$ where δp_i is a small perturbation to the current approximation of p_i.

4. The model

We apply our hybrid scheme to a simplified sediment transport model based on the 1D sediment conservation equation [1]

$$\frac{\partial z}{\partial t} = -\left(\frac{1}{1-\varepsilon}\right)\frac{\partial q}{\partial x}, \tag{10}$$

where $z(x,t)$ is the bathymetry, t is the time, q is the total (suspended and bedload) sediment transport rate, and ε is the sediment porosity. The transport rate q is a complex function of the water and sediment properties. For this work we use one of the most basic sediment tranport flux formula [16], $q = Au^n$, where $u = u(x,t)$ is the current in the x direction and A and n are parameters whose values need to be set. The parameter A is a dimensional constant whose value depends on various properties of the sediment and water. The derivation of the parameter n is less clear. It is usually set by fitting to field data and generally takes a value in the range $1 \leq n \leq 4$.

To solve (10) we assume that the water height h and flux F are constant in space and set $u(h-z) = F$. Equation (10) can then be re-written in the advection form [14]

$$\frac{\partial z}{\partial t} + c(z)\frac{\partial z}{\partial x} = 0, \tag{11}$$

where the bed celerity $c(z)$ is a function of the bed height z and parameters h, F, ε, A, n only. For the purpose of this work, we assume that h, F and ε

are known constant values but that the values of A and n are uncertain. To prevent unphysical solutions a small diffusive term is added to to the right hand side of (11). This equation is then solved numerically using a combined semi-Lagrangian Crank-Nicolson scheme based on that presented in [17].

5. Experiments & results

We have tested our scheme by running a series of identical twin experiments using an initially symmetric, isolated bedform, with initial profile given as a Gaussian hump. We assume that our numerical model is perfect and generate a reference or 'true' solution by running the model with set parameter values $A = 0.002\ \mathrm{ms}^{-1}$ and $n = 3.4$. This solution is used to provide pseudo-observations for the data assimilation and also to evaluate the performance of our scheme. The model is then re-run from a perturbed initial bathymetry and with incorrect starting values for the parameters A and n.

The assimilation process is carried out sequentially, with a new set of observations being assimilated every hour. The model was sampled on a regular grid with a spacing of $\Delta x = 1.0\ \mathrm{m}$ and timestep $\Delta t = 15$ min. The cost function was minimised iteratively using a quasi-Newton descent algorithm [18]. Observations were generated from the true solution at intervals of $25\Delta x$. They are assumed to be perfect and without any added noise.

For the observation error covariance matrix we set $\mathbf{R}_k = \mathbf{R} = \sigma_o^2\mathbf{I}$, where σ_o^2 is the observation error variance. Although the observations are perfect, specifying a non-zero observation error variance allows us to consider the impact of the accuracy of the observations on the assimilation without actually adding noise. This is a recognised practice, routinely used for the preliminary testing of data assimilation schemes with pseudo data (e.g. [8]). Results from a related set of experiments in which noisy observation errors are simulated by adding random error can be found in [14].

The state background error covariance matrix $\mathbf{B_{zz}}$ is given by the isotropic correlation function [19] $b_{ij} = \sigma_b^2\rho^{|i-j|}, i, j = 1, \ldots, m$, with $\rho = \exp(-\Delta x/L)$ where L is a correlation length scale that is adjusted empirically, and σ_b^2 is the background error variance. The parameter error covariance matrix $\mathbf{B_{pp}}$ is a fixed 2×2 matrix with parameter error variances σ_A^2 and σ_n^2 on the diagonal and off-diagonal elements σ_{An}. The state-parameter cross covariance matrix $\mathbf{B}_{\mathbf{zp}_k}$ is recalculated at each new assimilation time as described in section 3, with perturbations $\delta A = 10^{-5}$ and $\delta n = 10^{-2}$. At the end of each assimilation cycle the model parameters are updated and the state analysis is integrated forward using the model (with the new parameter values) to become the background state for the next analysis time.

Figure 1 illustrates the impact incorrect parameter estimates can have on the modelled bathymetry by comparing model runs performed with and without data assimilation over a 24 h period. For this example, the parameter A is initially over estimated ($A_0 = 0.02\text{ms}^{-1}$) and n under estimated ($n_0 = 2.4$). With no data assimilation (top), the model bathymetry rapidly diverges away from the truth. After 24 hours it has moved beyond the model domain. Running the model with the joint state-parameter assimilation scheme greatly improves the model predictions (bottom). At 24 hours it is almost impossible to distinguish between the predicted model bathymetry and the true bathymetry. The corresponding parameter updates are shown in figures 2(a) and (b). The scheme successfully recovers the true values of A and n to a high level of accuracy.

Experiments were repeated for a range of starting combinations of A and n, investigating the sensitivity of the parameter estimates to different error ratios, observation combinations and observation noise. The quality of the state and parameter estimates is highly dependent on the accuracy of the information fed into the assimilation algorithm. We do not present the results of these experiments here but refer the reader to [14] for further details and discussion. It was found that various factors can affect the convergence and accuracy of the parameter estimates, such as the quality of the initial background guesses, the estimated parameter error variances and cross covariances, the location and spatial frequency of the observations, the level of observational noise and the time between successive assimilations.

6. Conclusions

We have presented a novel method for joint state-parameter estimation and demonstrated its efficacy in the context of morphodynamic modelling. By combining ideas from the 3D Var and EKF data assimilation techniques we have developed a scheme that provides a flow dependent approximation of the state-parameter cross-covariances but which avoids the computational complexities associated with implementation of the full Kalman filter.

This new method has been tested using an idealised, 1D non-linear sediment transport model that has two uncertain parameters. The results are positive with the scheme able to recover the true parameter values to a good

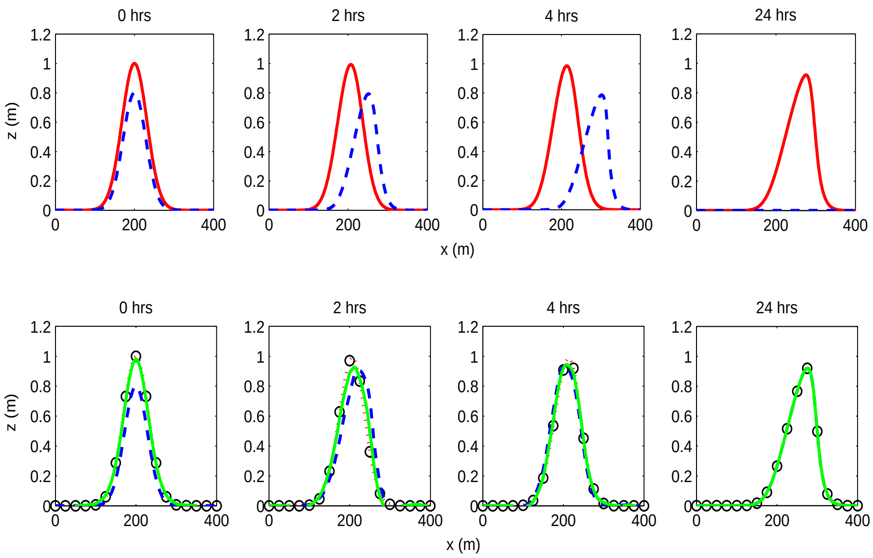

Figure 1: **Top**: model run with without data assimilation. **Bottom**: model run with data assimilation. The *dotted red line* represents the true bathymetry $\mathbf{z}^t$, the *dashed blue line* represents the model predicted (background) bathymetry $\mathbf{z}^b$, observations $\mathbf{y}$ are given by *black circles* and the analysis $\mathbf{z}^a$ is given by the *solid green line*.

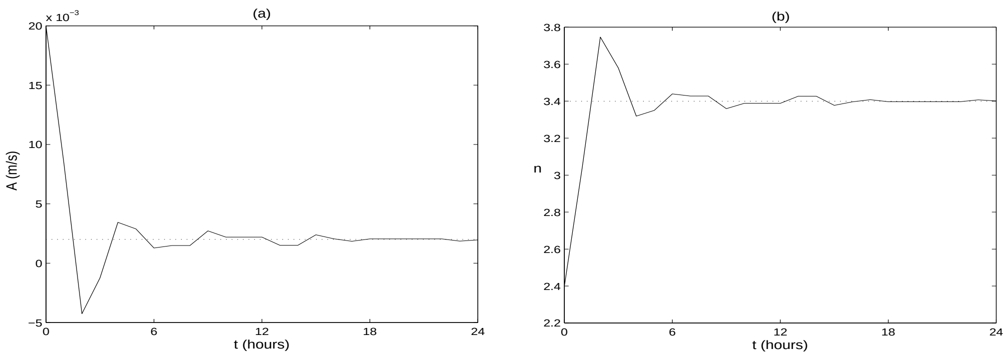

Figure 2: Parameter updates for initial estimates (a) $A_0 = 0.02\text{ms}^{-1}$ and (b) $n_0 = 2.4$. True parameter values (a) $A = 0.002\text{ms}^{-1}$ and (b) $n = 3.4$ are given by the dotted line.

level of accuracy. This has a positive impact on the predictive skill of the model. Our findings indicate that there is great potential for the use of 3D Var data assimilation for joint state-parameter estimation. In this paper we have focussed on application of the method to morphodynamic modelling but the versatility of the method has recently been demonstrated via a series of tests with a range of simple dynamical system models [20].

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