

THE REDUCED RANK TRANSFORM SQUARE ROOT FILTER FOR DATA ASSIMILATION

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Abstract: During the last decade, several suboptimal filtering schemes for data assimilation have been proposed. One of these algorithms, which has successfully been used in several applications, is the Reduced Rank Square Root filter. In this paper, a numerically more efficient variation, the Reduced Rank Transform Square Root filter, is introduced. A theoretical comparison of both filters is given and their performance is analyzed by comparing assimilation results on a magnetohydrodynamic example which emulates a space storm interacting with the Earth's magnetosphere. *Copyright ©2006 IFAC*

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1. INTRODUCTION

Data assimilation refers to methodologies that estimate the state of an environmental system from incomplete and inaccurate measurements. The Kalman filter, well known from linear control theory, is the optimal algorithm for assimilating measurements into a linear model. This technique recursively updates the estimate of the model-state when new measurements become available. However, for large-scale environmental systems, the task of state-estimation is very challenging, since the required spatial resolution leads to large-scale models, obtained by discretising partial differential equations, with a huge number of state variables, from 10^4 to 10^7 (Verlaan and Heemink, 1997; Groth *et al.*, 2000). As a consequence, the number of computations and the required storage for the Kalman filter become prohibitive. Therefore, during the last decade, several suboptimal filtering schemes for use in realistic and large-scale data assimilation applications have been developed.

One of these suboptimal filters, which has successfully been used in several applications, is the Reduced Rank

Square Root filter (Verlaan and Heemink, 1997). In this paper, we present a numerically more efficient variation, the Reduced Rank Transform Square Root filter and compare both filters by analyzing their assimilation results on a magnetohydrodynamic example which emulates a space storm interacting with the Earth's magnetosphere.

2. THE KALMAN FILTER

Consider the linear discrete time model

$$x_{k+1} = A_k x_k + B_k u_k + F_k w_k \quad (1)$$

and measurements

$$y_k = C_k x_k + v_k, \quad (2)$$

where $x_k \in \mathbb{R}^n$ is the state, $u_k \in \mathbb{R}^{m_u}$ is the input and $y_k \in \mathbb{R}^p$ is the measurement. The process noise $w_k \in \mathbb{R}^{m_w}$ and the measurement noise $v_k \in \mathbb{R}^p$ are assumed to be zero-mean white Gaussian and mutually uncorrelated with covariance matrices Q_k and R_k , respectively.

The Kalman filter yields optimal estimates x_k^a of the state x_k from noisy measurements y_k by minimizing the trace of the error covariance matrix $P_k^a \in \mathbb{R}^{n \times n}$, defined by

$$P_k^a \triangleq \mathcal{E} [(x_k - x_k^a)(x_k - x_k^a)^T]. \quad (3)$$

The Kalman filter equations can be expressed in two steps (Anderson and Moore, 1979), the forecast step (or time-update) where information about the system is used, and the analysis step (or measurement update) where information from the measurements is used. These steps are expressed as:

forecast step:

$$x_{k+1}^f = A_k x_k^a + B_k u_k, \quad (4)$$

$$P_{k+1}^f = A_k P_k^a A_k^T + F_k Q_k F_k^T, \quad (5)$$

and, analysis step:

$$L_k = P_k^f C_k^T (C_k P_k^f C_k^T + R_k)^{-1}, \quad (6)$$

$$P_k^a = P_k^f - L_k C_k P_k^f, \quad (7)$$

$$x_k^a = x_k^f + L_k (y_k - C_k x_k^f). \quad (8)$$

In large-scale environmental applications, the number of state variables is typically larger than the number of output variables, which in turn is much larger than the number of input variables, $n \geq m_w, p \gg m_u$. Under this assumptions, the computation time of the Kalman filter is dominated by (5) and takes $\mathcal{O}(n^3)$ flops. However, the system matrix A_k is typically obtained by discretising PDE's and hence is sparse. By exploiting this sparsity, the computational demand is reduced to $\mathcal{O}(n^2)$ flops. However, despite the computational power of present supercomputers, this does not make real-time estimation with the Kalman filter possible.

3. SUBOPTIMAL KALMAN FILTERS

Several suboptimal filtering schemes for use in large-scale applications have been developed. The number of computations and the storage requirements are reduced by approximating the Kalman filter equations.

Usually, a square root formulation is adopted. Potter and Stern (Potter and Stern, 1963) introduced the idea of factoring the error covariance matrix P_k into Cholesky factors, $P_k = S_k S_k^T$, and expressing the analysis step in terms of the Cholesky factor S_k , rather than P_k . While these algorithms are numerically better conditioned than the original Kalman filter equations, they are not guaranteed to more efficient, in contrast.

Suboptimal square root filters, on the other hand, gain speed, but loose accuracy by propagating a non-square $S_k \in \mathbb{R}^{n \times q}$ with very few columns, $q \ll n$. This leads to a huge decrease in computation times and storage requirements, while the computed error covariance matrix is still guaranteed to be positive definite.

4. THE REDUCED RANK SQUARE ROOT FILTER (RRSQRT)

The Reduced Rank Square Root filter (RRSQRT) (Verlaan and Heemink, 1997) is a square root algorithm based on an optimal lower rank approximation of the error covariance matrix. It is assumed that the matrix $F_k Q_k F_k^T$ is of low rank r , with $r \leq m_w \ll n$, such that a square root $F_k Q_k^{1/2} \in \mathbb{R}^{n \times r}$ can easily be found. The algorithm consists of three steps: the forecast step, the analysis step and the reduction step.

Forecast step

The forecast step is given by

$$x_{k+1}^f = A_k x_k^a + B_k u_k, \quad (9)$$

$$S_{k+1}^f = \begin{bmatrix} A_k S_k^a & F_k Q_k^{1/2} \end{bmatrix}, \quad (10)$$

where $S_k^a \in \mathbb{R}^{n \times q}$ is a square root of the optimal rank- q approximation of the error covariance matrix after the k -th analysis step. Notice that the number of columns in the covariance square root, and hence the rank of the error covariance matrix grows from q to $q+r$.

Analysis step

The RRSQRT has been proposed with a scalar analysis step (Verlaan and Heemink, 1997). This means that the estimates of the state and the error covariance square root need to be updated p times, one time for every component of the measurement-vector y_k . If the measurement noise is correlated, the measurements need to be transformed with $R_k^{-1/2}$. The resulting independent measurements can be processed one at a time.

Reduction step

The augmentation of the rank during the forecast step, could quickly blow up computation times. Therefore, the number of columns in S is reduced from $q+r$ to q by truncating the error covariance matrix $P = S S^T$ after the q largest eigenvalues and corresponding eigenvectors. The eigenvalue decomposition of P can efficiently be computed from the one of the much smaller matrix $S^T S \in \mathbb{R}^{(q+r) \times (q+r)}$. If the eigenvalue-decomposition of $S^T S$ equals

$$S^T S = X \Omega X^T, \quad (11)$$

it is straightforward to show that

$$(S X \Omega^{-1/2}) \Omega (S X \Omega^{-1/2})^T \quad (12)$$

is the eigenvalue-decomposition of P , and thus

$$\tilde{S} = [S X]_{:,1:q} \quad (13)$$

is a square root of the optimal rank- q approximation of P . Since $q, r \ll n$ this procedure is much faster than an eigenvalue decomposition directly on P .

When the process noise is negligible, speed-up can be obtained by assuming $Q_k = 0$. The update of the error covariance square root and the computation of the Kalman gain can then efficiently be implemented

by using the QR-decomposition. This leads to the Singular Square Root Kalman filter (SSQRTKF) (Barrero and De Moor, 2004).

5. THE REDUCED RANK TRANSFORM SQUARE ROOT FILTER

The SVD-based reduction is the most time consuming step of the RRSQRT. This motivates research to speed-up the reduction step. In this section, we propose a variant of the RRSQRT where the reduction is interweaved in the analysis step. To this aim, we adopt an analysis step where all the components of the measurement-vector are processed simultaneously, in contrast to the original formulation of the RRSQRT. Hence, this variant is very efficient when a large number of measurements are available, $p \gg q$. Since this variant uses a single transformation matrix to convert S_k^f into S_k^a , similar to the Ensemble Transform Kalman filter (Bishop *et al.*, 2001) and in the same time also reduces the rank of the error covariance matrix, we give it the name ‘‘Reduced Rank Transform Square Root filter’’ (RRTSQRT).

5.1 RRTSQRT Algorithm

The forecast step of the RRTSQRT is exactly equal to the one of the RRSQRT (9-10), and hence the rank of the error covariance matrix grows from q to $q+r$.

The analysis step is based on the Potter formulation

$$P_k^a = S_k^f (I - V_k^T D_k^{-1} V_k) S_k^{fT}, \quad (14)$$

where $V_k \triangleq C_k S_k^f$ and $D_k \triangleq V_k V_k^T + R_k$. For convenience of notation, we define the square matrix T_k as

$$T_k \triangleq (I - V_k^T D_k^{-1} V_k). \quad (15)$$

If the square root factorisation of T_k equals

$$T_k = G_k G_k^T, \quad (16)$$

it follows from (14) that

$$S_k^a \triangleq S_k^f G_k \quad (17)$$

is an exact matrix square root of P_k^a , $P_k^a = S_k^a S_k^{aT}$. In practical applications, G_k will be square. Hence S_k^a will have the same size as S_k^f and no reduction is done. Moreover, if $p \gg q$, it is prohibitive to evaluate (15) and factor the result consecutively. Inverting D_k , for instance, would require $\mathcal{O}(p^3)$ flops.

In the RRTSQRT, the combined analysis and reduction is done by computing a non-square G_k with fewer columns than rows. In addition, the computational burden for evaluating G_k is reduced. First, compute the $(q+r) \times (q+r)$ symmetric matrix $W_k \triangleq V_k^T R_k^{-1} V_k$. If C_k and R_k^{-1} are sparse, this takes $\mathcal{O}(p(q+r)^2)$ flops. Next, compute the eigenvalue decomposition of W_k ,

$$W_k = U_k \Lambda_k U_k^T, \quad (18)$$

and approximate W_k by putting the smallest r eigenvalues to zero, $\tilde{W}_k \triangleq \tilde{U}_k \tilde{\Lambda}_k \tilde{U}_k^T$, where $\tilde{U}_k \triangleq [U_k]_{:,1:q}$ and $\tilde{\Lambda}_k \triangleq [\Lambda_k]_{1:q,1:q}$. From (15), (18) and using the matrix inversion lemma, it is straightforward to show that

$$T_k = U_k (I_{q+r} + \Lambda_k)^{-1} U_k^T, \quad (19)$$

and hence, from (16),

$$G_k = U_k (I_{q+r} + \Lambda_k)^{-1/2}. \quad (20)$$

Approximating G_k by $\tilde{G}_k \triangleq \tilde{U}_k (I_q + \tilde{\Lambda}_k)^{-1/2}$, it follows from (17) that

$$\tilde{S}_k^a = S_k^f \tilde{U}_k (I_q + \tilde{\Lambda}_k)^{-1/2} \quad (21)$$

is an approximate matrix square root of P_k^a with a reduced number of columns. Notice that the lower rank approximation of W_k is needed to obtain an error covariance square root \tilde{S}_k^a with fewer columns than S_k^f . A best rank- q approximation of P_k^a is obtained under the conditions mentioned in the following theorem.

Theorem 5.1. Let all state variables be directly measurable, $p = n, C_k = I_n$, and let the components of the measurement noise vector be uncorrelated and have unit variances, $R_k = I_p$, then the RRTSQRT analysis step yields, starting from the $n \times (q+r)$ matrix S_k^f a $n \times q$ matrix \tilde{S}_k^a which is a square root of the optimal rank- q approximation of P_k^a .

Proof:

Under the assumption that $C_k = I_n$ and $R_k = I_p$, the matrix W_k simplifies to

$$W_k = S_k^{fT} S_k^f. \quad (22)$$

If the eigenvalue decomposition of W_k is given by (18) then, according to (17) and (20),

$$S_k^a = S_k^f U_k (I_{q+r} + \Lambda_k)^{-1/2} \quad (23)$$

is an exact matrix square root of P_k^a . The RRTSQRT approximates S_k^a by retaining the first q columns. We now prove that this is equivalent to making an optimal rank- q approximation of P_k^a .

An optimal rank- q approximation is obtained by approximating $P_k^a = S_k^a S_k^{aT}$ by his leading eigenvalues and corresponding eigenvectors. Similar to the reduction step in the RRSQRT, this SVD can be derived from the one of the much smaller matrix $S_k^{aT} S_k^a$, given by (from (23), (22) and (18))

$$S_k^{aT} S_k^a = \Lambda_k (I_{q+m} + \Lambda_k)^{-1}, \quad (24)$$

and hence diagonal. As a consequence, the matrix containing the eigenvectors of $S_k^{aT} S_k^a$ equals the identity matrix. And thus, according to (13), $\tilde{S}_k^a = [S_k^a]_{:,1:q}$ is a matrix square root of the best rank- q approximation of P_k^a . This equals the result we obtained with the RRTSQRT. \square

While the first condition of theorem 5.1 is very restrictive, the second condition can always be achieved by a transformation of the measurements. However, we will show in an example that, in the case where the

Table 1. Computational complexity of KF, RRSQRT and RRTSQRT.

	KF	RRSQRT	RRTSQRT
forecast step	$\mathcal{O}(n^2)$	$\mathcal{O}(nq)$	$\mathcal{O}(nq)$
analysis step	$\mathcal{O}(n^2p)$	$\mathcal{O}(np(q+r))$	$\mathcal{O}(nq(q+r))$
reduction step	–	$\mathcal{O}(n(q+r)^2)$	–

ratio $n/p \approx 10$, like for example in weather forecasting (Bishop *et al.*, 2001), the performance of the RRTSQRT is close to optimal.

The computation time of the RRTSQRT is dominated by (21), which takes $\mathcal{O}(nq(q+r))$ flops. This combined analysis and reduction is faster than a single analysis or reduction step in the RRSQRT, which have a computational burden of $\mathcal{O}(np(q+r))$ and $\mathcal{O}(n(q+r)^2)$ flops, respectively. Table 1 compares the computational complexity of the Kalman filter (KF), the RRSQRT and the RRTSQRT for the case where the system matrix A_k is sparse and $n > p, m_w \gg q$.

5.2 Properties

A first property of the RRTSQRT is that, just like the RRSQRT, it is algebraically equivalent to the Kalman filter for $q = n$. The proof is straightforward, and hence omitted.

A second property is that the RRTSQRT inherently solves for an ill-conditioned W_k -matrix. If W_k is ill-conditioned, the smallest eigenvalues and corresponding eigenvectors can correspond to numerical noise, reducing the performance of the filter. The RRTSQRT solves this problem by discarding the contributions from the noisy eigenvectors. Evensen solved the ill-conditioning problem of $C_k P_k^f C_k^T + R_k$ in the Ensemble Kalman filter in a similar way (Evensen and van Leeuwen, 1996).

Another property is that, like in the RRSQRT, the error covariance matrix is underestimated because of the reduction. Denoting the truncated part of P_k^a as \bar{P}_k^a , obeying

$$\bar{P}_k^a = P_k^a - \tilde{P}_k^a, \quad (25)$$

where $\tilde{P}_k^a \triangleq \tilde{S}_k^a \tilde{S}_k^{aT}$, then, since the RRSQRT makes an SVD-based lower rank approximation of P_k^a , the norm of the truncated part is minimal and equals the first eigenvalue of P_k^a that has been ignored,

$$\|\bar{P}_k^a\| = \lambda_{q+1}(P_k^a), \quad (26)$$

where $\lambda_{q+1}(P_k^a)$ is the $(q+1)$ -th eigenvalue of P_k^a . While (26) always holds for the RRSQRT, it only holds for the RRTSQRT under the conditions given in theorem 5.1. In all other cases, the RRTSQRT underestimates P_k^a more. Denoting the truncated part of G_k by \tilde{G}_k , the truncated part of P_k^a be written as

$$\bar{P}_k^a = (S_k^f G_k)(S_k^f G_k)^T - (S_k^f \tilde{G}_k)(S_k^f \tilde{G}_k)^T \quad (27)$$

$$= (S_k^f \tilde{G}_k)(S_k^f \tilde{G}_k)^T, \quad (28)$$

where $\tilde{G}_k \triangleq [G_k]_{:,q+1:q+r}$.

5.3 Preventing filter divergence

Since the error covariance matrix is underestimated, both the RRTSQRT and RRSQRT may suffer from filter divergence. Notice that this problem is more apparent in the RRTSQRT, since the error covariance matrix is more underestimated. However, from (28), the truncated part of the error covariance matrix can exactly be computed. Therefore, it is possible to correct for the underestimation. We extend two heuristic, but computationally efficient methods for preventing divergence to the case where the truncated part of the error covariance matrix can exactly be computed.

The first method is an extension of the covariance inflation technique, introduced by Anderson to prevent filter divergence in the Ensemble Kalman filter (Anderson and Anderson, 1999). Covariance inflation is an approach where the error covariance square root matrix is multiplied by a heuristically chosen inflation factor κ (mostly chosen between 1.01 and 1.05) to enlarge the covariances artificially. We propose to use a time varying inflation factor κ_k that accounts for the underestimation of the total variance. In other words, κ_k is chosen such that

$$\kappa_k \cdot \text{trace}(\tilde{P}_k^a) = \text{trace}(P_k^a). \quad (29)$$

Notice that $\text{trace}(\tilde{P}_k^a)$ and $\text{trace}(P_k^a)$, and thus κ_k can efficiently be computed from the singular values of \tilde{S}_k^a and S_k^a , respectively. The covariances are then inflated by replacing \tilde{S}_k^a by $\sqrt{\kappa_k} \tilde{S}_k^a$.

The second method is an extension of the technique introduced by Corazza (Corazza *et al.*, 2002), who found that adding small random perturbations to the error covariance square root after the analysis step, improved the stability of the filter. We extend this method by adding small random numbers with appropriate statistics to \tilde{S}_k^a . More precisely, it follows from (28) that, by replacing the i -th column of \tilde{S}_k^a by

$$[\tilde{S}_k^a]_{:,i} + \frac{1}{\sqrt{q-1}} S_k^f \tilde{G}_k v_i, \quad (30)$$

where the random numbers v_i are sampled from a normal distribution with average zero and variance one, the new error covariance matrix approaches P_k^a .

6. STATE ESTIMATION FOR 2D MHD FLOW

6.1 Introduction

Plasma, as a distinct state of matter, plays a crucial role in numerous branches of science and engineering. The Earth is constantly bombarded by a plasma emitted by the Sun, the ‘‘solar wind’’. The state and behaviour of the solar wind is referred to as ‘‘space weather’’. During flares and coronal mass ejections, the most energetic solar phenomena, magnetic clouds with a mass up to 10^{14} kg and speeds up to 2600 km/s are ejected, causing fluctuations in the terrestrial magnetic

field and causing problems with Earth-based systems. Plasma flow is the subject of magnetohydrodynamics (MHD), which involves both fluid dynamics and electrodynamics. Consequently, MHD is governed by coupled partial differential equations, including both the Navier-Stokes and Maxwell's equations.

This section is concerned with state-estimation for 2D MHD flow, which is motivated by the fact that sub-optimal filters could provide the initial conditions for a space weather forecast (Groth *et al.*, 2000). Starting from the ideal MHD equations, we first set up a 2D simulation that emulates a space storm interacting with the Earth's magnetosphere and then compare the assimilation results of the RRSQRT and RRTSQRT.

6.2 Space Weather forecasting example

We assume that the plasma acts as a single fluid, in which the separate identities of positively and negatively charged species are ignored. Furthermore, we assume that the plasma flow occurs in a non-relativistic regime and we neglect ionization and recombination. Also, we assume that the conductivity of the plasma is infinite. Under these simplifying assumptions, the resulting ideal MHD equations are (Kallenrode, 2000; Freidberg, 1987) (see table 2 for the explanation of the symbols)

Mass continuity

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{u}) = 0, \quad (31)$$

Adiabatic equation of state

$$\frac{d}{dt} \left(\frac{p}{\varrho^\gamma} \right) = 0, \quad (32)$$

Momentum equation (ignoring external forces)

$$\varrho \frac{\partial \mathbf{u}}{\partial t} + \varrho (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \mathbf{J} \times \mathbf{B}, \quad (33)$$

Ampere's law (ignoring displacement current)

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}, \quad (34)$$

Faraday's law

$$\nabla \times (\mathbf{u} \times \mathbf{B}) = \frac{\partial \mathbf{B}}{\partial t}, \quad (35)$$

Gauss's law

$$\nabla \cdot \mathbf{B} = 0. \quad (36)$$

The ideal MHD equations are discretised over a 24×44 grid, using a second order Rusanov scheme (Eymard *et al.*, 2000). Since each grid-point contains 6 variables, this results in a nonlinear system of order $n = 6336$.

In order to compare the assimilation results of the RRSQRT and the RRTSQRT, a twin experiment was carried out. A reference solution was generated with the nonlinear system subject to process noise with a low rank covariance matrix. The initial and boundary conditions were chosen to emulate the interaction of

Table 2. List of symbols

Symbol	Physical quantity
μ_0	permeability of free space
ϱ	mass density
p	pressure
γ	ratio of specific heats
\mathbf{u}	velocity
\mathbf{J}	current density
\mathbf{E}	electric field
\mathbf{B}	magnetic field

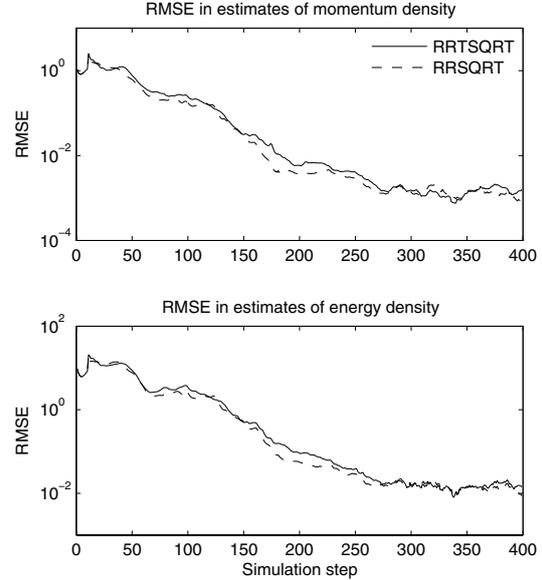


Fig. 1. RMSE in the estimates of the momentum density (top) and energy density (bottom) for the RRTSQRT (solid line) and RRSQRT (dashed line).

a space storm with the Earth's magnetosphere. At total of $p = 600$ observations were generated from the simulated data and measurement noise with a diagonal covariance matrix was added. Next, both filters were initialised with the same perturbed initial condition and error covariance square root matrix. The rank of the error covariance matrix was chosen to be $q = 250$. During the forecast step, the nonlinear system was numerically linearized around the current state estimate to obtain the system matrix A_k . Boundary conditions were assumed to be known.

6.3 Results

In figure 1, the Root Mean Squared Error (RMSE) in the estimates of the momentum density and the energy density are plotted for the RRTSQRT and RRSQRT as function of time. Both filters converge to the same RMSE-value. The speed of convergence for the RRTSQRT is only slightly slower than the one of the RRSQRT.

Figure 2 compares the errors in the estimates of the magnetic field magnitude and pressure for the RRTSQRT and RRSQRT at simulation step 100. The errors

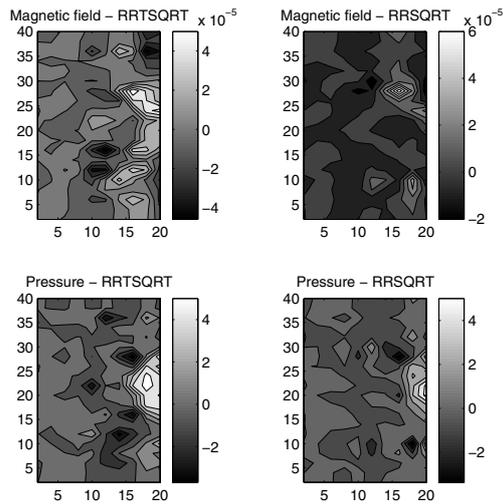


Fig. 2. Comparison between the errors in the estimates of the magnetic field magnitude (top) and pressure (bottom) for the RRTSQR (left) and RRSQR (right) at simulation step 100.

are largest in the region where the space storm (moving from the left hand side of the plots to the Earth at the right hand side) forms a bowshock and interacts with the magnetosphere, as can be seen in the right hand side of the figures. However, the residuals of both filters have the same order of magnitude.

While the reduction step of the RRSQR retained on average 99.2 percent of the total variance, the combined analysis and reduction step of the RRTSQR, retained 97.0 percent. This means that the optimal inflation factor is $\kappa = 1.015$, and hence is very close to the heuristically chosen factor in the EnKF.

7. CONCLUSIONS

The Reduced Rank Transform Square Root filter was introduced as a numerically more efficient variation of the Reduced Rank Square Root filter. Speed-up was obtained by adopting an analysis step with simultaneous processing, which in the same time performs the reduction. A theoretical study of both filters showed that, in general, the Reduced Rank Transform Square Root filter will underestimate the error covariance more than the Reduced Rank Square Root filter and hence is more sensitive to filter divergence. However, two techniques to prevent filter divergence were proposed.

The performance of both filters was analyzed by comparing their assimilation results on a magnetohydrodynamic example which emulates a space storm interacting with the Earth's magnetosphere. Simulation results confirm the theoretical study that the Reduced Rank Transform Square Root filter is slightly more sensitive to filter divergence, but almost as accurate and computationally less expensive than the Reduced Rank Square Root filter.

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