

# On the use of empirical orthogonal base functions in the analysis of GRACE-observed mass changes

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## Abstract

We use the well known statistical and data-adaptive method of the principal components/empirical orthogonal functions and its generalization, the multichannel singular spectrum analysis, to study the GRACE-observed mass variations in North America from high temporal resolution gravity field solutions. Both methods are able to extract the main mass variations, i.e., the mass increase in Hudson Bay, the mass decrease in the Alaskan glaciers and Greenland, and the annual hydrology cycle. Some peculiarities of the use of the orthogonal base functions, such as possible distortions in the orthogonal patterns, as well as the inference of the statistical significance of the extracted variability are discussed.

## 1. Introduction

The Gravity Recovery and Climate Experiment (GRACE) satellite mission (Tapley et al., 2004) operated by NASA and the German Aerospace Center (DLR) provides Earth gravity field solutions on a regular basis since March 2002 with a monthly and higher temporal resolution. These time series of gravity changes integrated in a vertical column are analyzed to infer mass variations in the interior, on the surface, or in the close exterior of the Earth such as the cycle of continental water storage, snow accumulation and melting, variations in the mass of the polar ice sheets and mountain glaciers, variations in the atmospheric surface pressure and ocean bottom pressure, and postglacial rebound (Wahr and Davis, 2002).

The conventional method that is applied in analyses of the GRACE-observed mass variations both on a global and regional scale is least-squares fitting to the time series of the spherical harmonic coefficients or the grid points of maps of variability, which provides estimates of the amplitude and phase of the annual and semi-annual cycles and possibly a trend. It takes into account GRACE errors and can handle discontinuous time series. Alternatively, the methods that are based on the empirical orthogonal functions can be used to derive changes in the periodic cycles as well as inter- and intra-annual mass variations. In this paper, we study and compare the method of the principal component/empirical orthogonal functions (PC/EOF) analysis and the generalization of this method, namely the mul-

tichannel singular spectrum analysis (MSSA). The PC/EOF analysis decomposes times series of single scalar geophysical fields in orthogonal spatial patterns and their time evolution. Examples include, but are not limited to, the modelling of inter-annual changes and long-term trends in sea level (Woolf et al., 2003), global sea surface temperature (Robertson and Mechoso, 1998), and coupled patterns of sea surface temperature and radar satellite altimetry sea surface heights (Leuliette and Wahr, 1999). In relation to GRACE, the PC/EOF analysis has been applied by Viron et al. (2006) to study global climate signals extracted from the GRACE-observed mass changes. Chambers (2006) analyzed the main signals of the seasonal steric sea level variations and Schrama et al. (2007) used PC/EOF to reduce the noise in the GRACE gravity field solutions. Rangelova et al. (2007) studied long-term and inter-annual variations in addition to the annual hydrology cycle in North America.

MSSA originates from the studies of the dynamics of chaotic systems using noise contaminated data but has also been applied in oceanography, meteorology and climate studies for analyzing the spatio-temporal variability of scalar fields (Ghil et al., 2002; Keppenne and Ghil, 1993; Plaut and Vautard, 1994; Jiang et al., 1995; Allen and Robertson, 1996). Vianna et al. (2007) applied the singular spectrum analysis, to which MSSA reduces in the case of a single time series, to derive the mean dynamic topography from GRACE data. The main difference with the PC/EOF method is that time-lagged fields are decomposed in orthogonal spatio-temporal patterns and principal component time series using the spatio-temporal covariance information in the data. In the ocean studies, MSSA is equivalent to the extended EOF analysis. The only difference is the number of time lags, which in the extended EOFs are much less compared to MSSA. The traditional PC/EOF analysis is a special case of MSSA when no time lags are introduced.

The main advantage of the use of both PC/EOF and MSSA stems from the fact that as non-parametric methods with data-dependent base functions they adapt to the analyzed data sets thus allowing for extraction of modulated periodic oscillations (Vautard and Ghil, 1989) while efficiently separating these signals from the random data errors. The main disadvantage is that due to the imposed orthogonality of the base functions distortions in the extracted patterns are possible. Moreover, mixing of the spectral modes can be encountered usually in short data series. Both PC/EOF and MSSA require uninterrupted data in space and time. In the case of missing GRACE gravity field solutions, data gaps can be bridged by least-squares interpolation.

We apply both PC/EOF and MSSA to the grids of continental water mass variations in North America derived from weekly GRACE gravity field data. Although these fields have low spatial resolution (approximately 700 km half-wavelength), the constructed uninterrupted time series contains 313 epochs and spans six complete years which allows us to demonstrate the efficiency of both methods.

## 2. Principal component/Empirical orthogonal functions analysis

We present the theory of the PC/EOF analysis using equations and definitions given by Jolliffe (2002). Gridded or scattered data are organized in a  $(n \times p)$  matrix  $\mathbf{D}$ , where  $n$  is the number of observations (time epochs) and  $p$  is the number of variables (data points). The data matrix  $\mathbf{D}$  is decomposed by singular value decomposition as follows:

$$\mathbf{D} = \mathbf{U}_D \mathbf{\Lambda}_D^{1/2} \mathbf{E}_D^T, \quad (1)$$

where  $\mathbf{U}_D$  and  $\mathbf{E}_D$  are  $(n \times n)$  and  $(p \times p)$  orthonormal matrices. The column vectors of  $\mathbf{E}_D$  define the EOF loading patterns (also called spatial amplitudes).  $\mathbf{\Lambda}_D$  is a diagonal matrix of rank  $r \leq \min(n, p)$  which contains the spectrum (eigenvalues)  $\sqrt{\lambda_i}$ ,  $i=1, \dots, r$ . The principal component (PC) time series are computed from the column vectors of  $\mathbf{P}_D$  where

$$\mathbf{P}_D = \mathbf{U}_D \mathbf{\Lambda}_D^{1/2} \quad (2)$$

The approximated signal variability is the best rank  $m$  approximation of  $\mathbf{D}$  using the selected  $m$  PCs, as follows:

$${}_m \hat{\mathbf{D}} = {}_m (\mathbf{P}_D \mathbf{E}_D^T). \quad (3)$$

If the PC/EOF analysis is applied with time-centered data, i.e., the mean from each column of the data matrix  $\mathbf{D}$  is removed, the diagonal elements of the matrix  $\mathbf{\Lambda}_D$  are the variances explained by each principal component in terms of the percentage of the total data variance. Usually, the orders of the PCs define their significance and the first several modes represent the dominant signal variability in the data.

According to Benzi et al. (1997), a pertinent weakness of PC/EOF is that the orthogonal modes, in which the data are decomposed, do not necessarily represent physical variability. When physical processes are analyzed, rotated PC/EOF should be used in order to properly represent the physical relations in the data. In addition, rotation detects undesirable effects (Richman, 1985), such as domain shape dependence, i.e., the signal changes with the change in the domain shape and size. A commonly applied algorithm is the *varimax* rotation of either EOF patterns or PC time series (Preisendorfer, 1988). Rotation maximizes the variance of the squared covariances between each rotated principal component and each of the original principal component time series. This results in few large loading patterns and many close to zero patterns. Therefore, rotation helps one to discriminate among the modes and simplifies the interpretation while revealing the physical variability in the data. As demonstrated by Rangelova and Sideris (2008), the varimax rotation of the signal modes facilitated the interpretation of the GRACE-derived geoid variability in North America.

In addition to the rotation, the methods for selecting the significant principal

components in the approximation step are often a subject of discussion. Generally, three groups of methods exist. The first group includes the methods based on the amount of the data variance explained. The *ad hoc* rule of thumb is to retain the PCs that explain at least 70% of the data variance (Valle et al., 1999). Another method is North's rule of thumb (North et al., 1982) which states that if the error of the eigen-value is larger than or comparable with the difference between two adjacent eigen-values then it is unlikely that these eigen-values represent separate modes. A very simple method is the inspection of the leveraging point of the spectrum where the rapid decline of the signals part of the spectrum transitions to the gradually decreasing part of the noise. The second group includes the time history methods that test the principal component time series for being random samples of a white noise process. One commonly applied method is the Kolmogorov-Smirnov (KS2) rule given by Preisendorfer (1988). The third group comprises the space-map methods based on the comparison of the EOF patterns with known geophysical patterns of variability.

### 3. Multichannel singular spectrum analysis

The main steps of the MSSA computational procedure are given following Allen and Robertson (1996):

1. For a data set  $\mathbf{d}(d_{il;t=1,T;l=1,L})$ , which consists of  $T$  observations (time epochs) each with  $L$  variables (channels) and chosen  $M$  time lags (a lag-window), form a *data trajectory matrix*  $\mathbf{D}$  using  $M$  lagged copies of the channels  $l=1,L$

$$\mathbf{D}_l \begin{pmatrix} d_{1l} & d_{2l} & \cdots & d_{Ml} \\ d_{2l} & d_{3l} & \cdots & d_{M+1l} \\ \vdots & \vdots & \cdots & \vdots \\ d_{Nl} & d_{N+1l} & \cdots & d_{Tl} \end{pmatrix}, 1 \leq l \leq L \quad (4)$$

where  $N = T - M + 1$  is the number of the overlapping views of the series for each point in the channel. Form the trajectory matrix  $\mathbf{D}$  of size  $(N \times ML)$ , as follows:

$$\mathbf{D} = (\mathbf{D}_1 \quad \mathbf{D}_2 \quad \dots \quad \mathbf{D}_L) \quad (5)$$

2. Apply singular value decomposition of  $\mathbf{D}$ , as follows:

$$\mathbf{D} = \eta \mathbf{P}_D \mathbf{\Lambda}_D^{1/2} \mathbf{E}_D^T, \quad \eta = \max(N, LM) \quad (6)$$

where  $\eta$  is a normalization factor. The matrix  $\mathbf{P}_D$  contains  $N$  orthonormal vectors called spatio-temporal principal components that are also eigen-vectors

of the lag-covariance matrix  $\mathbf{C}_D^{(P)} = (LM)^{-1} \mathbf{D} \mathbf{D}^T$ . The matrix  $\mathbf{E}_D$  contains  $M$  orthonormal vectors called spatio-temporal empirical orthogonal functions, also eigen-vectors of the lag-covariance matrix  $\mathbf{C}_D^{(E)} = (N)^{-1} \mathbf{D}^T \mathbf{D}$ . The diagonal entries of the eigen-spectrum  $\mathbf{\Lambda}_D = \mathbf{P}_D^T \mathbf{C}_D^{(P)} \mathbf{P}_D = \mathbf{E}_D^T \mathbf{C}_D^{(E)} \mathbf{E}_D$  are proportional to the data variance in the PCs (EOFs).

3. Filter out the spatiotemporal EOFs of no interest:

$$\mathbf{D}' = \mathbf{D} \mathbf{E}_D (\mathbf{I} - \mathbf{K}) \mathbf{E}_D^T \quad (7)$$

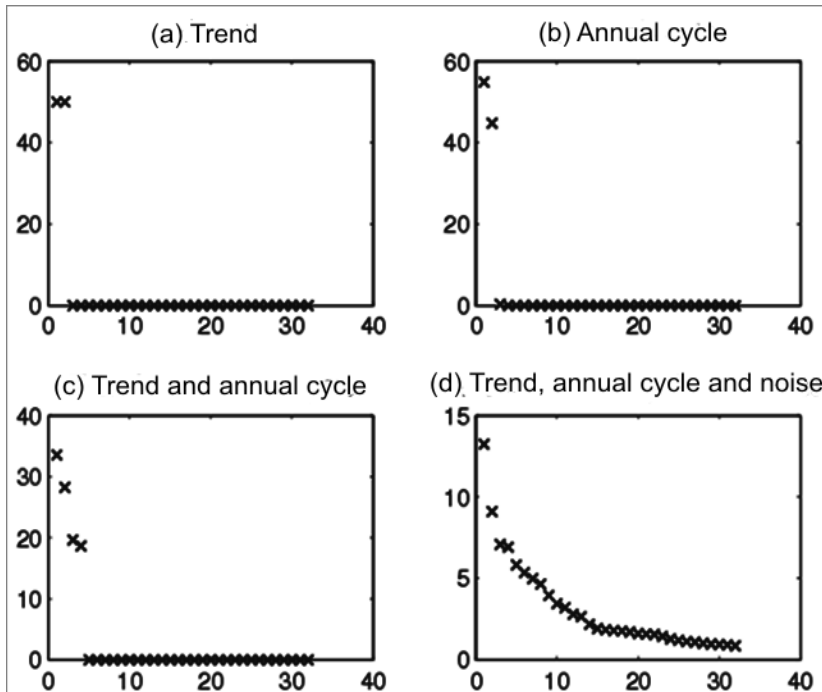
where  $\mathbf{K}$  is a diagonal matrix with  $K_{ii} = 0$  if the  $i^{\text{th}}$  EOF is retained and  $K_{ii} = 1$  if the  $i^{\text{th}}$  EOF is filtered out.  $\mathbf{D}' = (\mathbf{D}'_1 \quad \mathbf{D}'_2 \quad \cdots \quad \mathbf{D}'_L)$  contains the filtered augmented time series for all channels.

4. Reconstruct the filtered series for each channel by averaging along the diagonals of  $\mathbf{D}'_l, l = 1, L$  as shown by Golyandina et al. (2001, p.17).

In order to study the capabilities of the MSSA to extract annual variations and a trend from relatively short spatiotemporal series, we simulated a series of 60 epochs of monthly water mass variations using the annual amplitude and phase of the GLDAS/Noah model (Rodell et al, 2004) in North America and the ICE-5G (VM2) postglacial rebound model of Peltier (2004). Random noise was simulated from the residuals in the weighted least-squares fit to the GRACE-derived monthly water mass variations. The residuals are spatially correlated due to the GRACE system and processing of the GRACE measurements, post-processing smoothing of the data errors and the residual geophysical signals not accounted for by the least-squares fit.

The trend generates an eigen-pair of modes which explain equal amounts of the data variance (Figure 1a). It requires the largest possible lag-window, which however cannot exceed a half of the length of the time series when the number of the overlapping views is minimal. Ideally, each of the modes of the annual cycle should also explain 50% of the data variance. To extract this periodic oscillation, the size of the lag-window should be at least double the wavelength of the periodic signal. At the same time, the number of the overlapping views, which determines the statistical significance of the extracted oscillation, should be large enough in order to decrease the dependence on the lag-window (observed on Figure 1b) and to ensure good spatio-temporal localization in the reconstruction step. Therefore, the requirements for extracting periodic oscillations and trend-like variations are conflicting with each other and a good balance cannot be achieved for the relatively short GRACE series, in which case the trend and periodic modes tend to mix (Figure 1c). As a result, the trend PC time series show oscillations while the periodic PC time series show an apparent trend. If correlated noise in space and time (of geophysical origin) is present in the data, “non-genuine” oscillations can be generated in the low frequency band of the eigen-spectrum in the presence of the

trend and can mistakenly be taken as true signals (Allen and Robertson, 1996). The correlated GRACE noise can further enhance the spectral mixing of the trend and annual modes (Figure 1d). If the annual hydrology cycle is of interest, any known trends should be removed prior the analysis of the GRACE time series.



**Figure 1:** Eigen-spectra of simulated GRACE data series. The vertical axis shows the percentage of the data variance explained by each mode (horizontal axis)

As in the PC/EOF analysis, the significant modes can be determined upon the inspection of the leveraging point of the eigen-spectrum. However, this simple method is inefficient in the presence of correlated noise. The modes of true oscillations with small variances and low signal-to-noise ratio could be buried in the eigen-spectrum and discarded when the significant variations are decided by the cut-off rule. A generalisation of the Monte Carlo singular spectrum analysis algorithm can be used to construct a test to identify these oscillations (Allen and Robertson, 1996). While GRACE data are subject to correlated noise in space, i.e., north-south stripes in the maps of the weekly mass variations, this noise is of different nature than the “red noise” in the geophysical systems that is also likely present in some form in the GRACE-observed water mass variations. The magnitudes of the GRACE correlated errors are largely reduced by means of the post-processing smoothing. Therefore, we do not study how these errors propagate in the eigen-spectrum of the mass variations.

## 4. Data

We analyze a series of water mass variations  $\Delta h$  expressed in cm of water equivalent height (WEH) that are synthesized for each time epoch  $t$  and geographical location (co-latitude  $\theta$  and longitude  $\lambda$ ) from the weekly GFZ GRACE gravity field solutions given by the changes (with respect to the mean) of the spherical harmonic cosine and sine coefficients,  $\Delta C_{lm}$  and  $\Delta S_{lm}$ , of the maximum degree  $l$  and order  $m$  30, as follows (Wahr et al., 1998):

$$\Delta h(\theta, \lambda, t) = \frac{\alpha_e \rho_{ave}}{3 \rho_w} \sum_{l=2}^{30} \sum_{m=0}^l \frac{2l+1}{1+k_l} W_l \bar{P}_{lm}(\cos\theta) [\Delta C_{lm}(t) \cos(m\lambda) + \Delta S_{lm}(t) \sin(m\lambda)] \quad (8)$$

In this equation,  $\bar{P}_{lm}(\cos\theta)$  are the fully normalized associated Legendre functions of degree  $l$  and order  $m$  and  $W_l$  are the weighting coefficients of a smoothing isotropic Gaussian filter;  $\rho_w$  is the water density of  $1000 \text{ kg/m}^3$ ,  $\rho_{ave}$  is the average density of the Earth,  $5517 \text{ kg/m}^3$ ,  $k_l$  is the load Love number of degree  $l$  and  $a_e$  is the mean radius of the Earth.

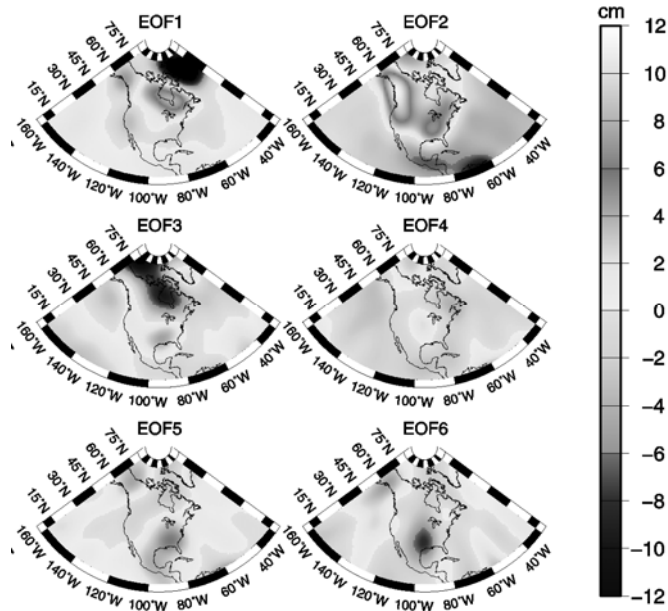
The GRACE errors are smoothed by means of a Gaussian averaging filter with a radius of 700 km, which roughly corresponds to the spatial resolution of the weekly data. The time series consists of 313 epochs between week #5 of 2004 and week #4 of 2010. Thus, the data set is a complete 6-year series of weekly water mass changes with respect to the mean field for the same time period. In the construction of the data matrix  $\mathbf{D}$ , the variables (channels) are the grid point water mass changes and the observations are the temporal changes of the grid points.

In addition to the continental water mass variability and postglacial rebound, the eigen-spectrum of the data covariance matrix of the GRACE-observed mass changes in North America likely contains errors in the de-aliasing models of atmospheric variability, tides and ocean signals, leakage of the ocean signals over the continents, and correlated errors. Because of the complexity of the GRACE errors and the known variability, we have found that the ad hoc rule of thumb is the most efficient technique for selecting the retained principal components.

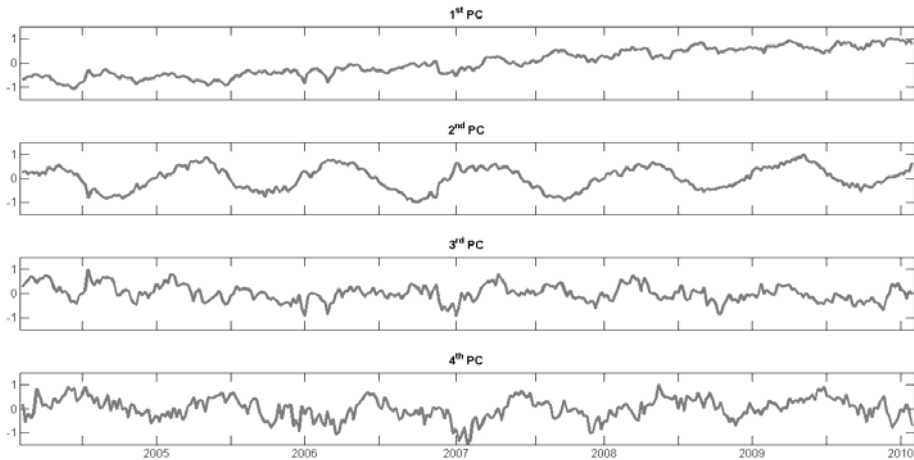
## 5. Results

### 5.1 PC/EOF analysis

Figure 2 shows the first six EOF loading patterns. The first EOF represents the secular mass increase over Hudson Bay associated with the postglacial rebound signal, as well as the mass decrease in south-eastern Greenland and Alaska due to the rapid ice sheet and glaciers melting. The time evolution of this EOF is a trend as shown in Figure 3 by the first PC time series, which is normalized by dividing



**Figure 2:** EOF loading patterns of the weekly GRACE-observed mass variations in North America; units are cm WEH



**Figure 3:** Normalized principal component (PCs) time series of the weekly GRACE-observed mass variations in North America

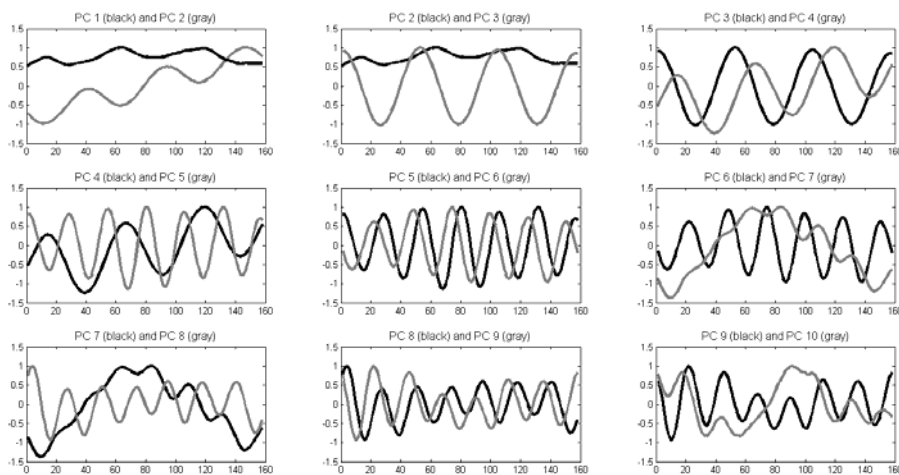
with the maximum value. Therefore, the EOF multiplied by the same maximum represents the magnitude of the signal in cm WEH. The trend mass variations represent about 44% of the total data variance. The second EOF shows the pattern of the snow accumulation and melting in the Western Cordillera and Quebec-Labrador and accounts for about 20% of the data variance. The second PC time



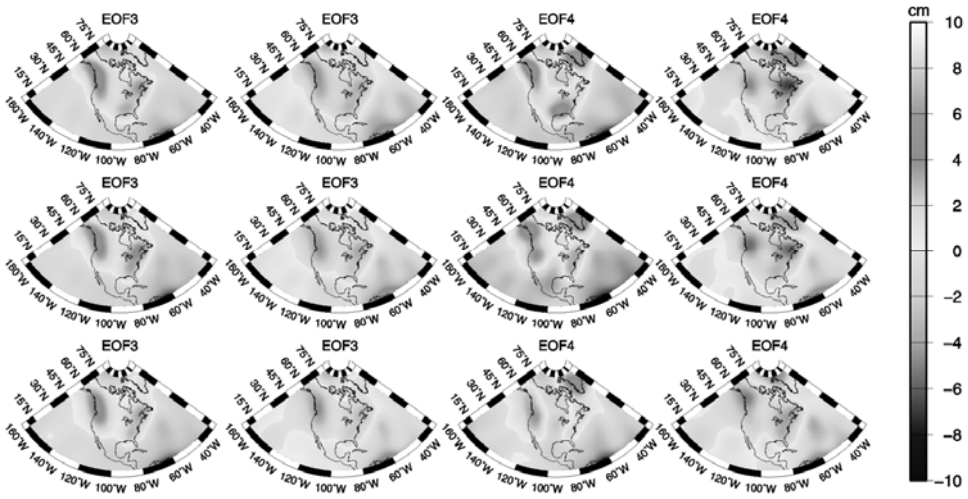
series clearly shows the more gradual late fall and winter snow accumulation with a maximum in April and the rapid spring melting. The lowest water content for North America is reached in September/October. The third mode shows mostly dipole variability (11%) over North America. The corresponding PC time series does not show structured signal behaviour. The fourth, fifth and sixth modes explain low percentage of the data variance (approximately 3% each). We show only the fourth PC which accounts for the time evolution of the hydrologic signal in St. Lawrence River and Mississippi basins and the US high plains and shows an annual cycle with December/January lows and May/June highs.

## 5.2 MSSA

The parameters of the analysis are as follows. The lag-window is 156 epochs, which is the maximum possible window and at the same time a multiple of the annual cycle. This allows us to analyze the trend, annual and semi-annual variations without varying the lag-window in each case. As in the PC/EOF analysis, the trend is the most dominant signal identified by the first and second modes in Figures 4 and 5 but contributes only 33% to the total variance. The third and fourth modes account for the annual cycle with 24% of the data variance. Clear spectral mixing of the trend and annual modes is seen in both figures. If the water mass variations were the sole focus of this analysis then the geodynamic postglacial rebound signal should have been removed using the most accurate available model which would leave the annual cycle as the signal with the largest variance in North America. However, as shown in Rangelova and Sideris (2008), any residual mass variations due to the imperfect postglacial rebound model will be present in the hydrology EOF loading patterns.



**Figure 4:** Normalized spatio-temporal principal component (PCs) time series of the weekly GRACE-observed mass variations in North America



**Figure 5:** Spatio-temporal EOF cosine (left) and sine (right) loading patterns of the weekly GRACE-observed mass variations in North America; units are cm WEH

The third pair (fifth and sixth modes), which corresponds to the semi-annual variations, explains only 5.2% of the total data variance and is mixed with the seventh, eighth and ninth modes. The largest semi-annual patterns are located over the oceans. Without further analysis of the GRACE-observed residual ocean signal and restoring the main part from the background models used in the GRACE data processing, it is difficult to assess if the extracted semi-annual variability is indeed a real signal. It should be noted that the conventional PC/EOF analysis does not see semi-annual variability or more precisely it is not able to extract the low-variance signal from the noisy data.

Figure 5 shows the three maximums and minimums in the annual sine and cosine loading patterns in cm WEH after multiplying the EOFs with the maximums of the corresponding PC time series. The third EOF is the pattern of the snow mass variability in the east and west mountain regions. While this EOF pattern does not change in time, the fourth EOF shows large variations both in space and time. There is an apparent reduction in the amplitudes that compensates for the positive trend in the fourth PC times series in Figure 4. Further evidence that the trend and annual signals are not effectively separated is found in the trend EOFs which contain patterns associated with the annual hydrology variations. Part of the problem comes from the fact that in some areas, such as the Alaskan glaciers, Hudson Bay and Laurentide, grid points exhibit both trend and annual variations, which in this case are virtually inseparable. This effect is further enhanced by the low spatial resolution of the GRACE mass variations. However, the main factor for this spectral mixing is the relatively short data series. An analysis of a 10-year time series of synthetic mass variations computed from postglacial rebound and hydrology mod-

els shows that if the GRACE data noise is disregarded the effect of the spectral mixing becomes irrelevant. The main reason for this improvement is the increased statistical significance of the annual cycle.

## 6. Conclusions

We analyzed 6 years of GFZ weekly GRACE water mass changes in North America using the conventional principal components/empirical orthogonal functions (PC/EOF) analysis and the multichannel singular spectrum analysis (MSSA). Both methods are able to extract the main mass variations, i.e., the mass increase in Hudson Bay and the mass decrease in the Alaskan glaciers and Greenland and the annual hydrology cycle, from the noisy data, but the MSSA could not separate well the trend and annual signals, both appearing to explain large portions of the total data variance. The main reason is likely the fact that while increasing the lag-window size we were not able to control the statistical significance of the extracted periodic variability. As GRACE continues to provide data, the problem will become less significant, but the computational load will eventually increase significantly. This is the main obstacle that does not allow analyses of series of maps of global mass variability, in which case PC/EOF has a clear advantage. Nonetheless, MSSA will be more relevant in the studies of the GRACE-derived ocean mass changes where spatio-temporal variations of the EOFs may be more pronounced than on land. Furthermore, as shown in our examples, MSSA is able to extract a low-variance semi-annual signal which was not the case for the PC/EOF analysis. Whether this signal is of geophysical origin is yet to be verified; nevertheless, it may be advantageous to apply MSSA in the studies of the water balance in large river basins with a large semi-annual cycle such as Congo or to study low-variance inter-annual signals.

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