Supplement of

Development and evaluation of 0.05° terrestrial water storage estimates using Community Atmosphere Biosphere Land Exchange (CABLE) land surface model and assimilation of GRACE data

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Supplement

Pseudocodes of GRACE DA

CABLE LSM is written in Fortran90, while the GRACE DA module can be written in any programming language, e.g., Fortran, Python, Matlab. In this study, the processing is performed in a Unix environment with Fortran compiler, and NetCDF library installed. Comprehensive details on CABLE installation and simulation are given in [https://trac.nci.org.au/trac/cable/wiki/CableUserGuide](https://trac.nci.org.au/trac/cable/wiki/CableUserGuide). A single-core central processing unit (CPU) and 16 GB memory are sufficient to carry out the simulation, but higher computational power helps to speed up the process. The processing details of GRACE DA are clearly described in Sect. 3 and Fig. 3. Below is the pseudocode of the processing.

**S1. Main program**

Define $N_{lat}$ = Length of latitude of the study domain, $N_{lon}$ = Length of longitude

Define $N_{time}$ = Number of simulation epoch, $N_{state}$ = number of state variables, $N_{ens}$ = number of ensemble members

Set first processing year and month

While processing year ≠ last year and month ≠ last month

Perturb forcing data and parameter of the processing year and month (see S2 below)

Perform model propagation of all ensemble members for one month

If GRACE data of the processing year and month are available

Print “Performing GRACE DA”

Perturb GRACE data of the processing year and month (see S2 below)

Collect ensemble model TWS states in matrix $A$ (see Sect. 3.1)

Collect perturbed TWS observation in matrix $D$ (see Sect. 3.1)

Define matrix $H$ (see Eq. 3 and S3 below)

Compute TWS monthly update ($\Delta A$) using Kalman equation (Eq. 4)

Divide TWS monthly update by a number of days ($\Delta A/N_{\text{day}}$) to obtain the daily update

Reinitialize initial states

For ensemble member $j$

For process day $d$

Add TWS daily update $j$ to TWS initial states of day $d$

Perturb forcing and parameter of year, month, and day $d$ (see S2 below)

Perform model propagation of ensemble $j$ for day $d$
Save simulation output of ensemble \( j \) for day \( d \) in memory

End
End
Else
Print “Missing observations, skip GRACE DA”
Do nothing
End
Collect result, e.g., compute ensemble mean of states (see S4 below)
Set processing year and month to the next processing year and month
End

S2. Perturbation
Obtain forcing data, parameter, or observation from input
Obtain the uncertainty (standard deviation, \( std \)) of forcing data, parameter, or observation from input
Obtain correlation length (\( L \)) of forcing data and observation from input
If the input is forcing data
Define matrix \( F \); dimension is 4D (\( N_{lat}, N_{lon}, N_{time}, N_{ens} \))
If the input is precipitation or shortwave radiation
Generate multiplicative noise based on lognormal distribution with given \( std, N_{ens}, L \)
Else if the input is temperature
Generate additive noise based on a normal distribution with given \( std, N_{ens}, L \)
End
For each ensemble member \( j \)
Apply the generated noise to nominal value and store in \( F[ :, :, :, j] \)
End
Else if the input is parameter or observation
Define matrix \( P \); dimension is 3D (\( N_{lat}, N_{lon}, N_{ens} \))
Generate additive noise based on a normal distribution with given \( std \) and \( N_{ens} \)
For each ensemble member \( j \)
Apply the generated noise to the nominal value and store it in \( P[ :, :, j] \)
Else if the input is observation

Define matrix \( \text{OBS} \); dimension is 3D \((N\text{lat}, N\text{lon}, N\text{ens})\) to store perturbed monthly TWS

Generate additive noise based on a normal distribution with given \( \text{std}, N\text{ens}, L \) \((L \text{ is optional})\)

For each ensemble member \( j \)

Apply the generated noise to the nominal value and store it in \( \text{OBS}[::,::,j] \)

End

End

S3. Setting matrix \( \text{H} \)

Obtain model and mascon coordinate (latitude, longitude) from input

Determine \( \text{H} \) matrix dimension based on the number of model grid cells inside mascon cells

Define zero matrix \( \text{H} \)

For mascon grid cell \( i \)

Search for all model grid cells \( (k) \) inside mascon \( i \), and create a row vector

Assign \( 1/k \) element to the row vector

Place the row vector at \((i,k)\) position of the matrix \( \text{H} \) \(\text{(Eq. 3)}\)

End

S4. Saving ensemble results

Each ensemble output can be obtained from the memory

Allocate matrix \( \text{B} \); dimension is 5D \((N\text{lat}, N\text{lon}, N\text{time}, N\text{state}, N\text{ens})\) to store ensemble outputs

For ensemble output \( j \)

Collect daily estimates of all estimated variables in matrix \( \text{B}[::,::,::,::,j] \)

End

Compute ensemble mean value of the matrix \( \text{B} \); the output is a 4D matrix \((N\text{lat}, N\text{lon}, N\text{time}, N\text{state})\)

Compute ensemble standard deviation value of the matrix \( \text{B} \); the output is a 4D matrix

Save monthly ensemble mean and standard deviation in the desired file format (e.g., NetCDF)