



NERO GRAV

New Refined Observations of Climate Change from Spaceborne Gravity Missions

International Spring School
Neustadt an der Weinstraße, Germany, March 12, 2025

Stochastic Modeling of GRACE/GRACE-FO Data

Michael Murböck (TU Berlin)

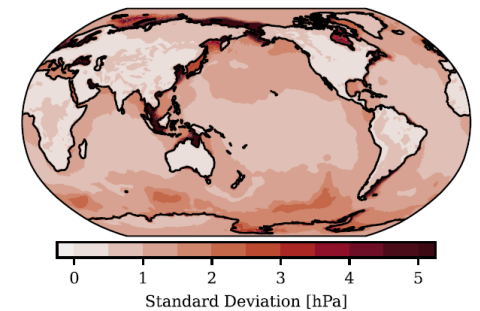
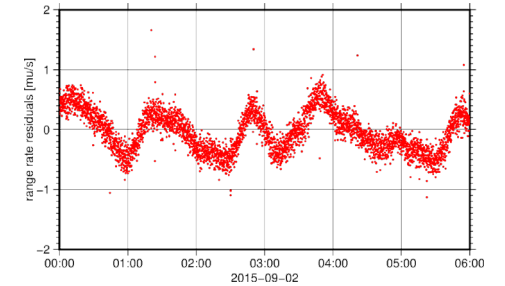
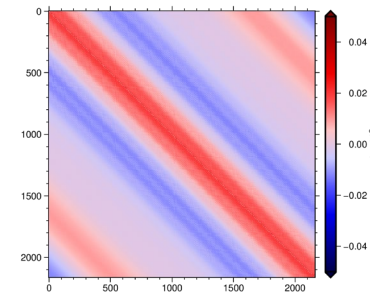
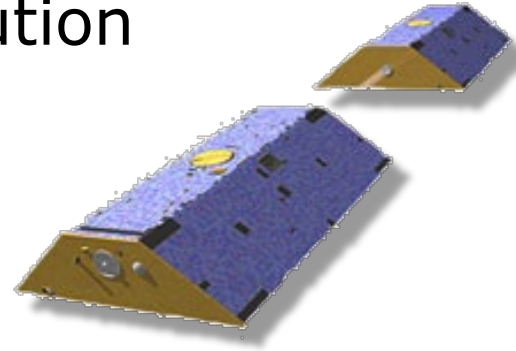


Technische
Universität
München



Overview

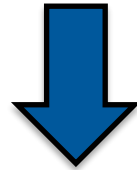
- From measurements to gravity field solution
 - Least squares adjustment
- Residual analysis
- Weight matrix of instrument noise
- Background model noise
 - Example: non-tidal AOD model
- Summary



From measurements to gravity field solution

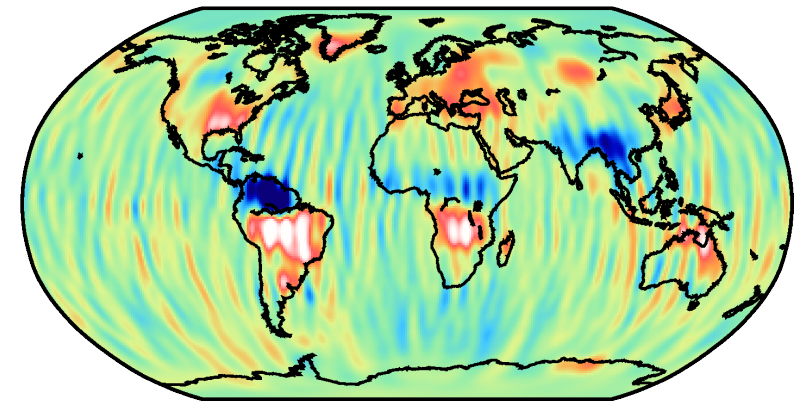
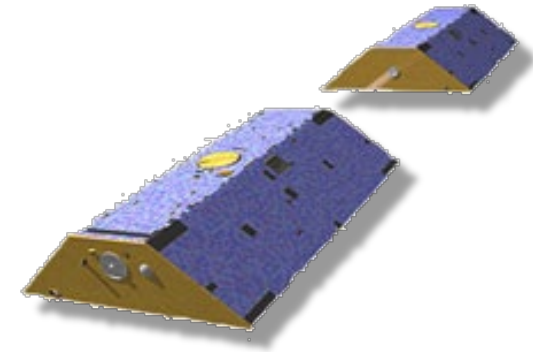
Measurements

- Range-rate data between the satellites
- Accelerometer data
- Star camera data
- ...



Monthly gravity field of the Earth

- Spherical harmonics coefficients
- or Mascons
- or ...



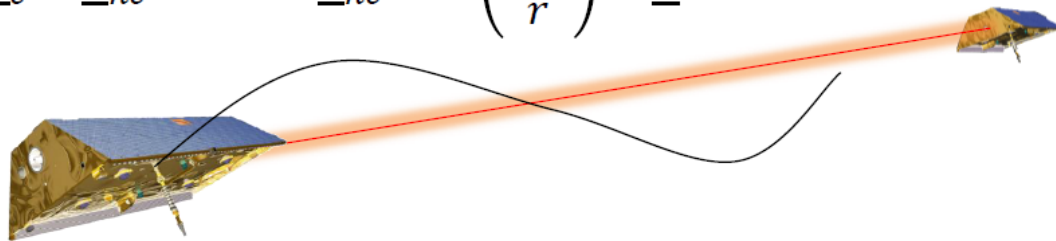
From measurements to gravity field solution

6. GRACE observation equation



Equation of motion

$$\ddot{\underline{r}} = \underline{a}_c + \underline{a}_{nc} = \nabla V + \underline{a}_{nc} = \nabla \left(\frac{GM}{r} \right) + \underline{d}$$



Observations:

- (biased) range ρ
- range rate $\dot{\rho}$
- range acceleration $\ddot{\rho}$

Numerical orbit integration \rightarrow position+velocity \rightarrow range/range rate

Observation equation

$$y(t) = f\left(t, \overline{\underline{r}}, \overline{\underline{\dot{r}}}, \overline{\underline{x}}, \overline{\underline{d}}, \underbrace{cal, emp, \dots}_{\text{Calibration/empir. parameters}}\right) = f_0\left(t, \underbrace{\underline{r}_0, \underline{\dot{r}}_0, \underline{x}_0}_{\text{A-priori models}}, \dots\right) + \delta f$$

Orbit (ACC meas.)
Force models

\downarrow
 \downarrow

\uparrow
 \uparrow

Gravity field parameters
Obs. Residuals \rightarrow input to adjustment

$$\underline{x} = \{\overline{C}_{nm}, \overline{S}_{nm}\}$$

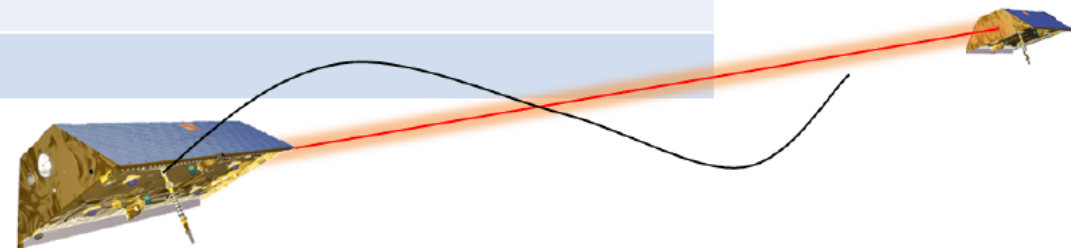
From Level-1B Instrument Data to Level-2 Spherical Harmonics (Gruber, TUM)

From measurements to gravity field solution

6. Methods of Earth's gravity field recovery from GRACE observations



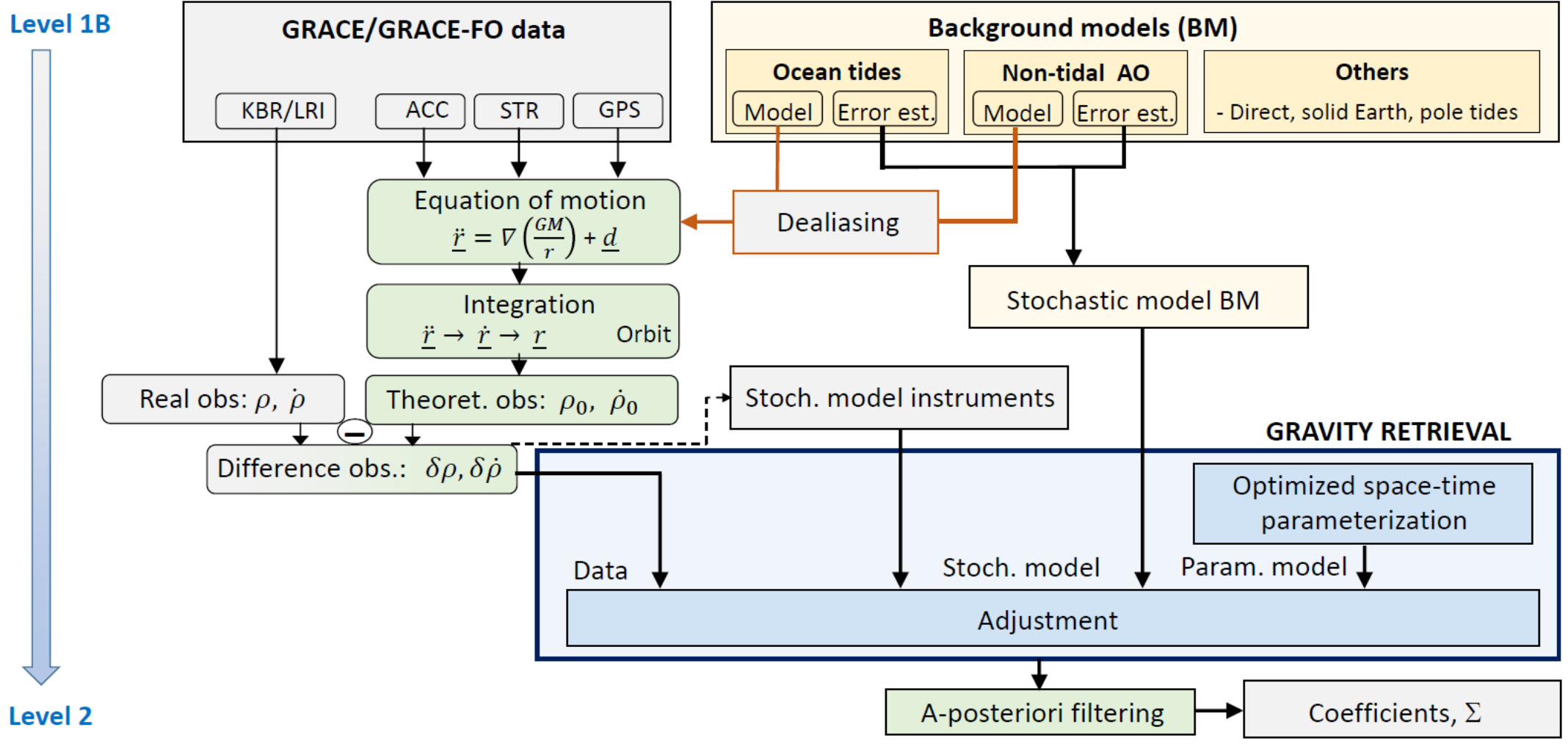
Method	Observations	Reference
Variational equations	$\rho, \dot{\rho}$	Tapley et al. (2004), GRL
Celestial mechanics approach	$\rho, \dot{\rho}$	Beutler et al. (2010), J. Geod.
Short-arc approach	$\rho, \dot{\rho}$	Mayer-Gürr et al (2006), Ph.D. Thesis
Energy balance approach	$\dot{\rho}$	Han et al. (2006), J. Geophys. Res.
Acceleration approach	$\ddot{\rho}$	Liu (2008), Ph.D. Thesis
Line of Sight Gradiometry	$\ddot{\rho}/\rho$	Keller & Sharifi (2005), J. Geod.
...		



From Level-1B Instrument Data to Level-2 Spherical Harmonics (Gruber, TUM)

From measurements to gravity field solution

6. Gravity field processing – overview

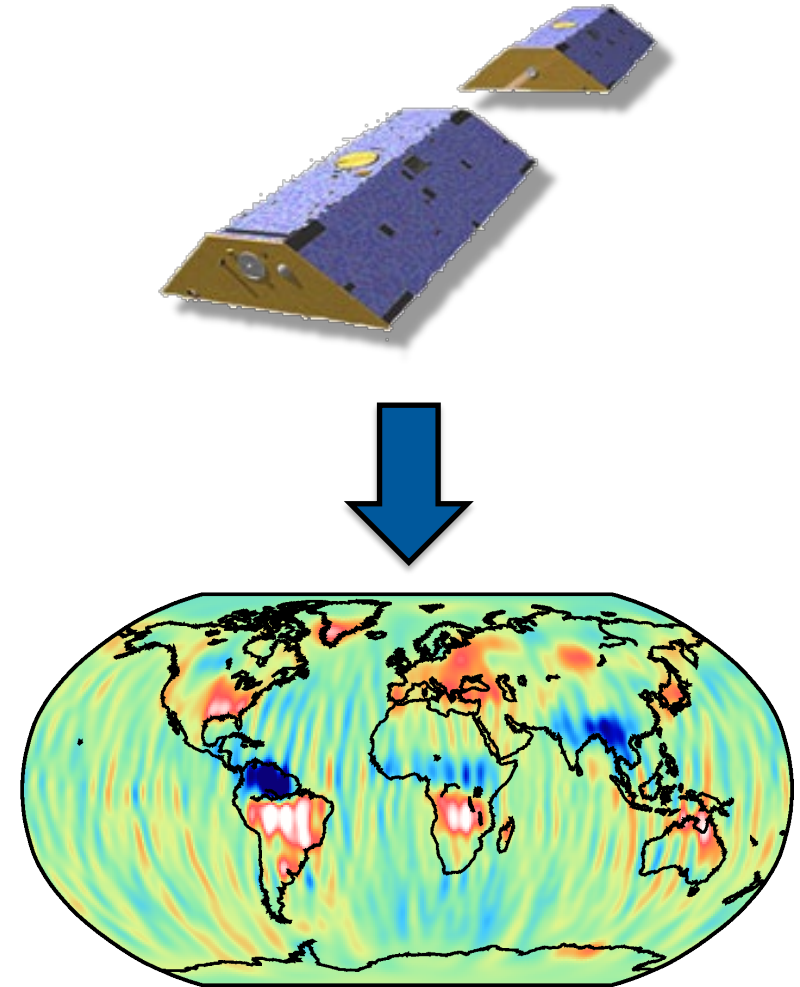


From Level-1B Instrument Data to Level-2 Spherical Harmonics (Gruber, TUM)

Least squares adjustment

- Prediction of the observations (range rate data) by a model

$$y(t) = f(\quad ??? \quad)$$

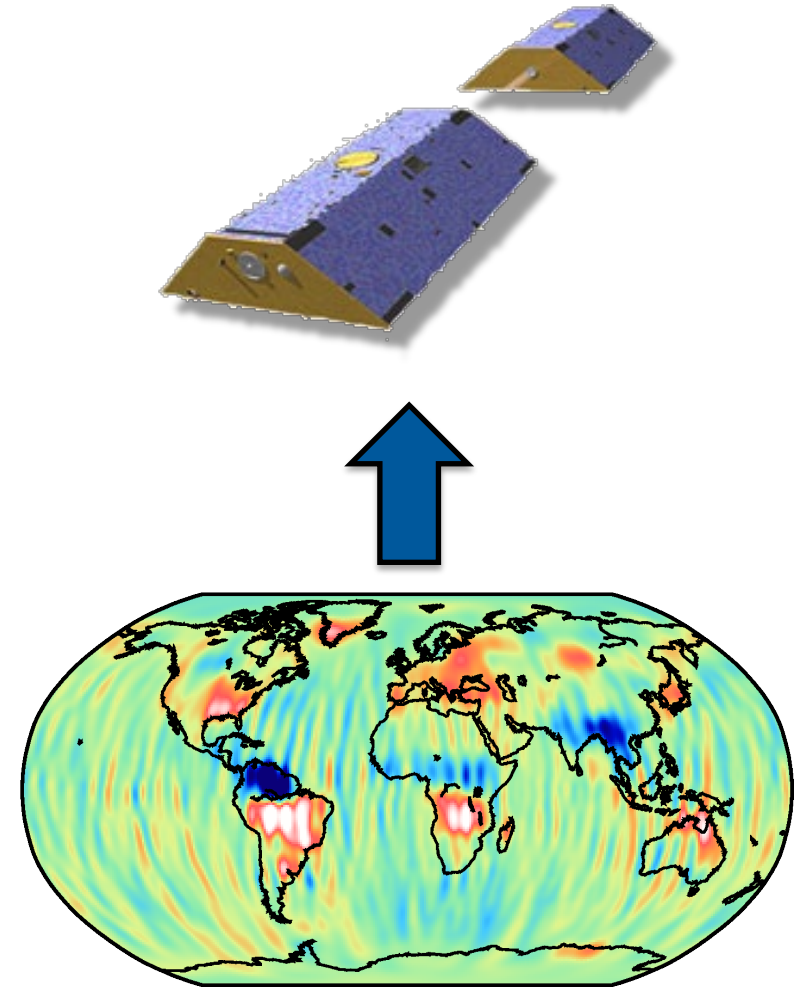


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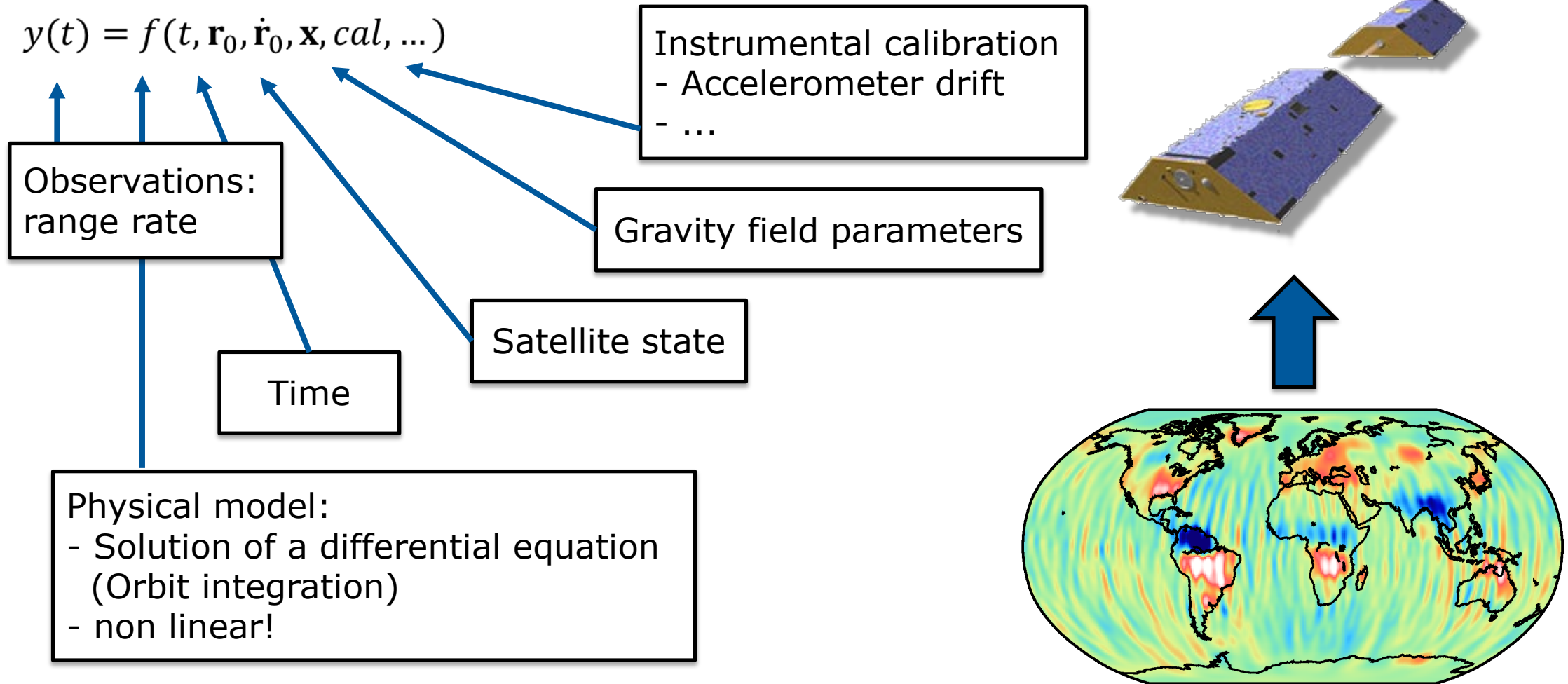
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↑
Observations:
range rate



Least squares adjustment

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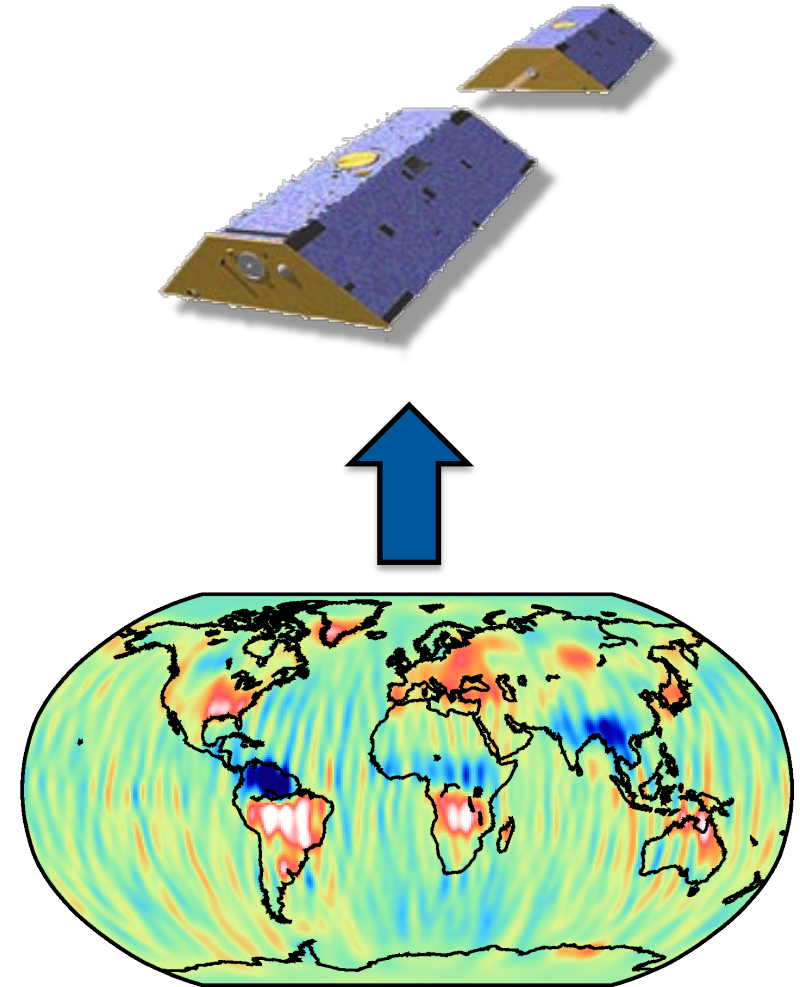
Least squares adjustment

- Prediction of the observations (range rate data) by a model

$$y(t) = f(t, \mathbf{r}_0, \dot{\mathbf{r}}_0, \mathbf{x}, cal, \dots)$$

- Linearization by a truncated Taylor series

$$y = f(\mathbf{x}_0) + \left. \frac{\partial f}{\partial \mathbf{x}} \right|_0 (\mathbf{x} - \mathbf{x}_0) + \dots$$



Least squares adjustment

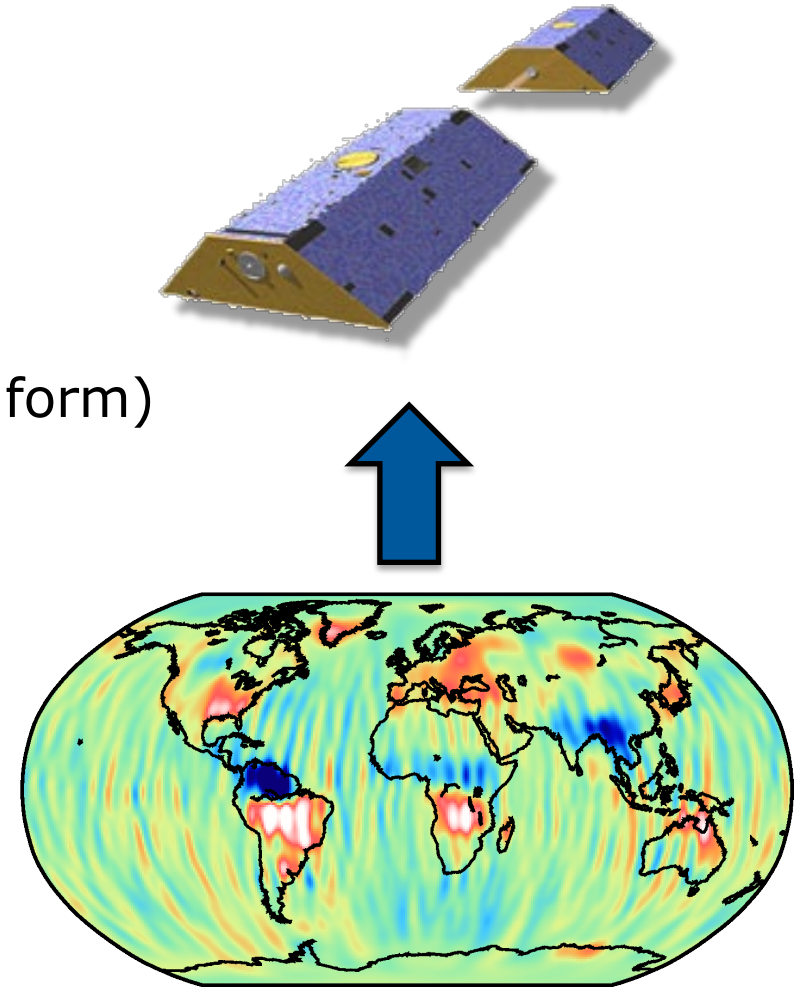
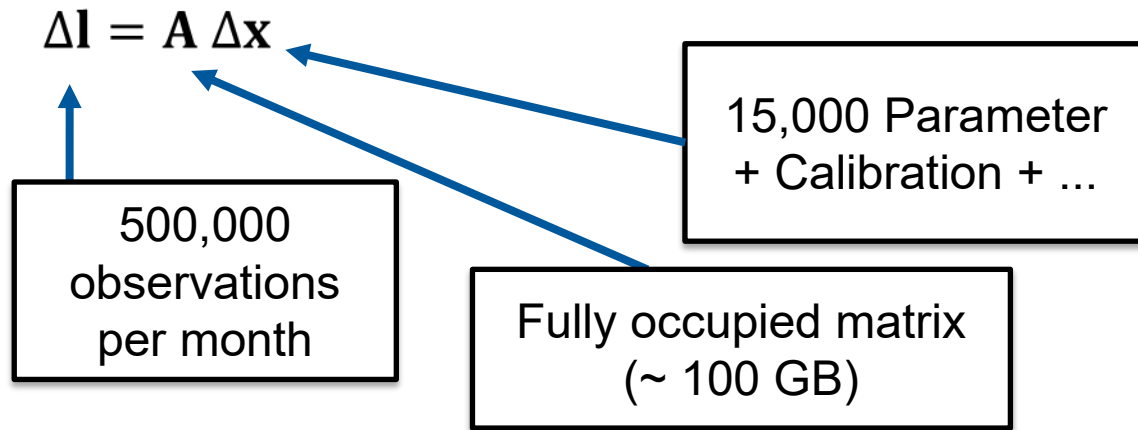
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- Linearization by a truncated Taylor series

$$y - f(\mathbf{x}_0) = \left. \frac{\partial f}{\partial \mathbf{x}} \right|_0 (\mathbf{x} - \mathbf{x}_0) + \dots$$

- Linear, overdetermined system of equations (in matrix form)



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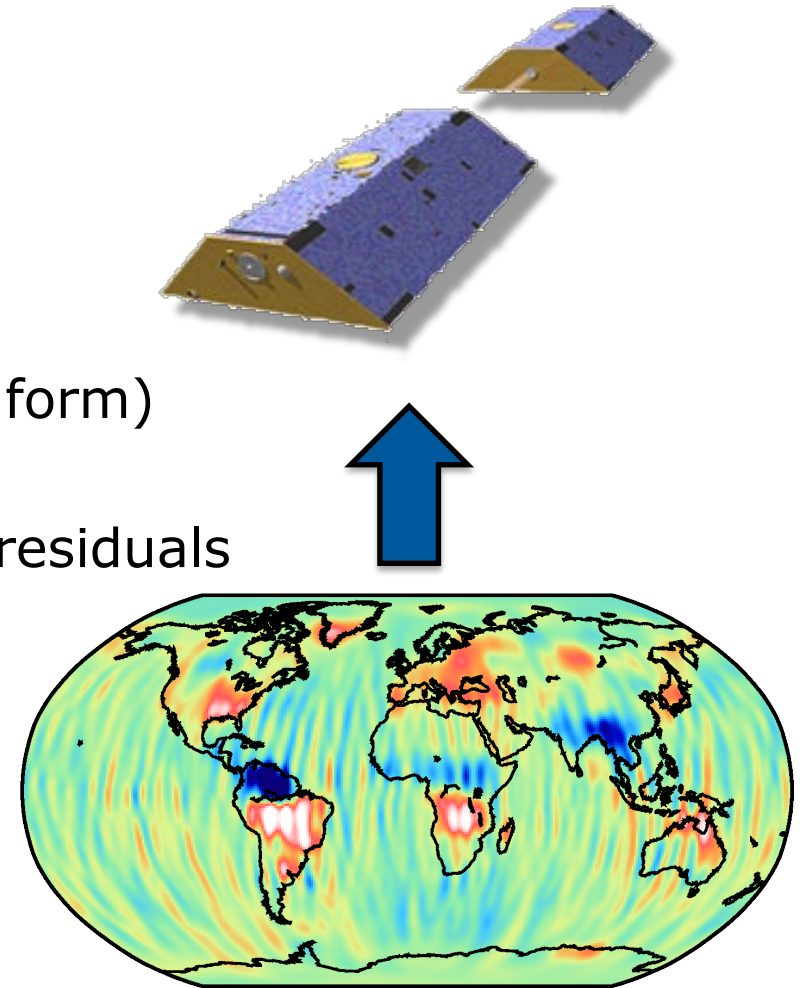
$$\Delta \mathbf{I} = \mathbf{A} \Delta \mathbf{x}$$

- Solution by minimizing the weighted quadratic sum of residuals

$$\|\Delta \mathbf{I} - \mathbf{A} \cdot \Delta \mathbf{x}\|_{\mathbf{P}}^2 \rightarrow \min$$

- Solution

$$\Delta \hat{\mathbf{x}} = (\mathbf{A}^T \mathbf{P} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{P} \Delta \mathbf{I}$$



Least squares adjustment

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Reduced observation vector

$$\Delta \mathbf{I} = (y - f(\mathbf{x}_0))$$

is a mixture of all instruments and models

- Differentiated Ranging Instrument noise
- Integrated Accelerometer noise
- Aliasing errors from background models
 - Atmosphere, ocean mass variations
 - Ocean tides
- ...

The the post-fit residuals (How good is the fit?)

$$\hat{\mathbf{e}} = \Delta \mathbf{I} - \mathbf{A} \cdot \Delta \hat{\mathbf{x}}$$

tell us something about the noise

The weight matrix

$$\mathbf{P} = \Sigma^{-1}$$

should consider the noise of the observation vector

⇒ Inverse of the noise covariance matrix



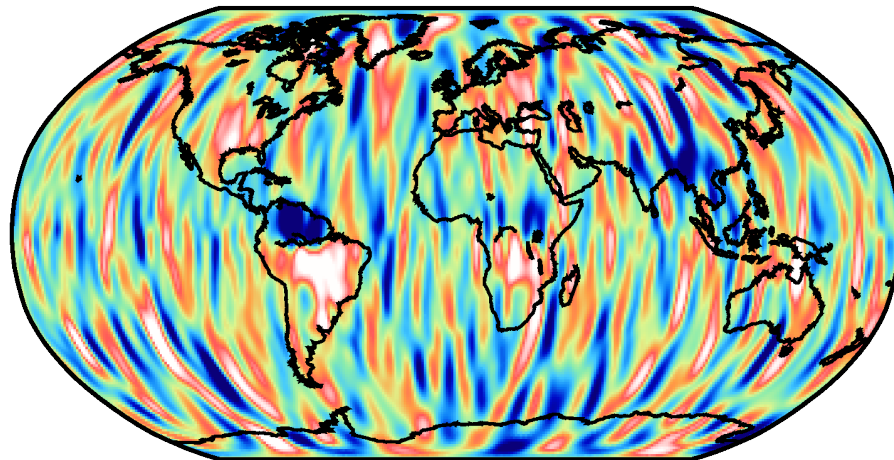
Least squares adjustment

- Almost every method for gravity field recovery is based on least squares adjustment

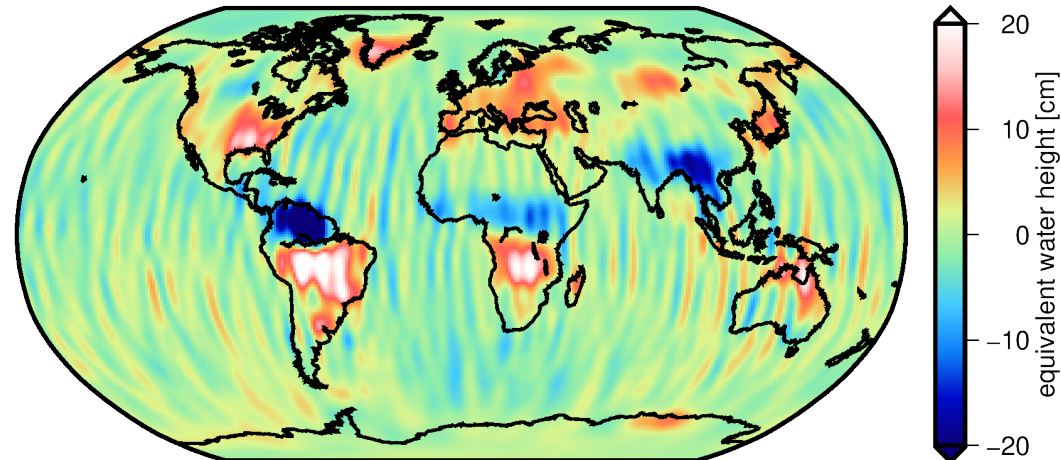
$$\|\Delta\mathbf{l} - \mathbf{A} \cdot \Delta\mathbf{x}\|_{\mathbf{P}}^2 \rightarrow \min$$

- This talk is only about the weight matrix \mathbf{P}

No weight matrix



Weight matrix

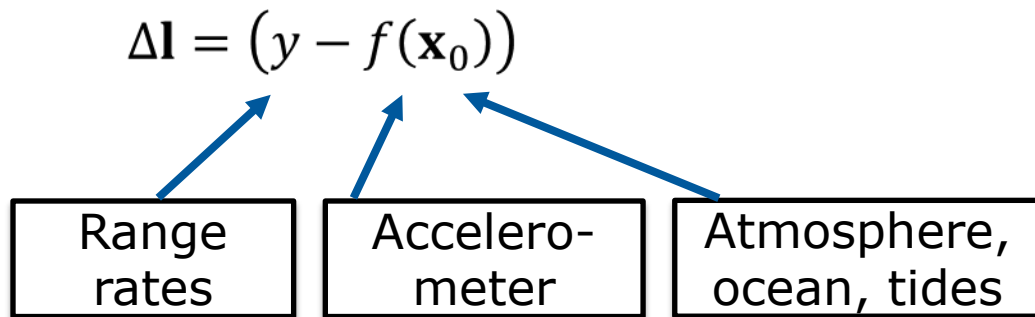


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- The weight matrix should consider the noise of the reduced observation vector $\mathbf{P} = \Sigma^{-1}$
- The reduced observation vector contains different noise sources



Least squares adjustment

- Almost every method for gravity field recovery is based on least squares adjustment

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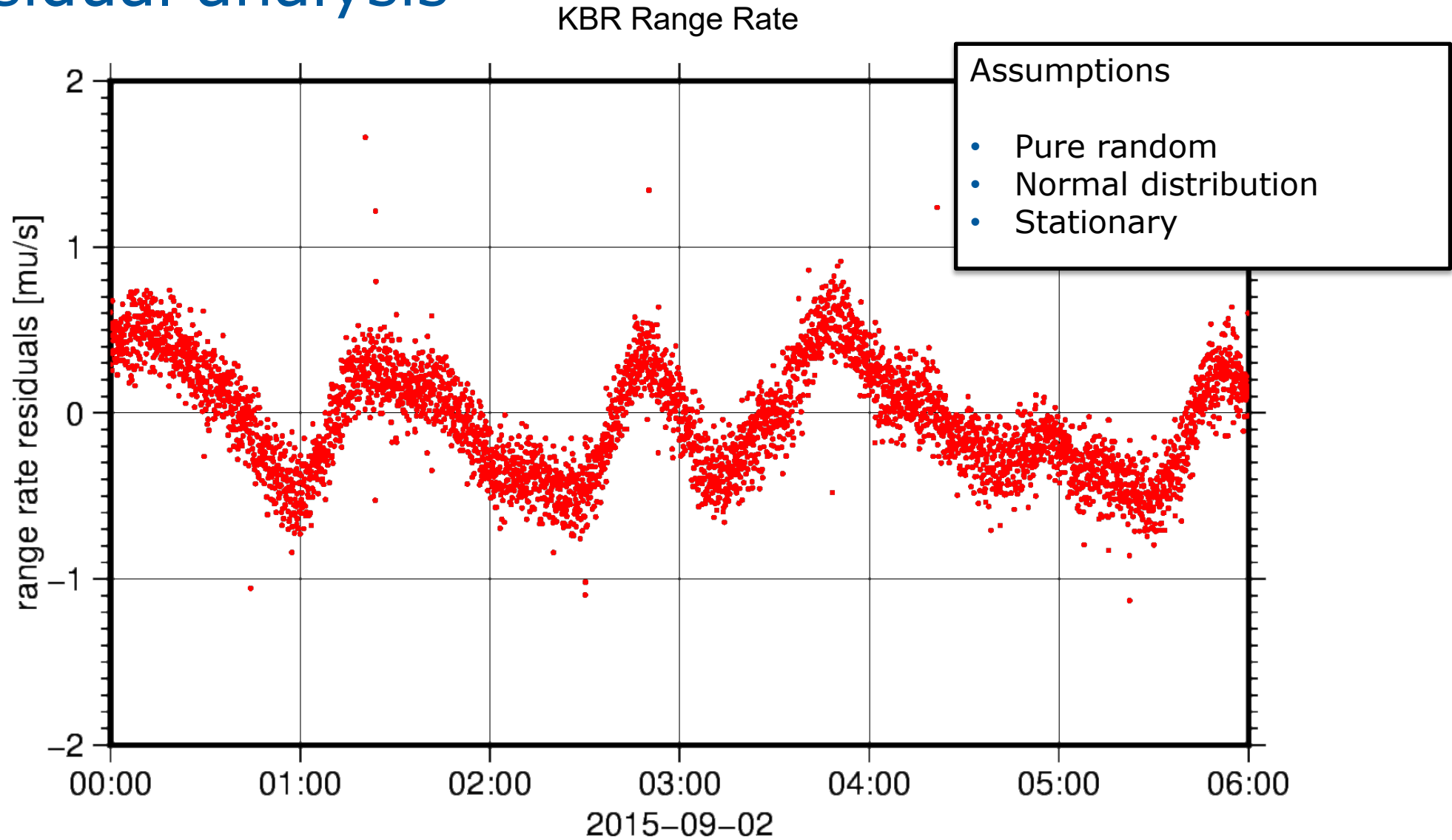
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$$\Delta\mathbf{l} = (y - f(\mathbf{x}_0))$$

- We can analyze the post-fit residuals to understand the noise

$$\hat{\mathbf{e}} = \Delta\mathbf{l} - \mathbf{A} \cdot \Delta\hat{\mathbf{x}}$$

Residual analysis



Residual analysis

- Assumption of a stationary noise

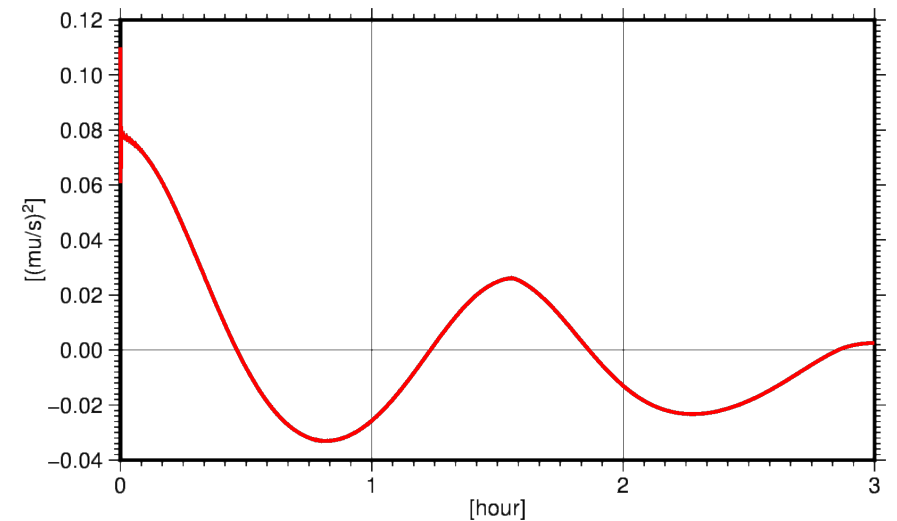
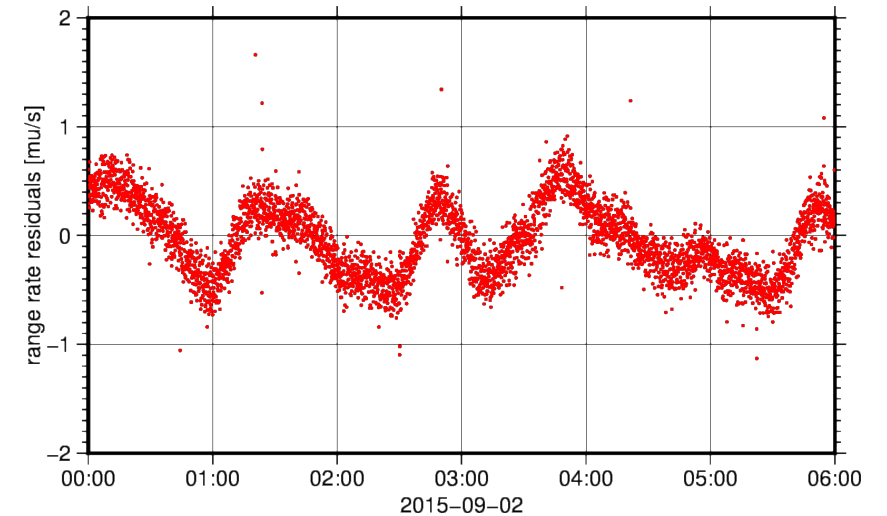
$$RMS^2 = \frac{1}{N} \sum_{i=0}^N \hat{e}^2(t_i)$$

- Neighboring residuals are correlated:
Estimation of the covariance

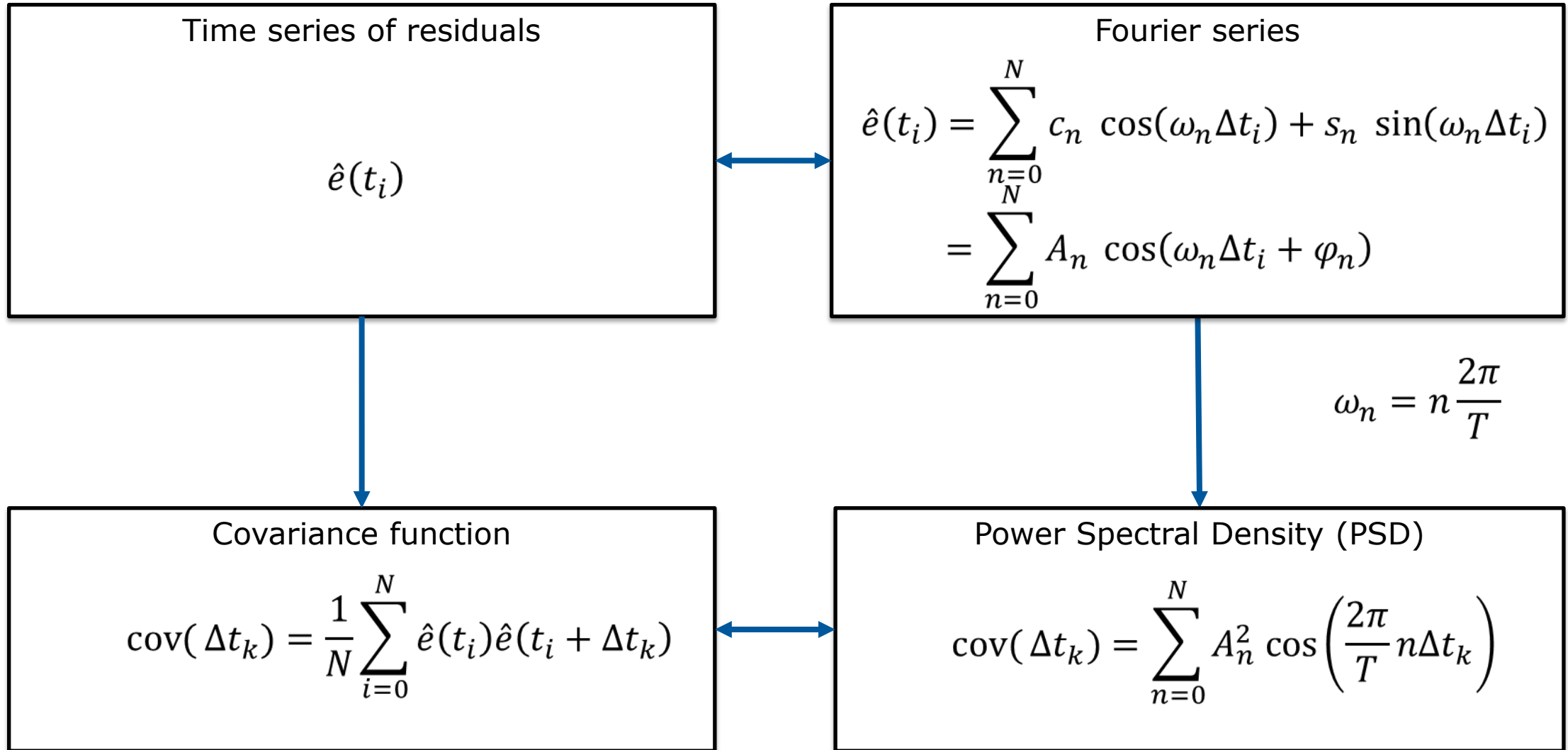
$$\text{cov}(\Delta t_k) = \frac{1}{N} \sum_{i=0}^N \hat{e}(t_i) \hat{e}(t_i + \Delta t_k)$$

- The covariance function can be expressed by the amplitudes of a power spectrum (PSD)

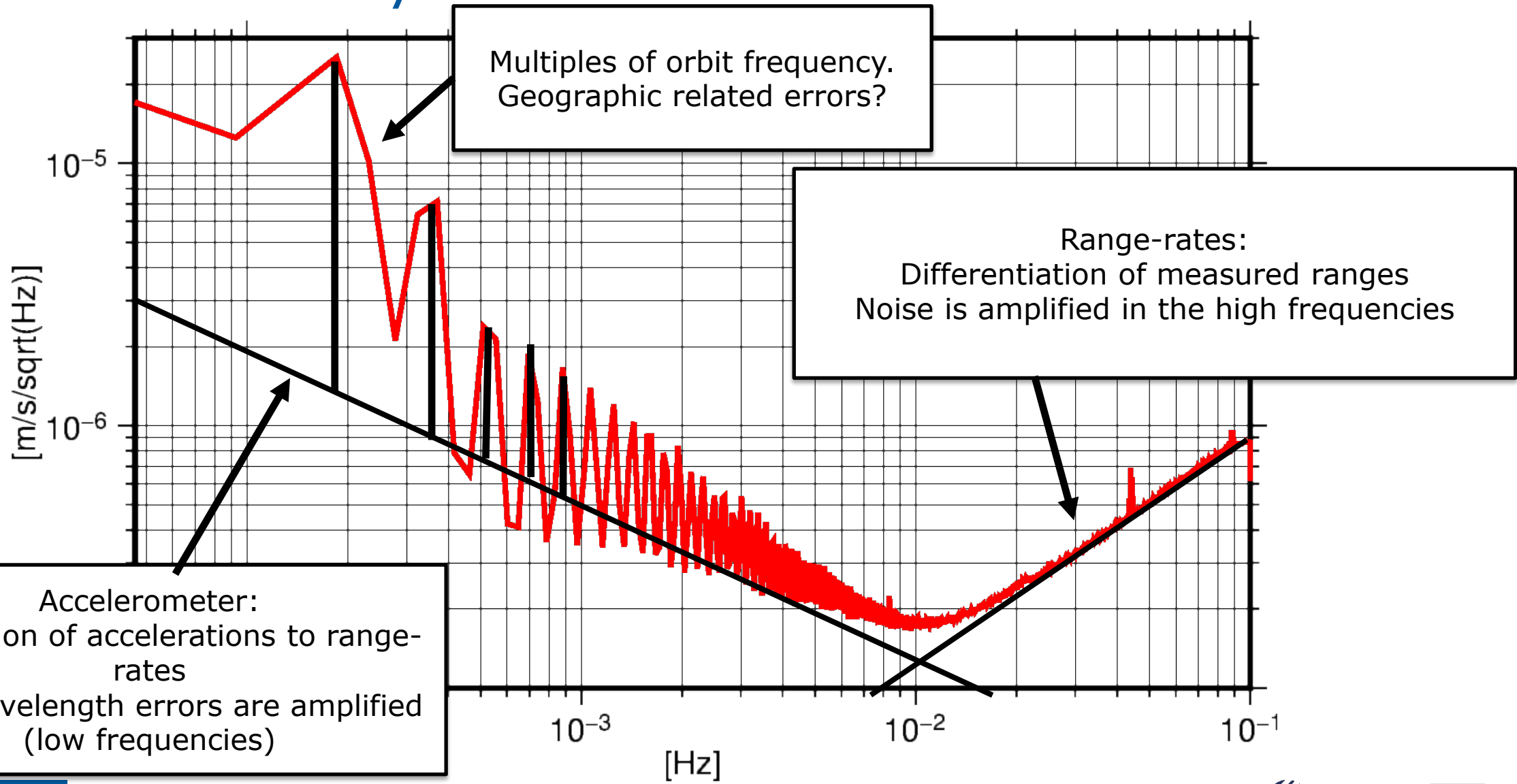
$$\text{cov}(\Delta t_k) = \sum_{n=0}^N a_n^2 \cos\left(\frac{2\pi}{T} n \Delta t_k\right)$$



Residual analysis



Residual analysis



Weight matrix of instrument noise

- Estimation of the covariance function

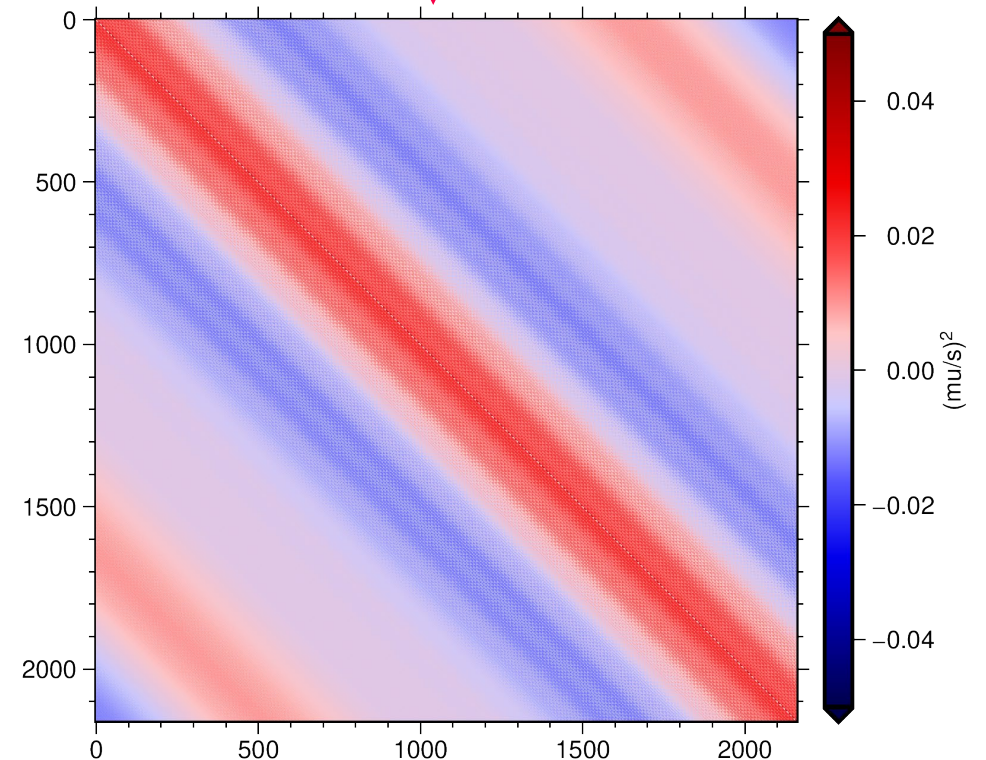
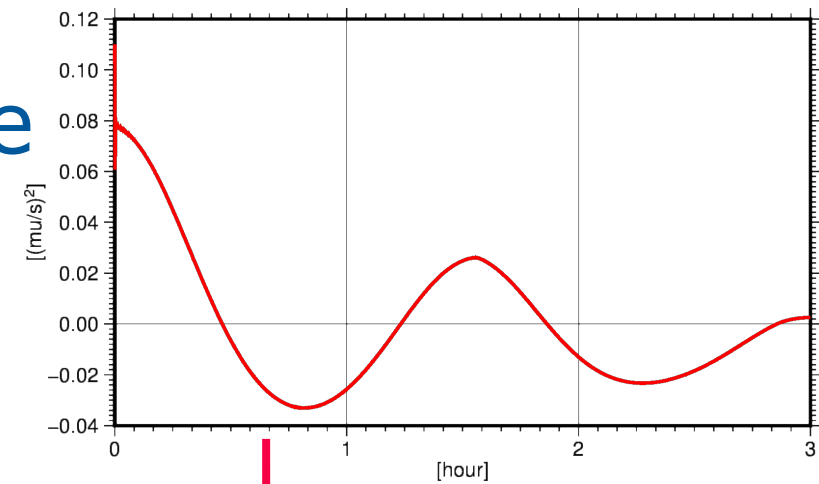
$$\text{cov}(\Delta t_k) = \frac{1}{N} \sum_{i=0}^N \hat{e}(t_i) \hat{e}(t_i + \Delta t_k)$$

- Assumption of a stationary noise process:
 - Covariance matrix is a Toeplitz matrix
 - Can be described by the covariance function

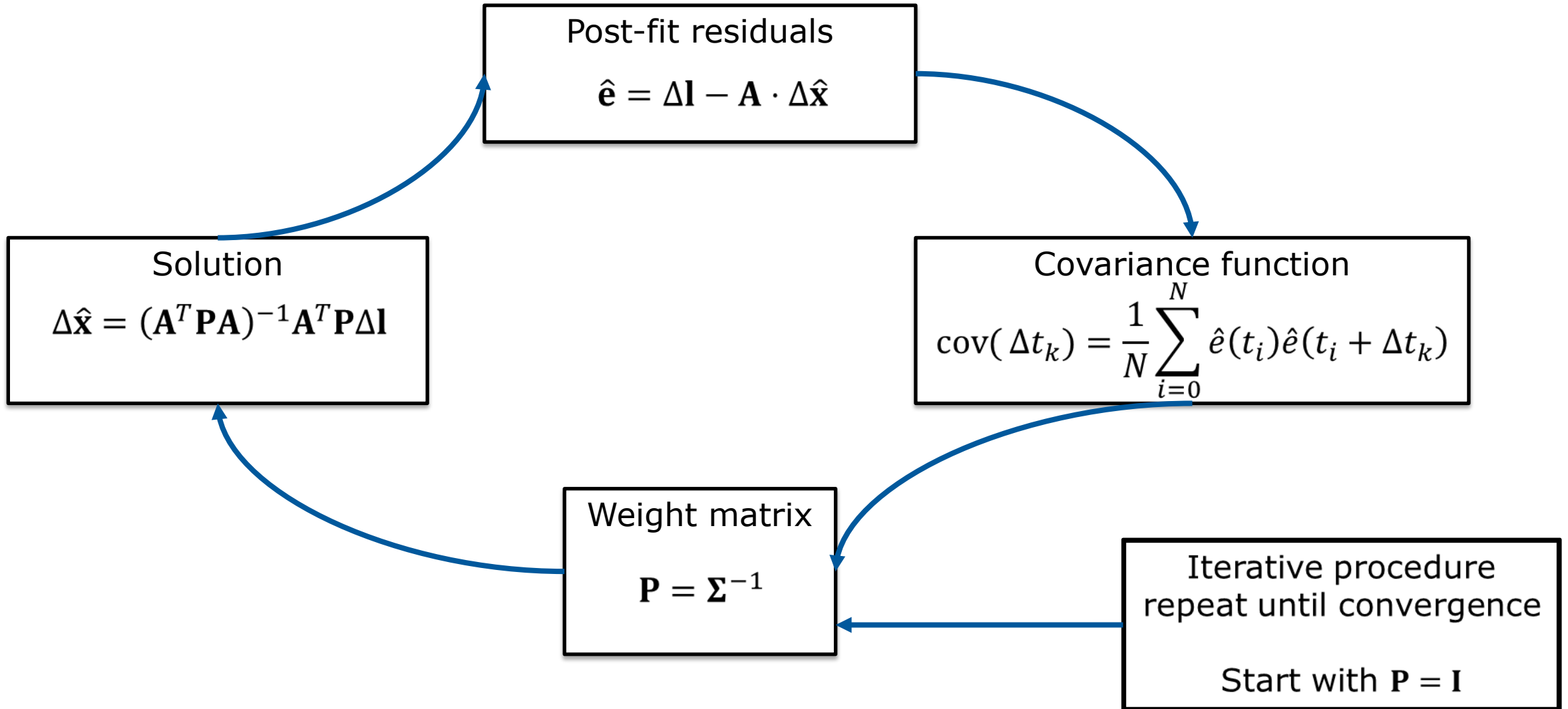
$$\Sigma = \begin{pmatrix} \text{cov}(\Delta t_0) & \text{cov}(\Delta t_1) & \text{cov}(\Delta t_2) & & \\ \text{cov}(\Delta t_1) & \text{cov}(\Delta t_0) & \text{cov}(\Delta t_1) & \dots & \\ \text{cov}(\Delta t_2) & \text{cov}(\Delta t_1) & \text{cov}(\Delta t_0) & & \\ & \vdots & & & \end{pmatrix}$$

- Weight matrix

$$\mathbf{P} = \Sigma^{-1}$$

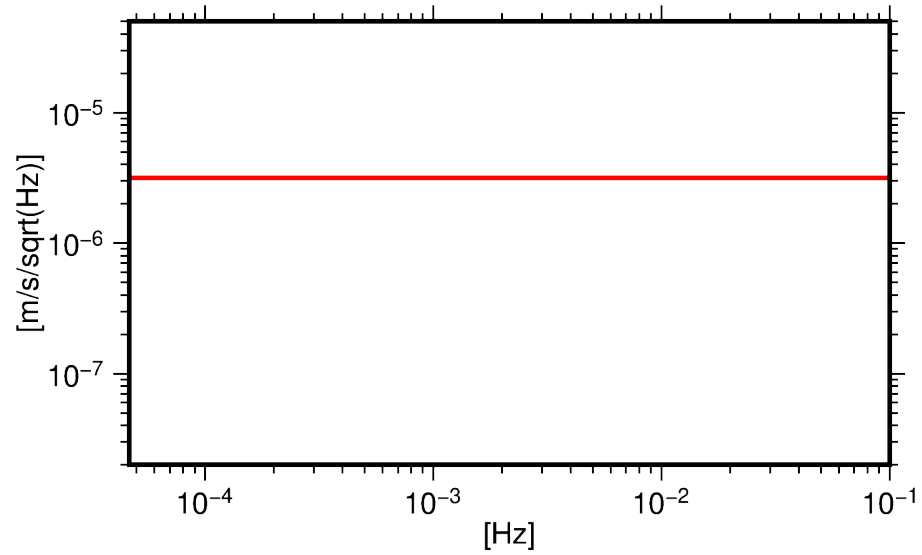


Weight matrix of instrument noise

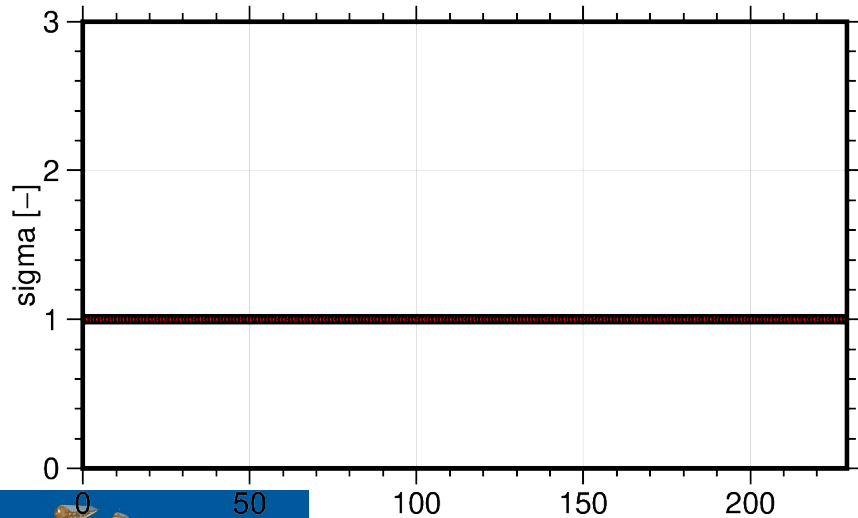


0. iteration

PSD range rate residuals (2010-02)

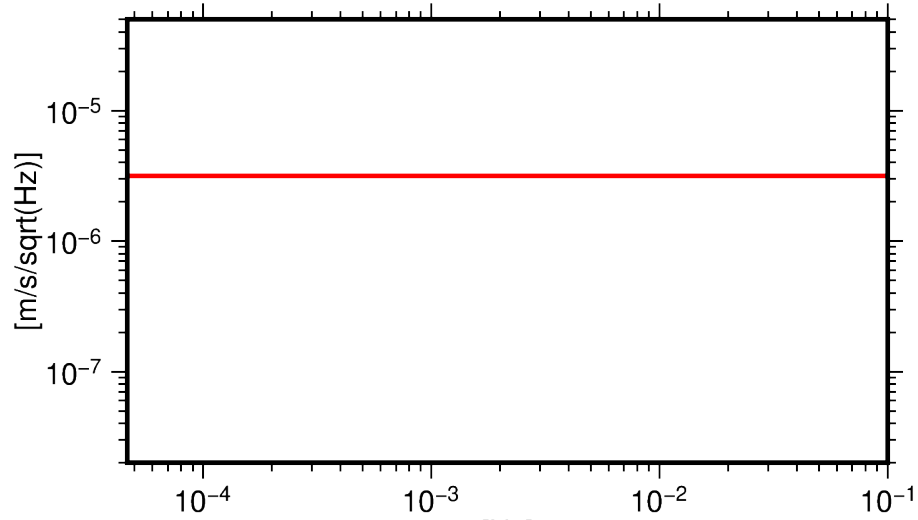


arc sigmas (2010-02)

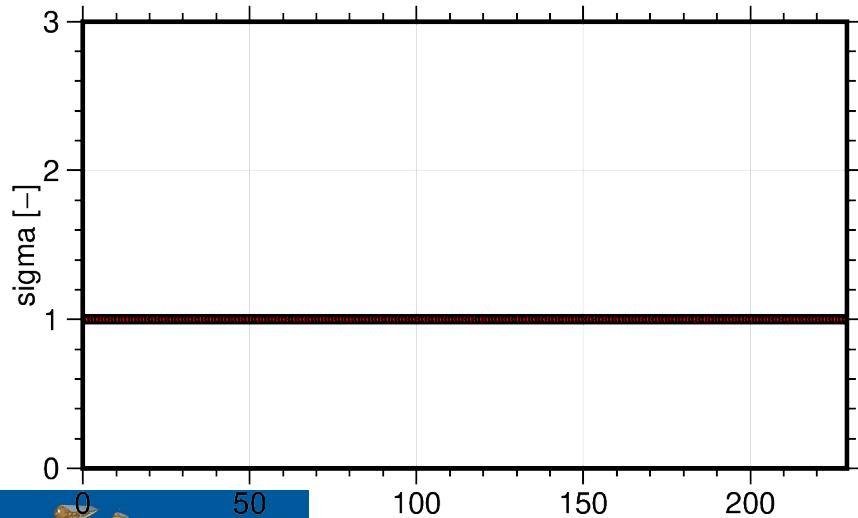


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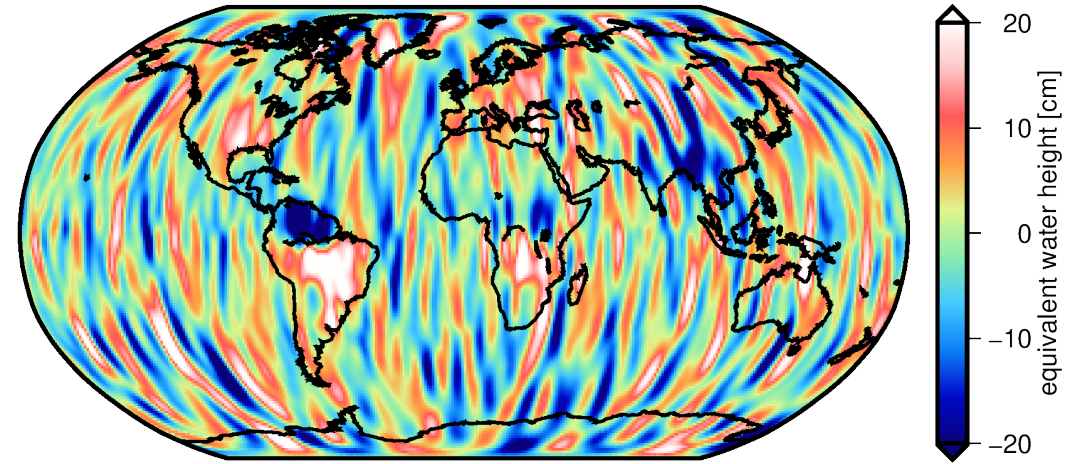


First weight matrix

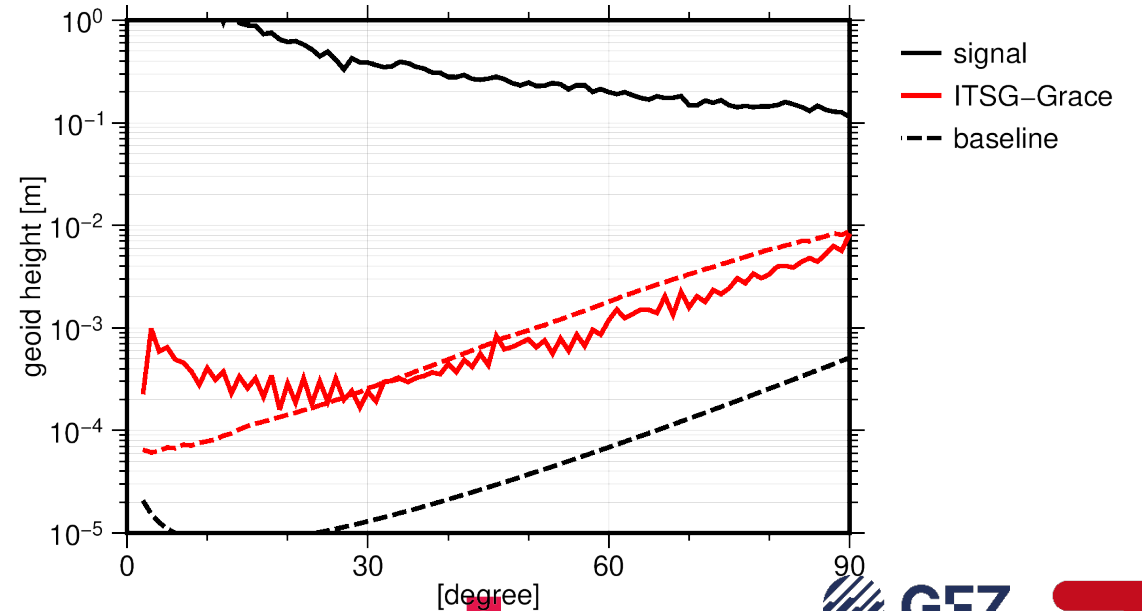


Least squares adjustment

Gaussian filter 350 km

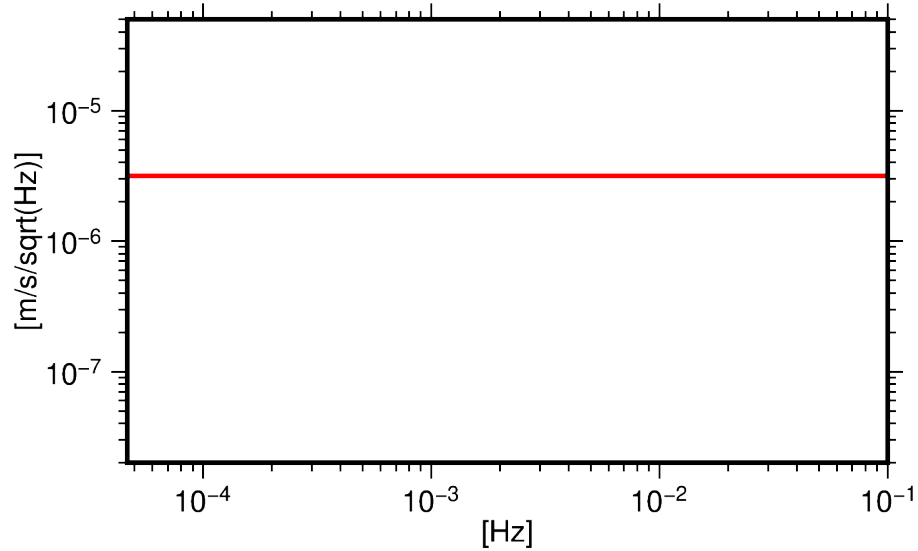


degree amplitudes (2010-02)

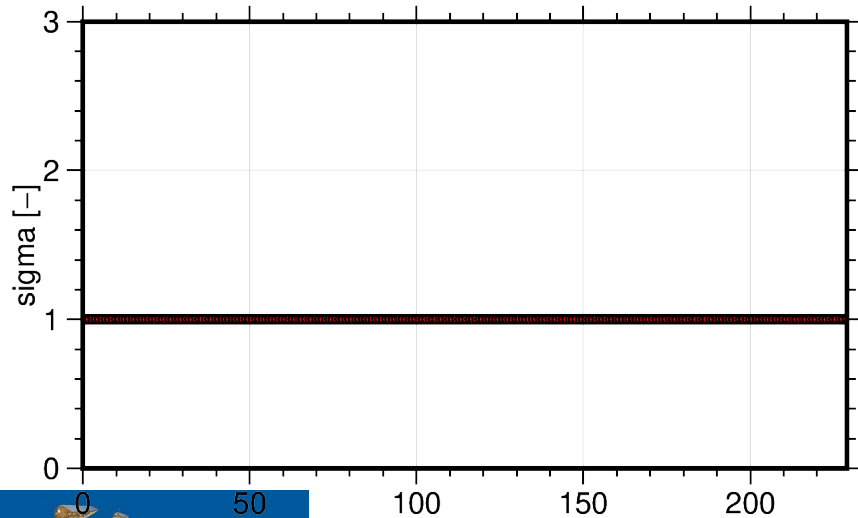


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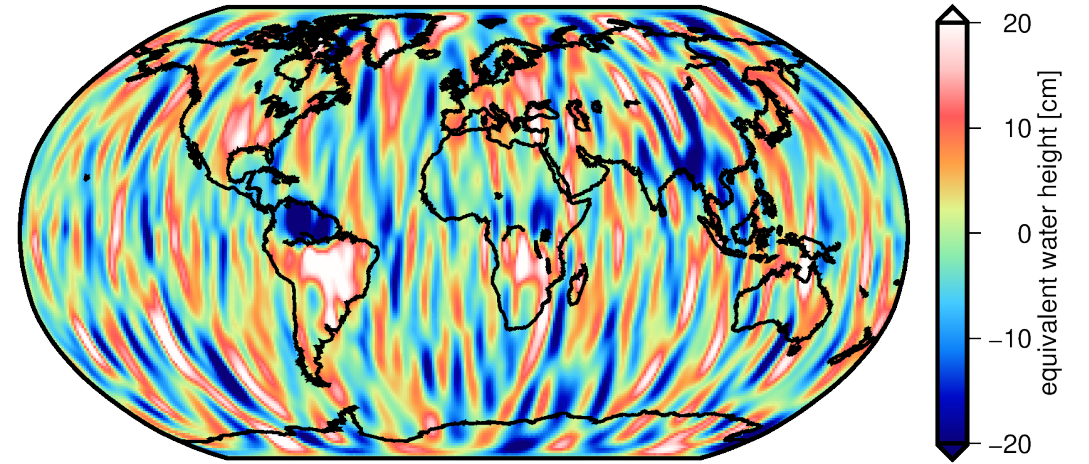
PSD range rate residuals (2010-02)



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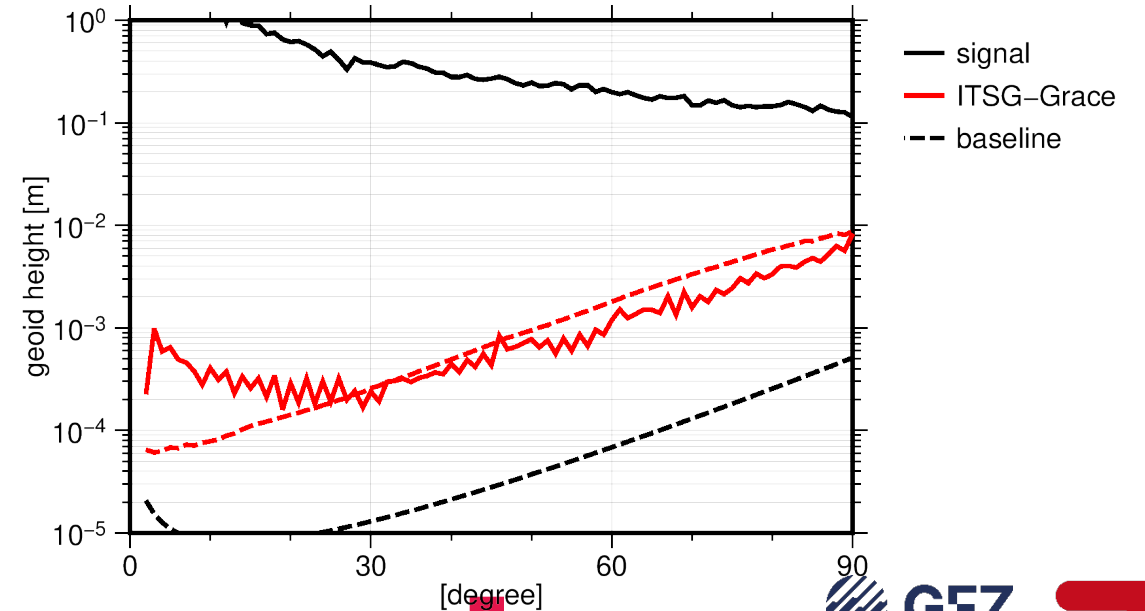


Post-fit residuals



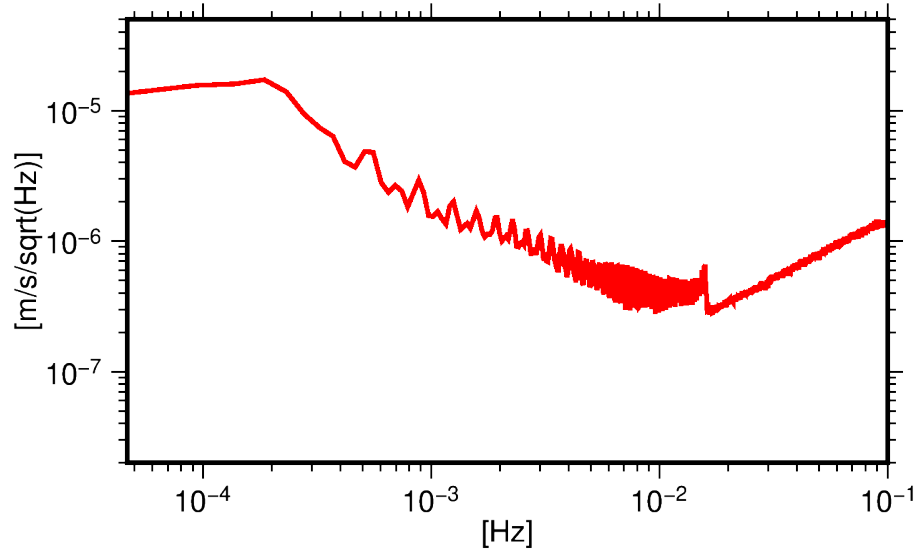
Estimate new covariance matrix

degree amplitudes (2010-02)

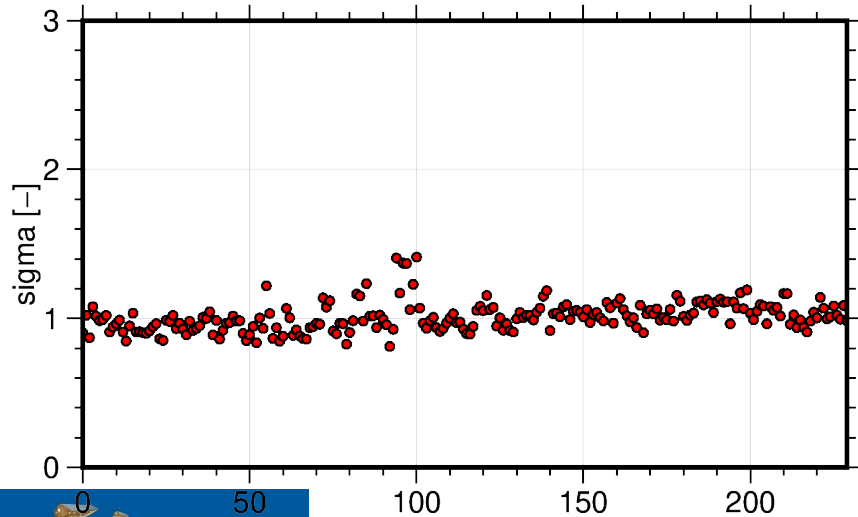


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arc sigmas (2010-02)

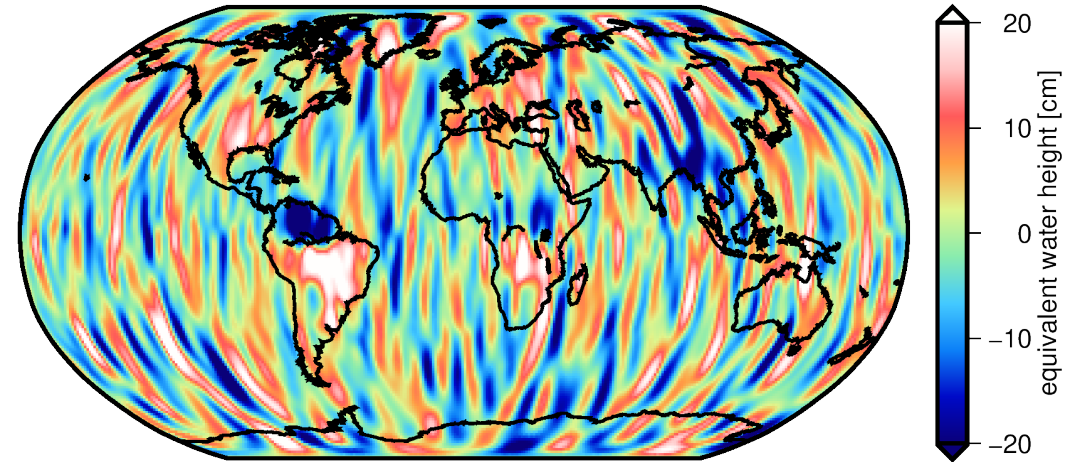


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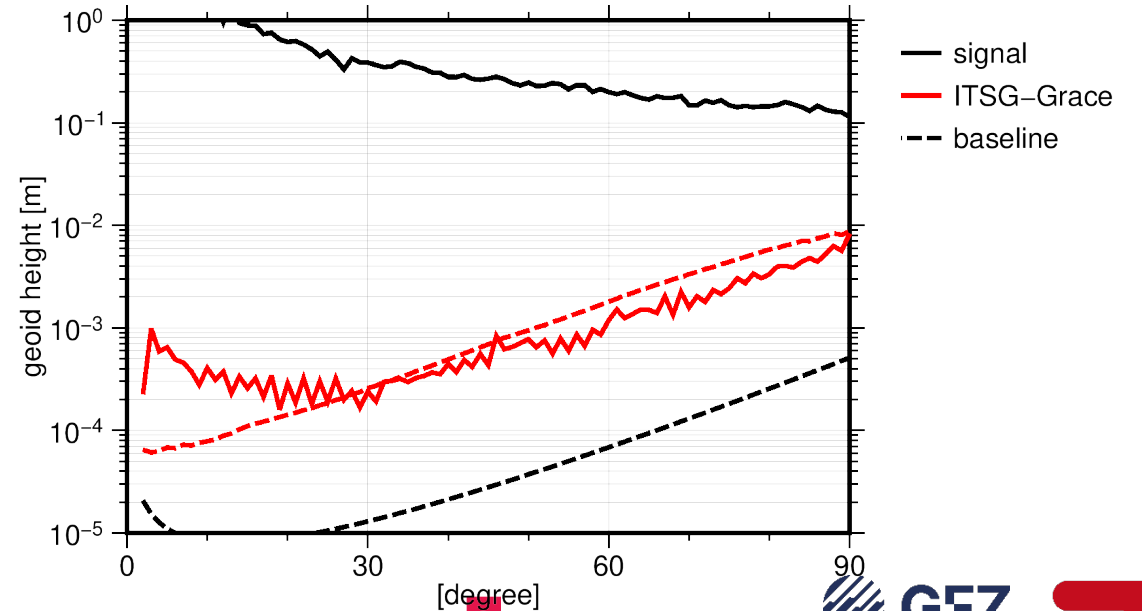


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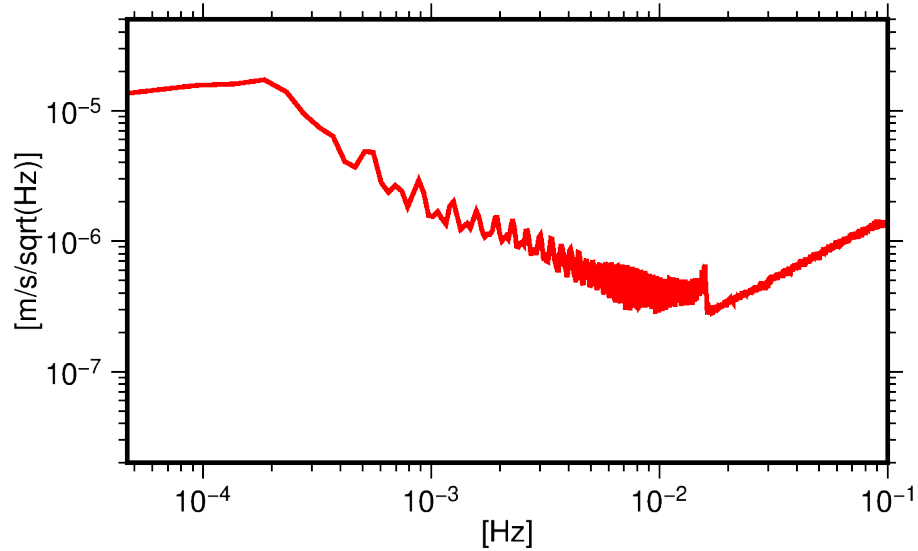


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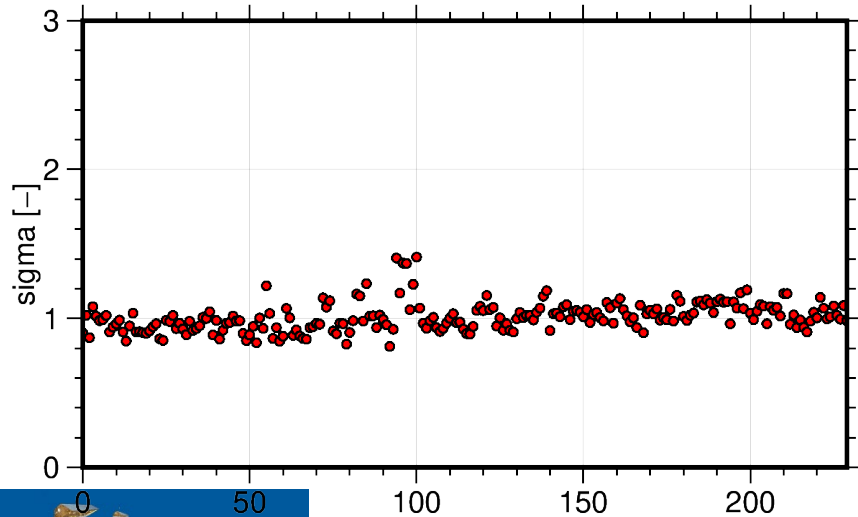


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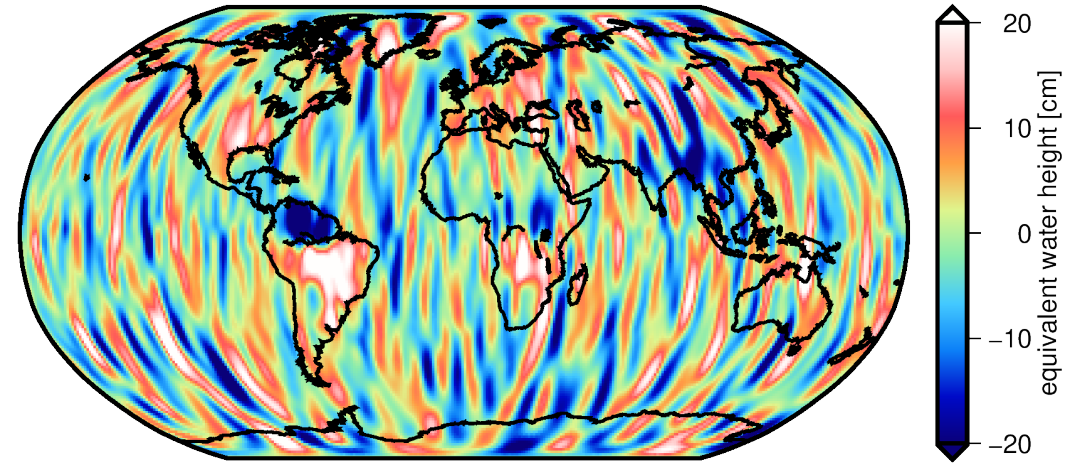


New weight matrix

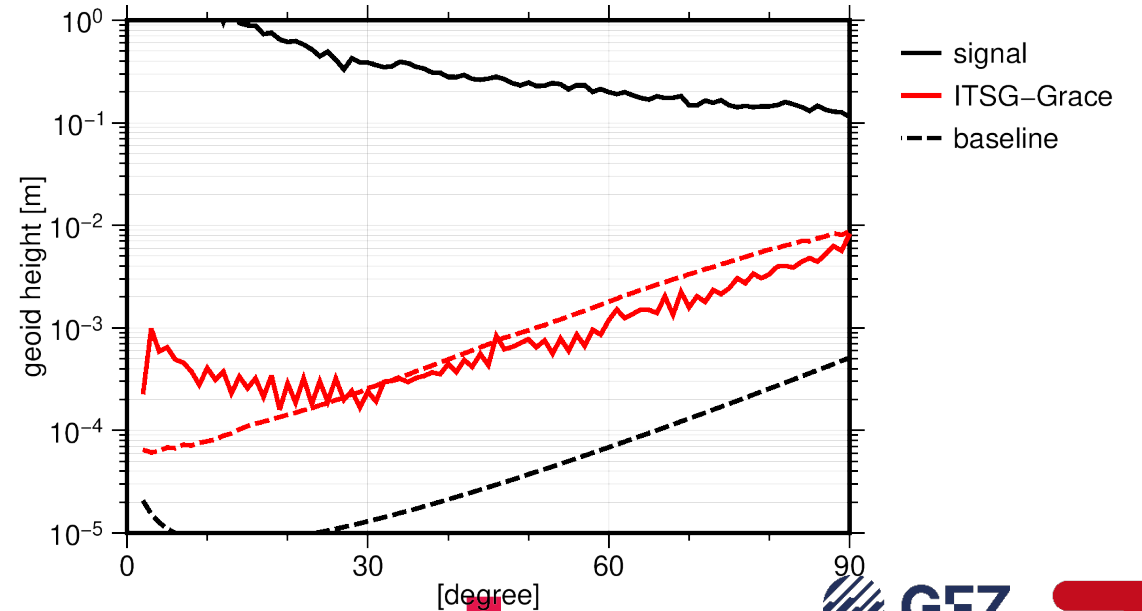


Least squares adjustment

Gaussian filter 350 km

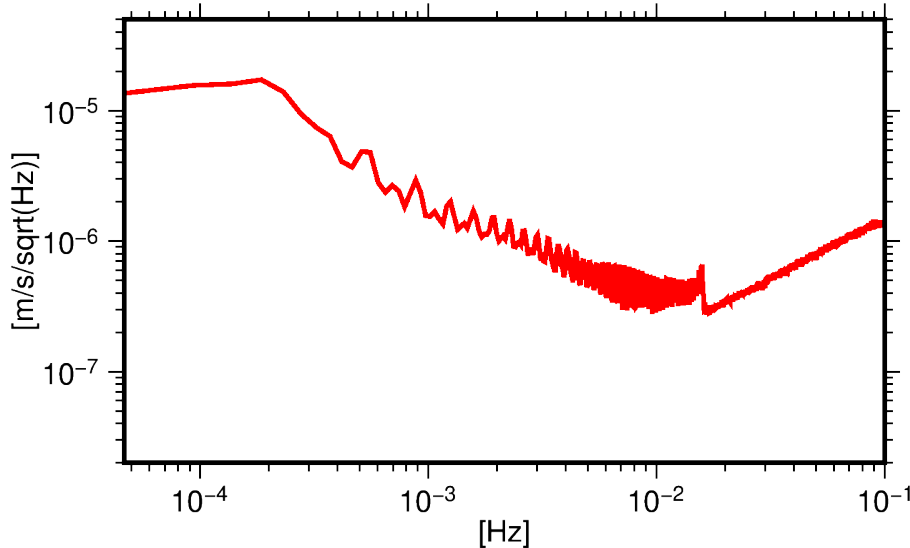


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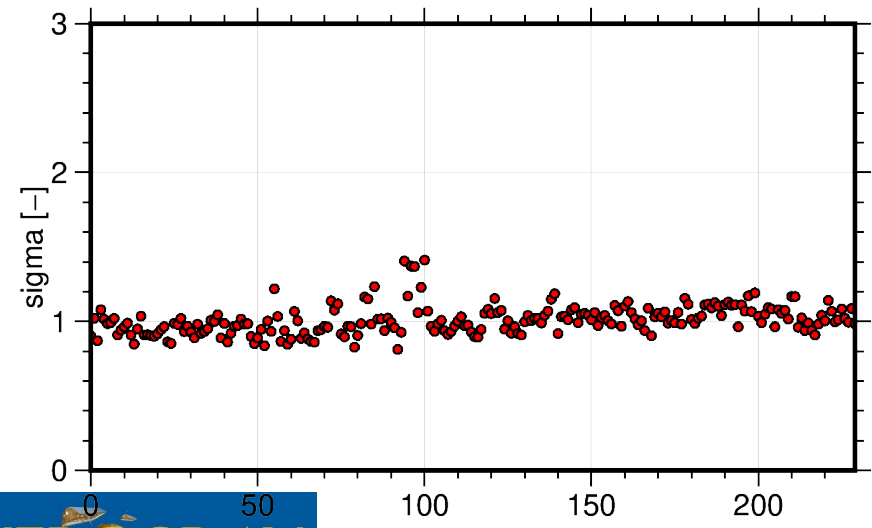


1. iteration

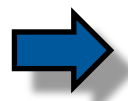
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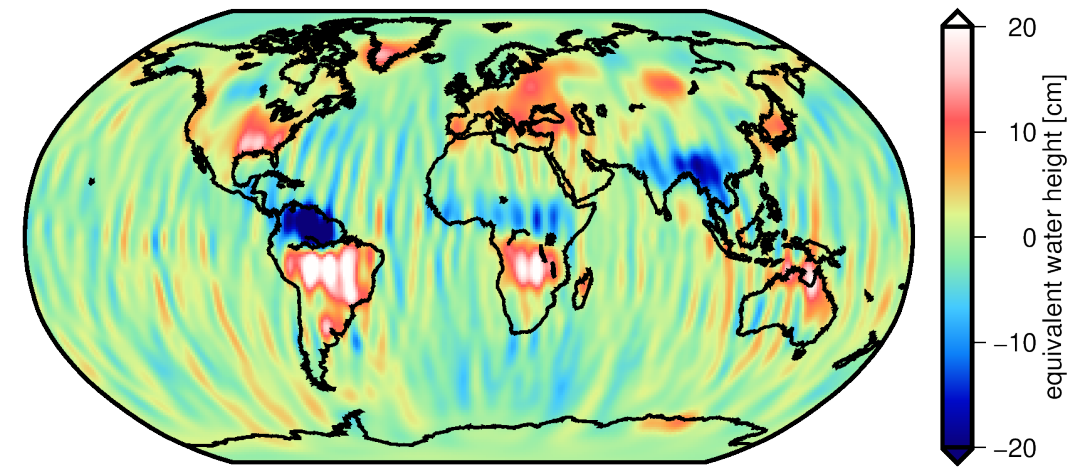


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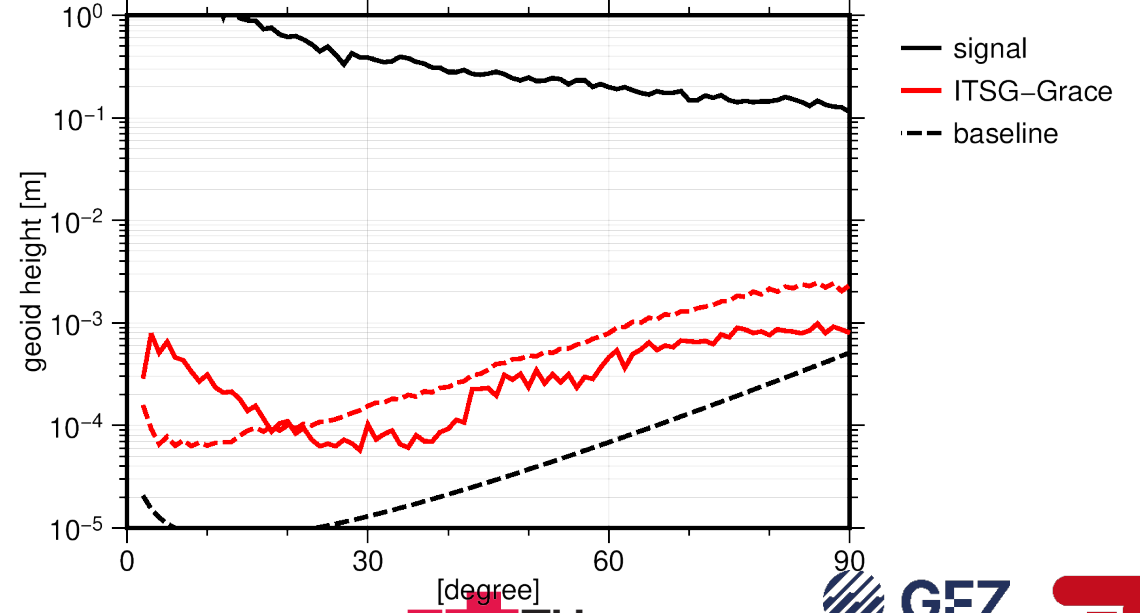


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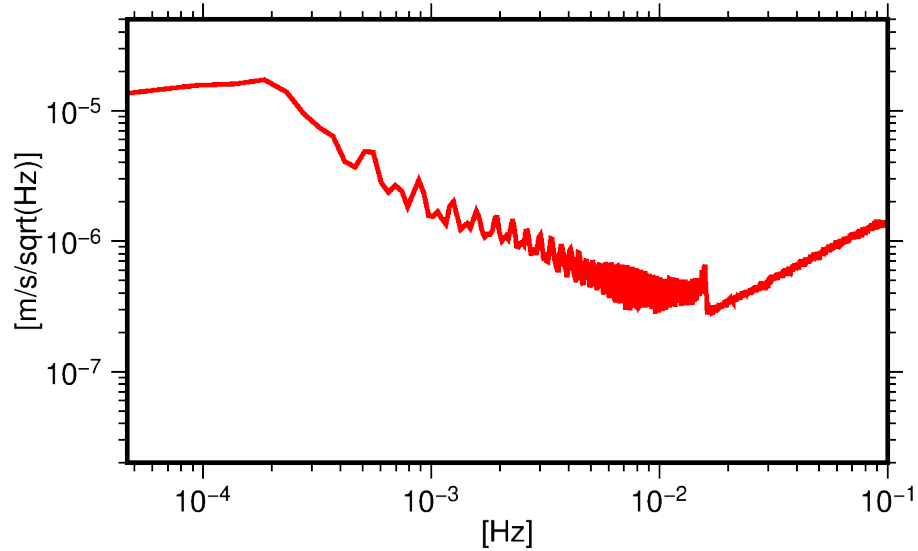


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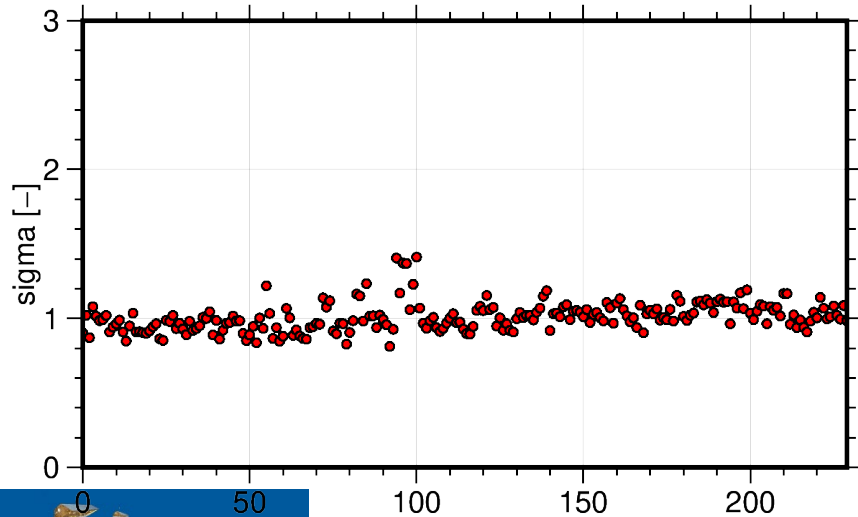


1. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

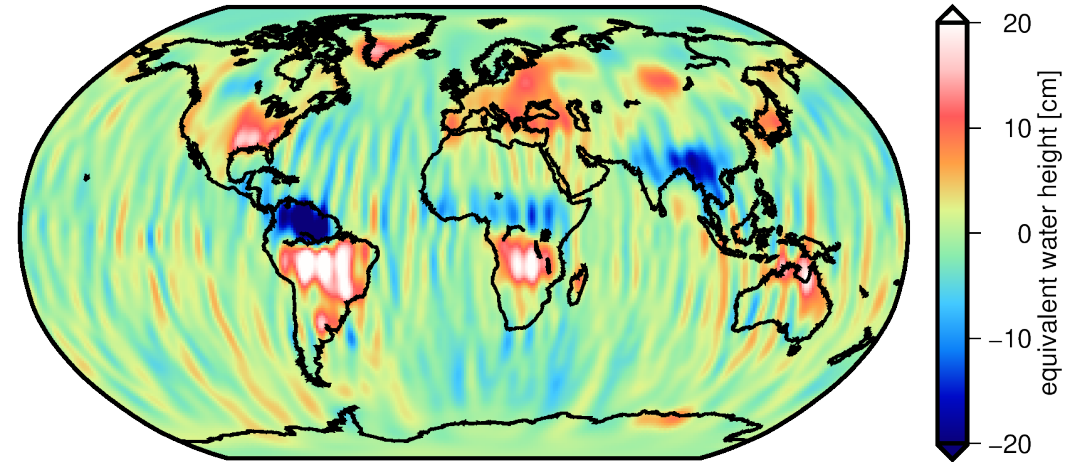


Post-fit residuals

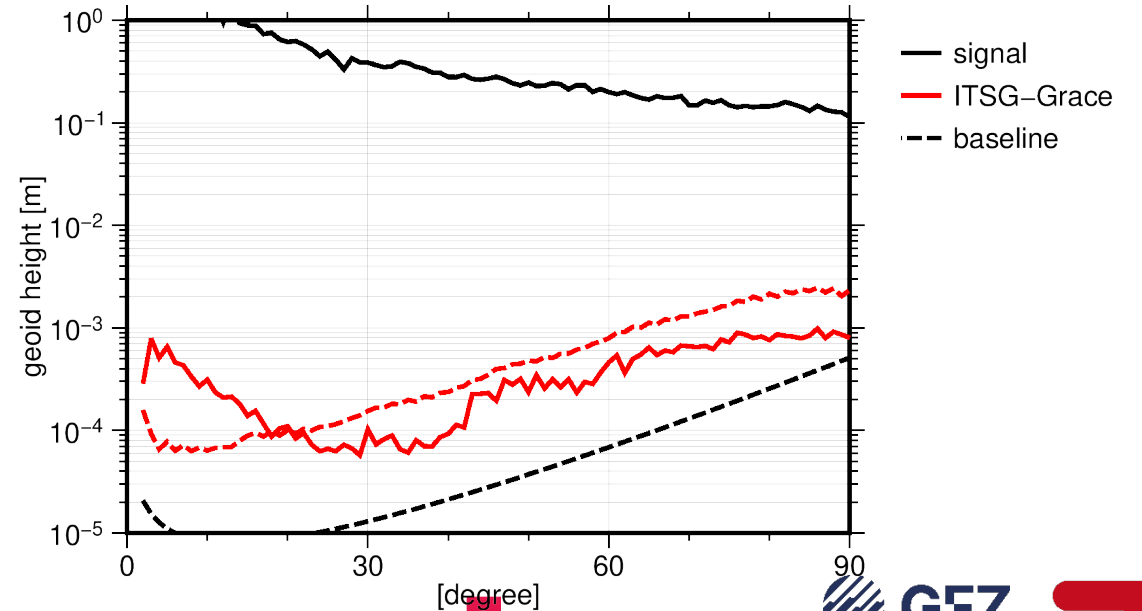


Estimate new covariance matrix

Gaussian filter 350 km

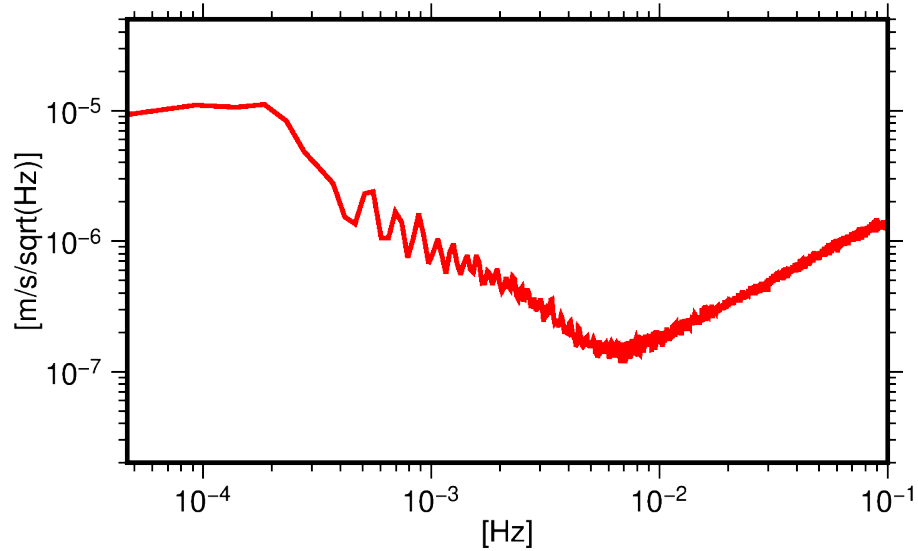


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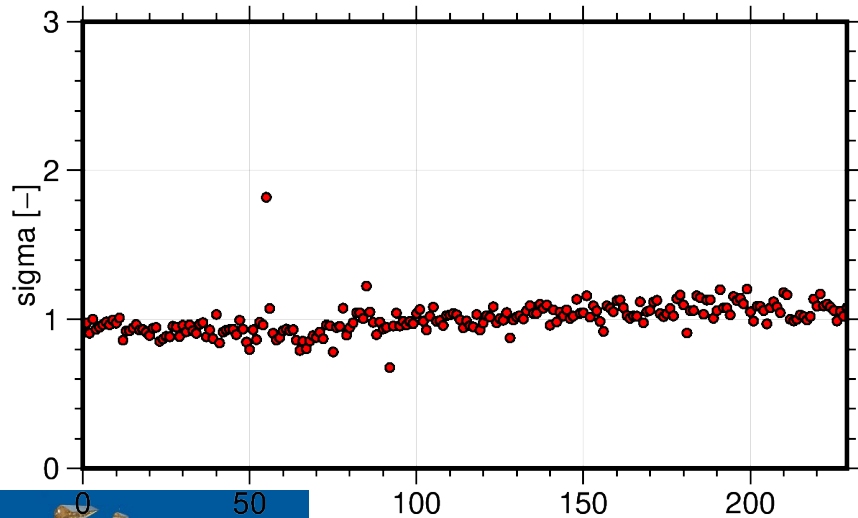


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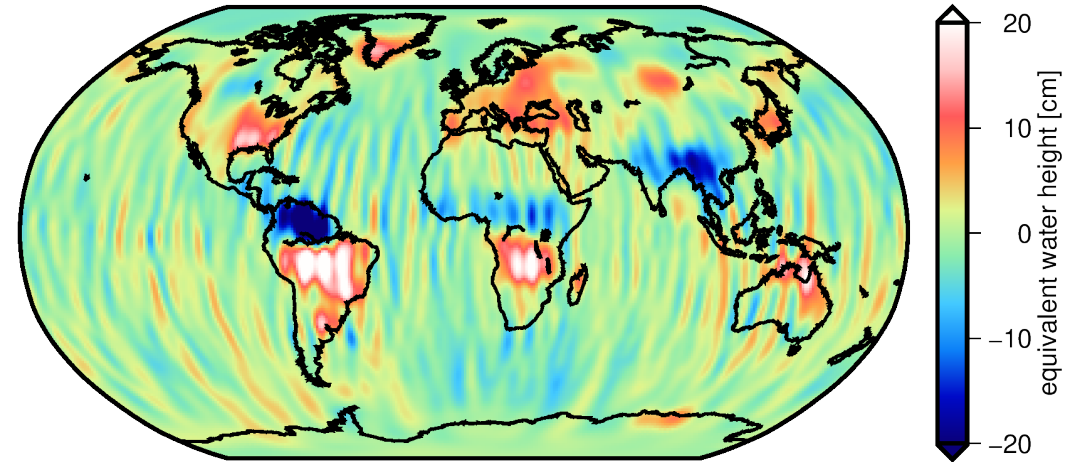


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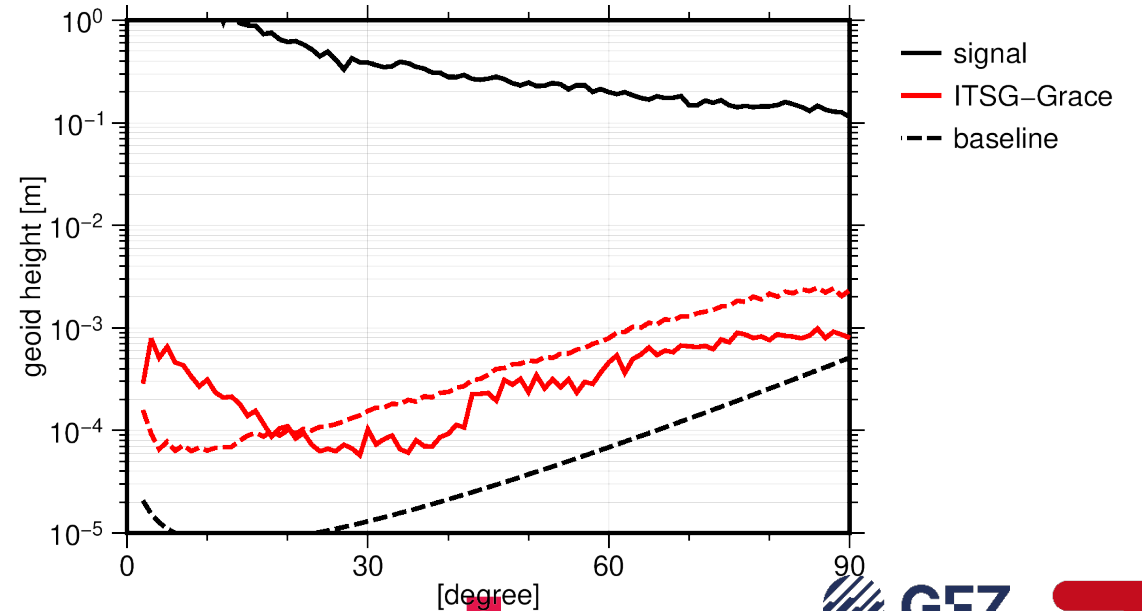


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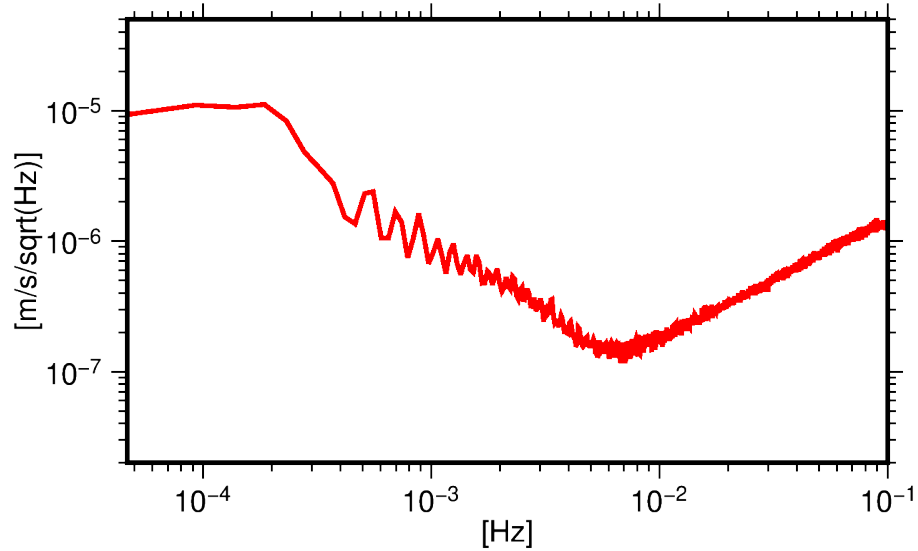


degree amplitudes (2010-02)

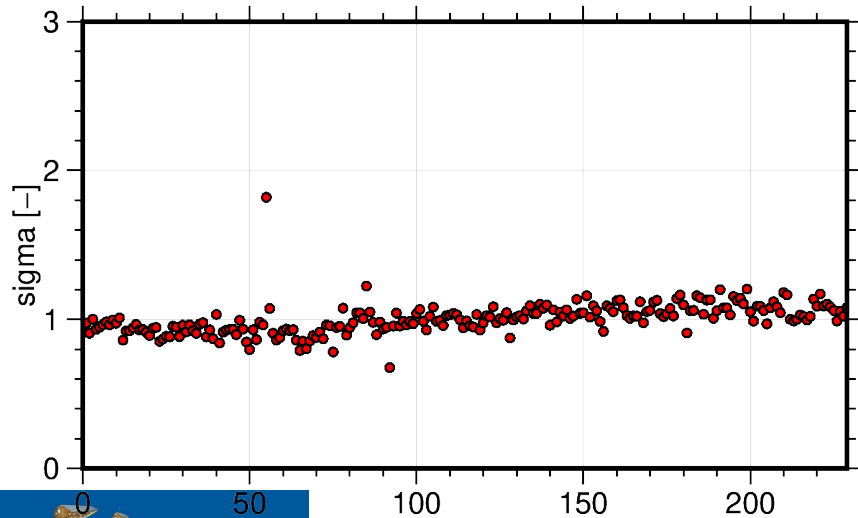


1. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

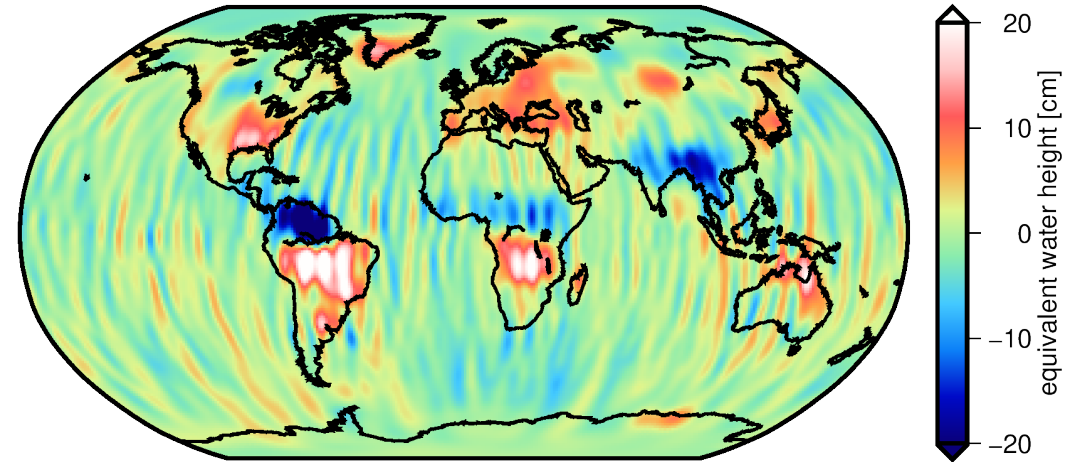


New weight matrix

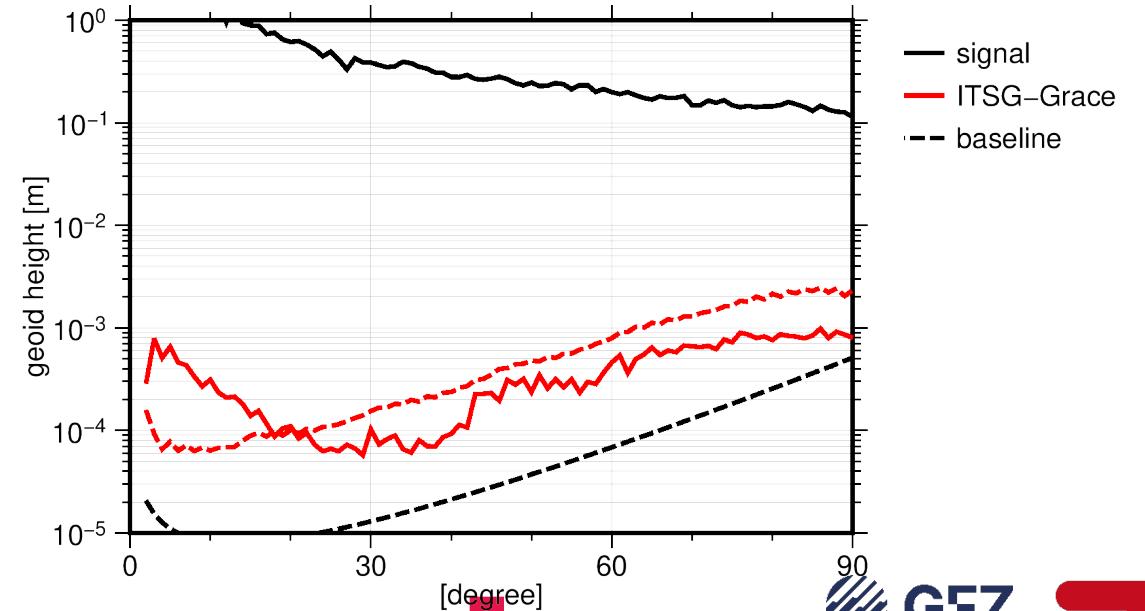


Least squares adjustment

Gaussian filter 350 km

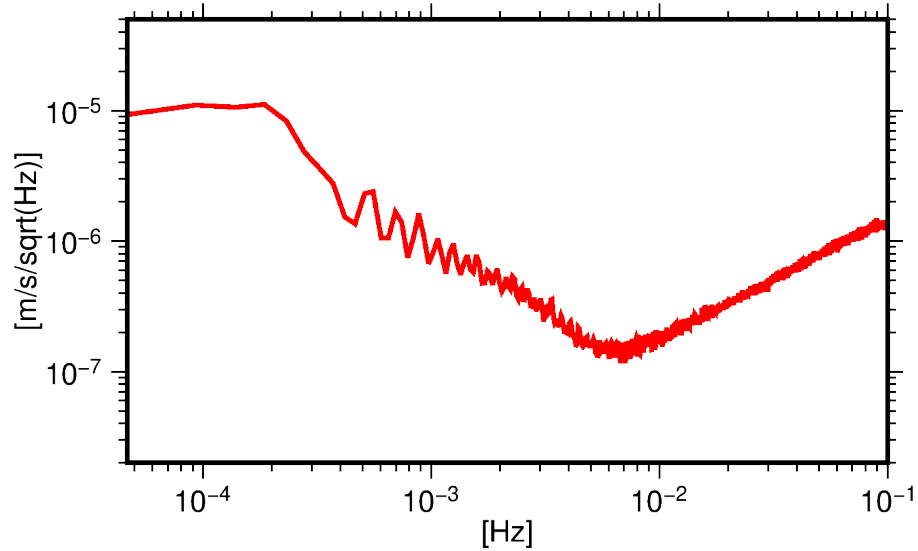


degree amplitudes (2010-02)

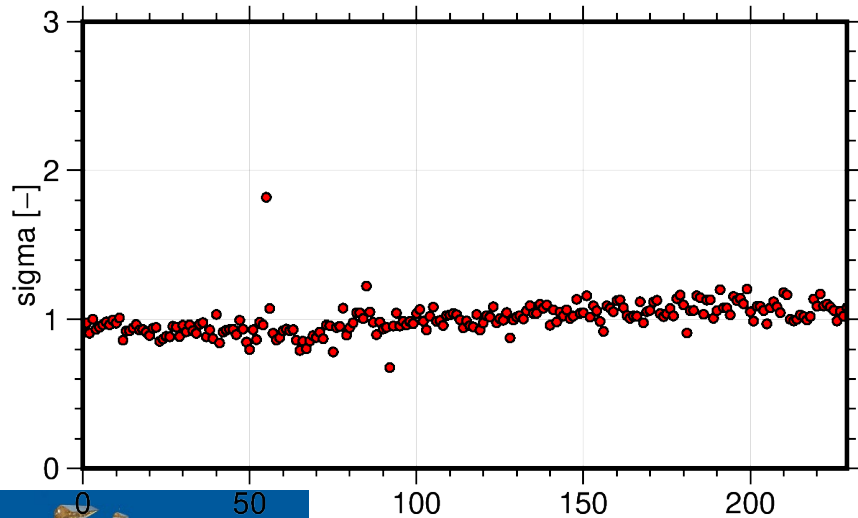


2. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

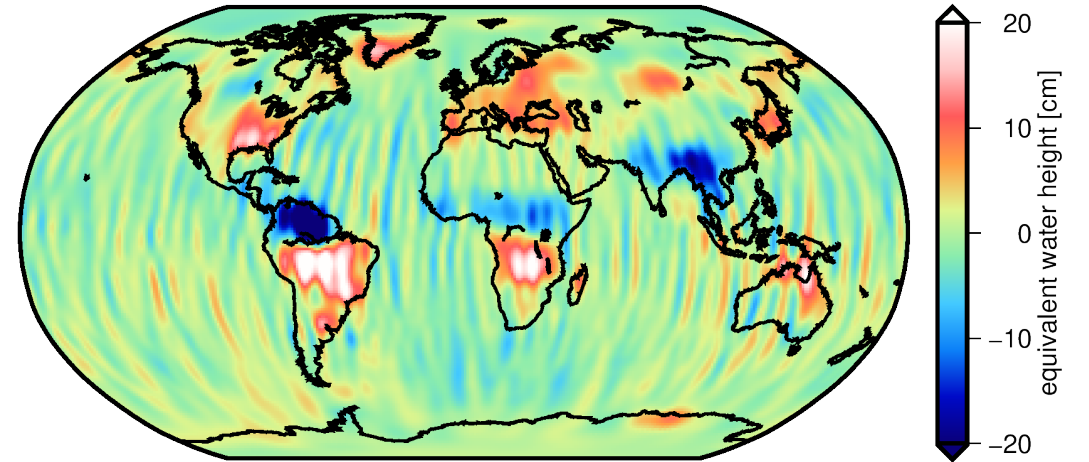


New weight matrix

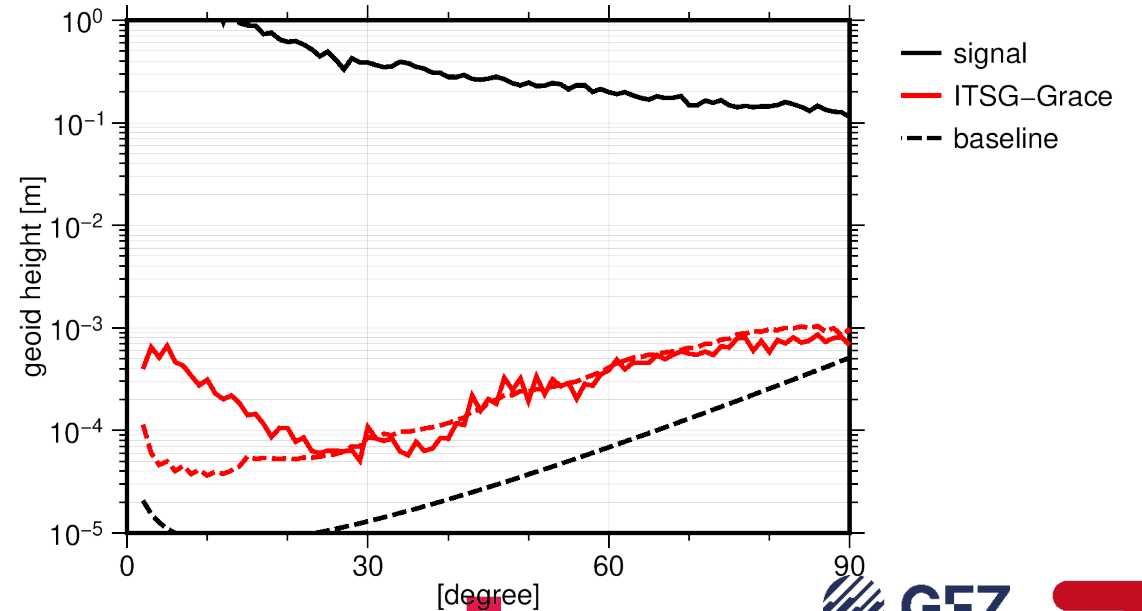


Least squares adjustment

Gaussian filter 350 km

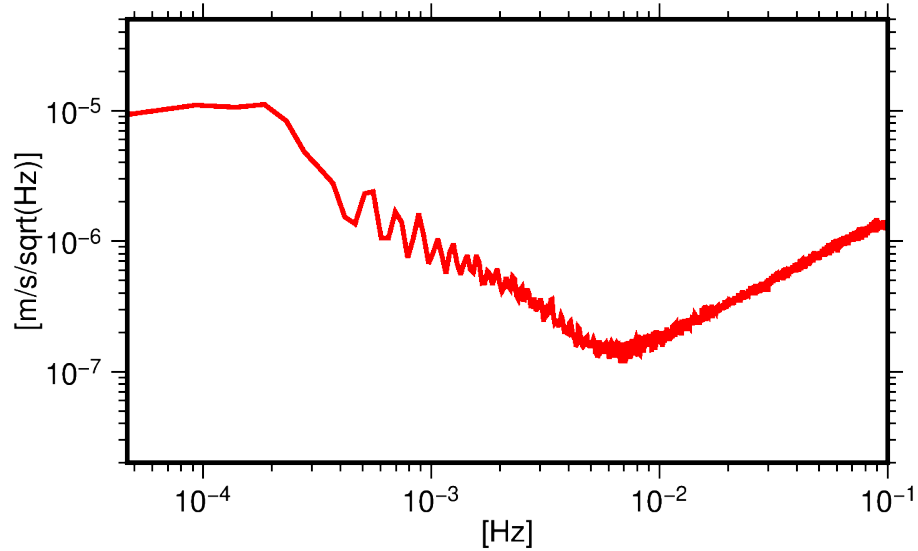


degree amplitudes (2010-02)

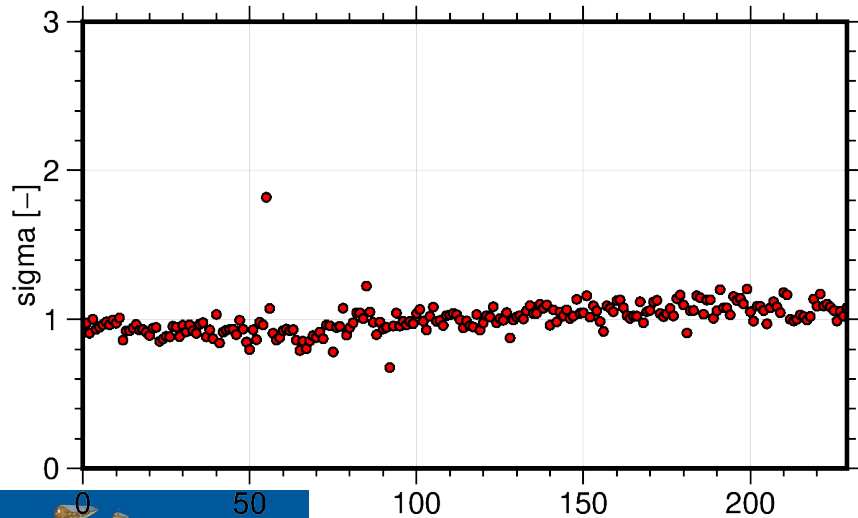


2. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

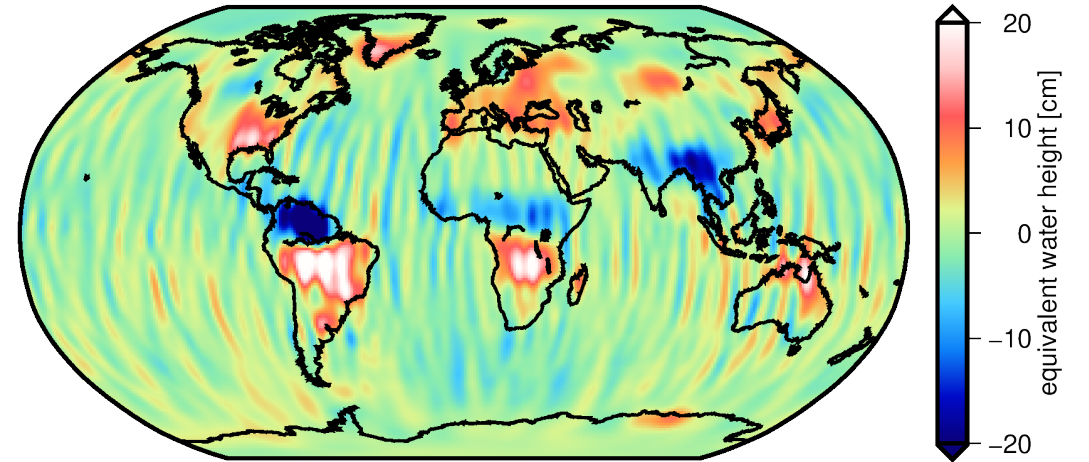


Post-fit residuals

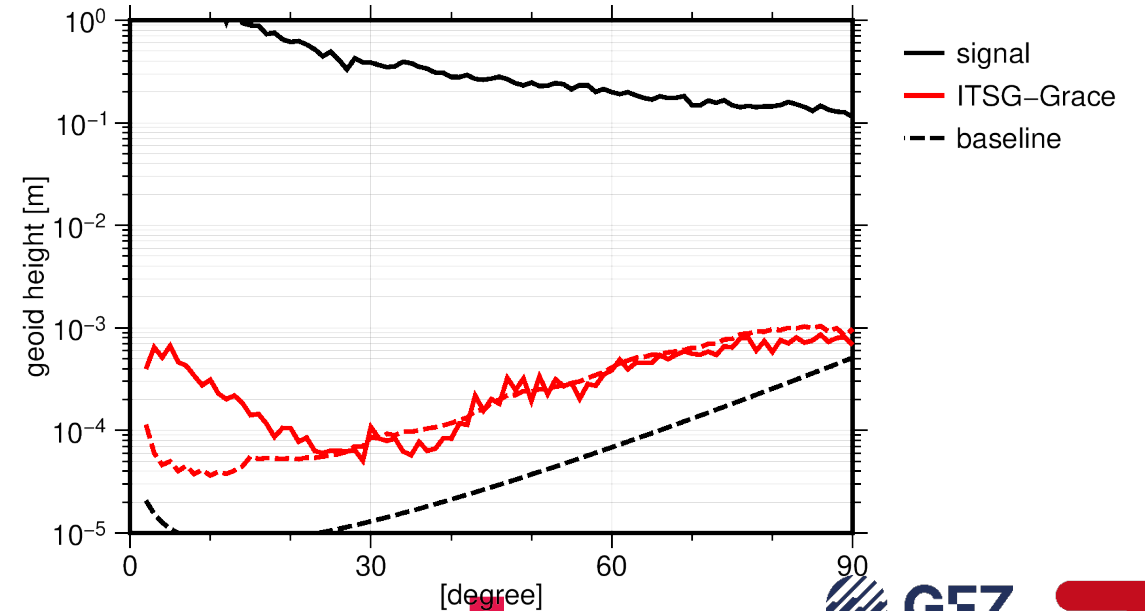


Estimate new covariance matrix

Gaussian filter 350 km

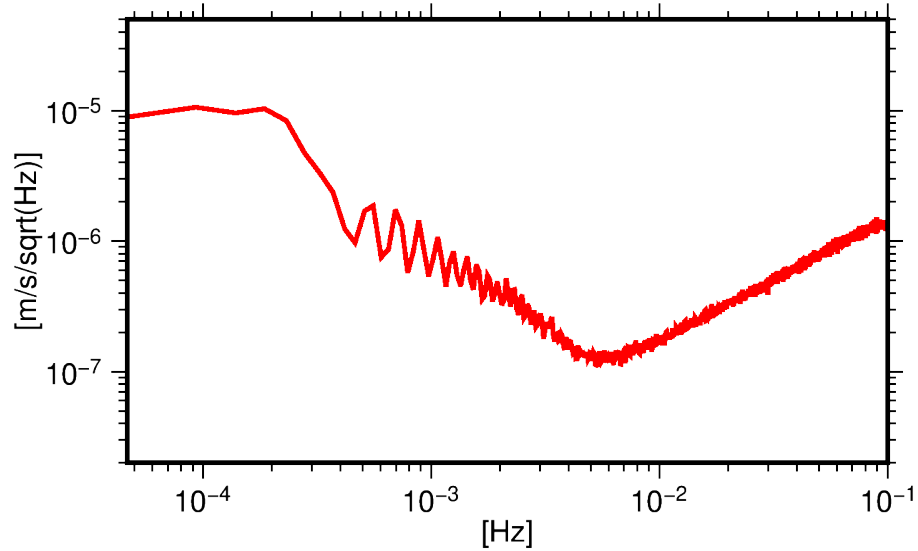


degree amplitudes (2010-02)

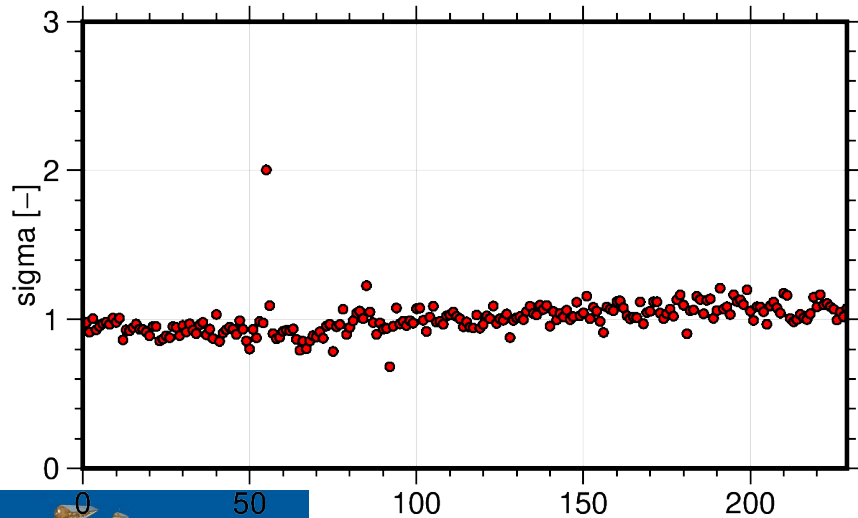


2. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

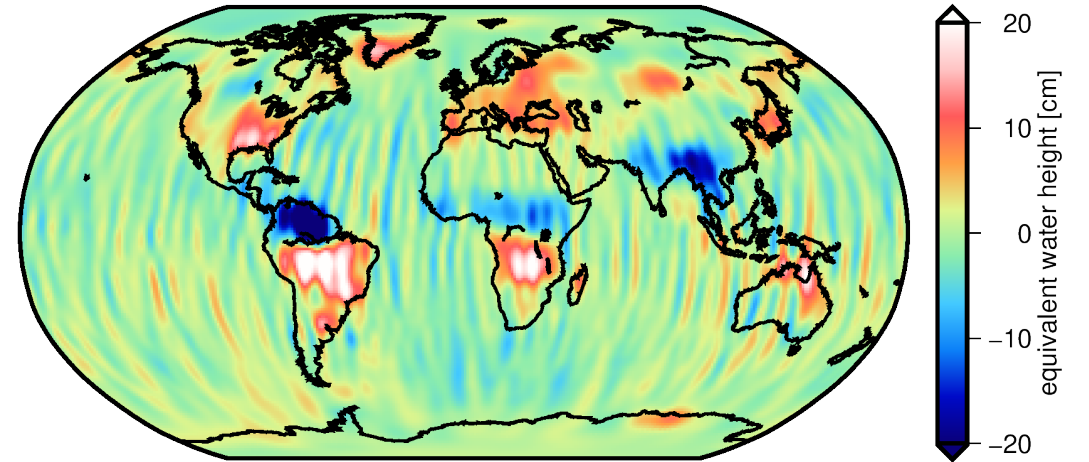


Post-fit residuals

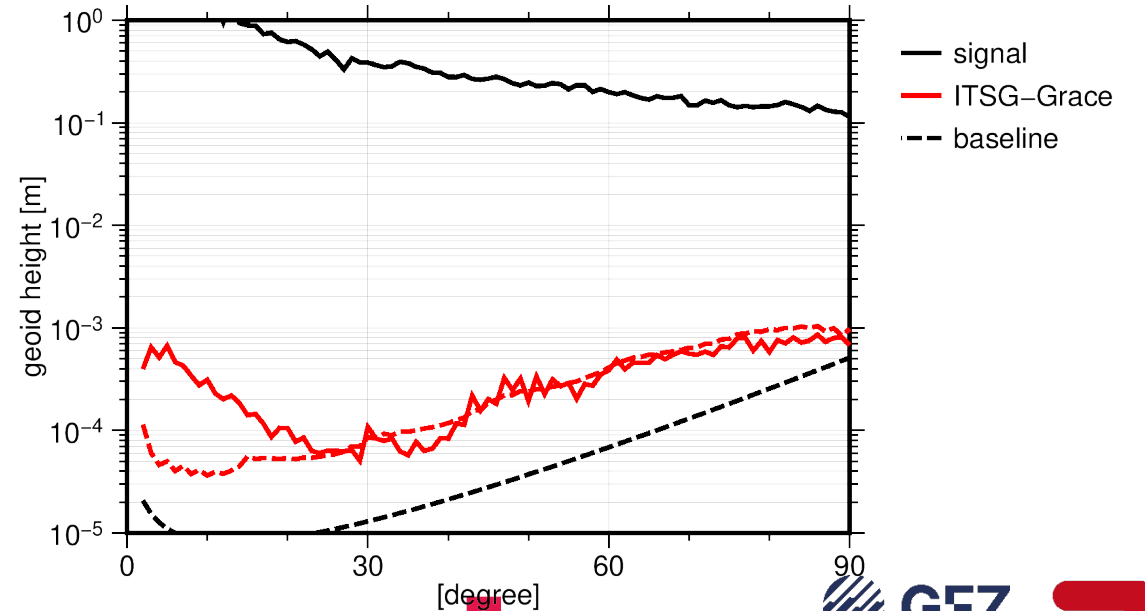


Estimate new covariance matrix

Gaussian filter 350 km

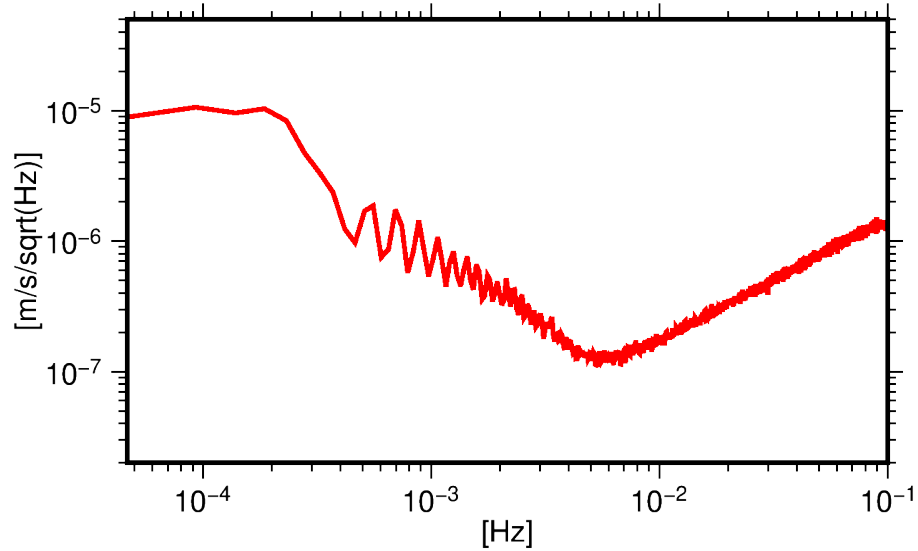


degree amplitudes (2010-02)

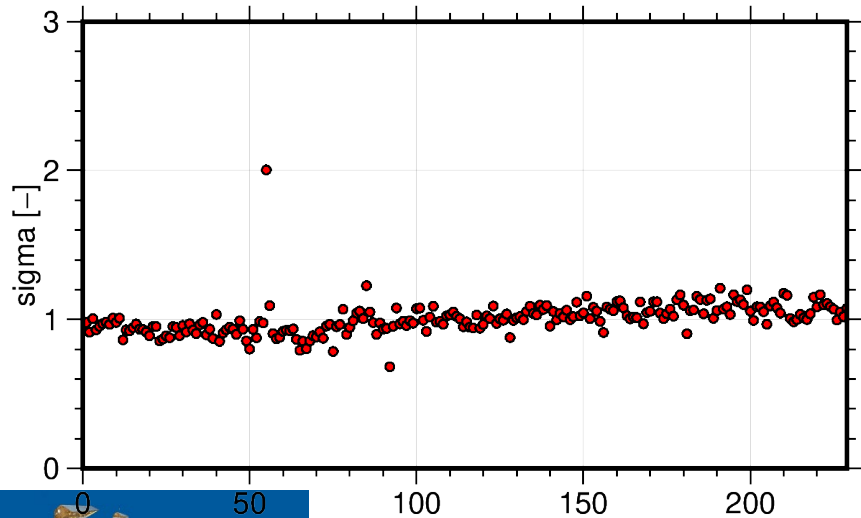


2. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)

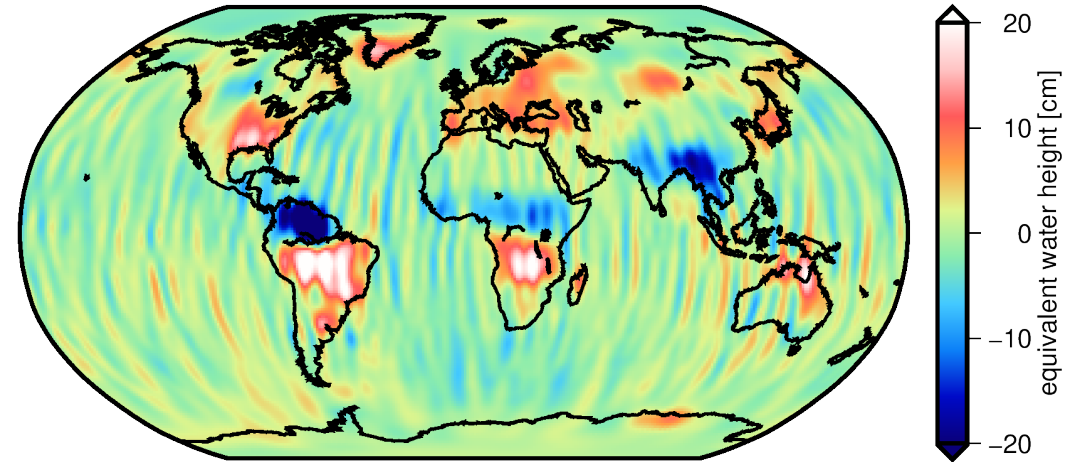


New weight matrix

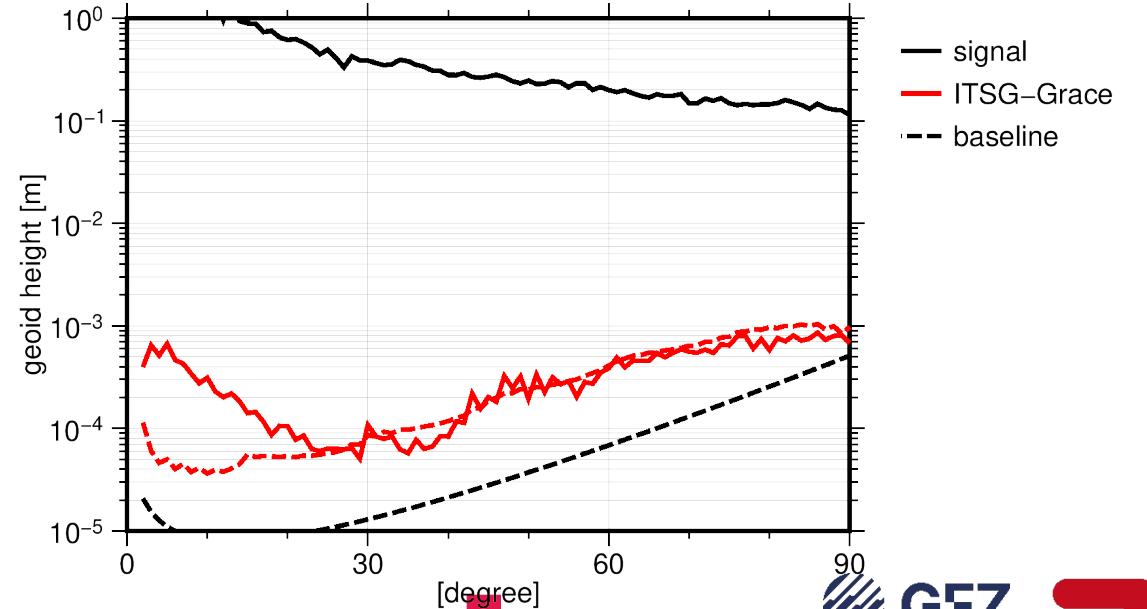


Least squares adjustment

Gaussian filter 350 km

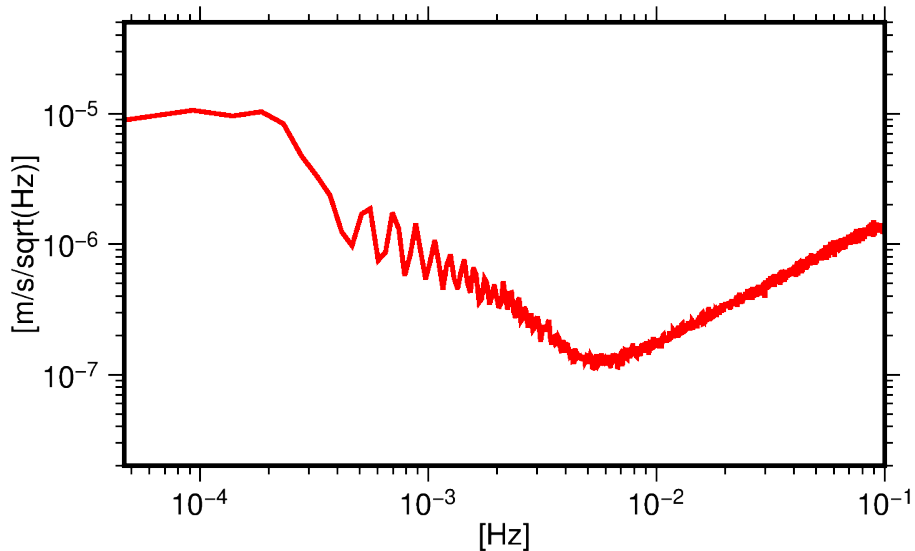


degree amplitudes (2010-02)

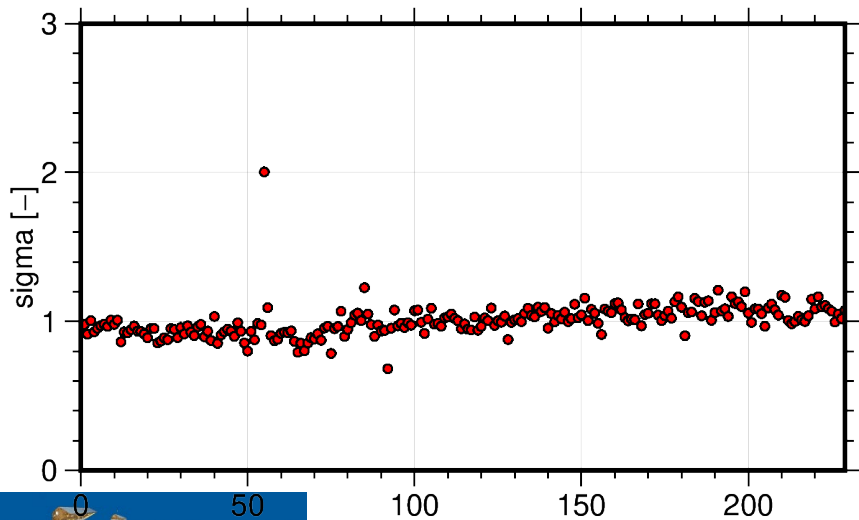


3. iteration

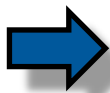
PSD range rate residuals (2010-02)



arc sigmas (2010-02)

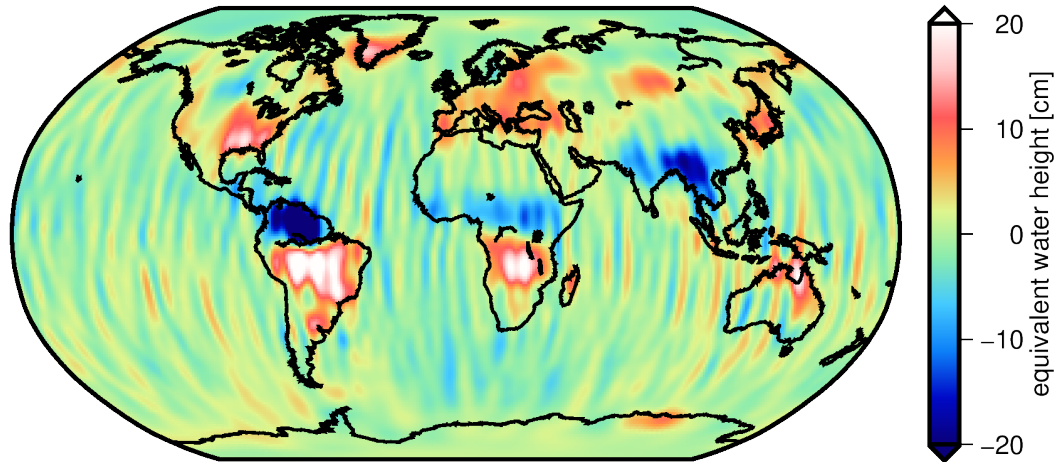


New weight matrix

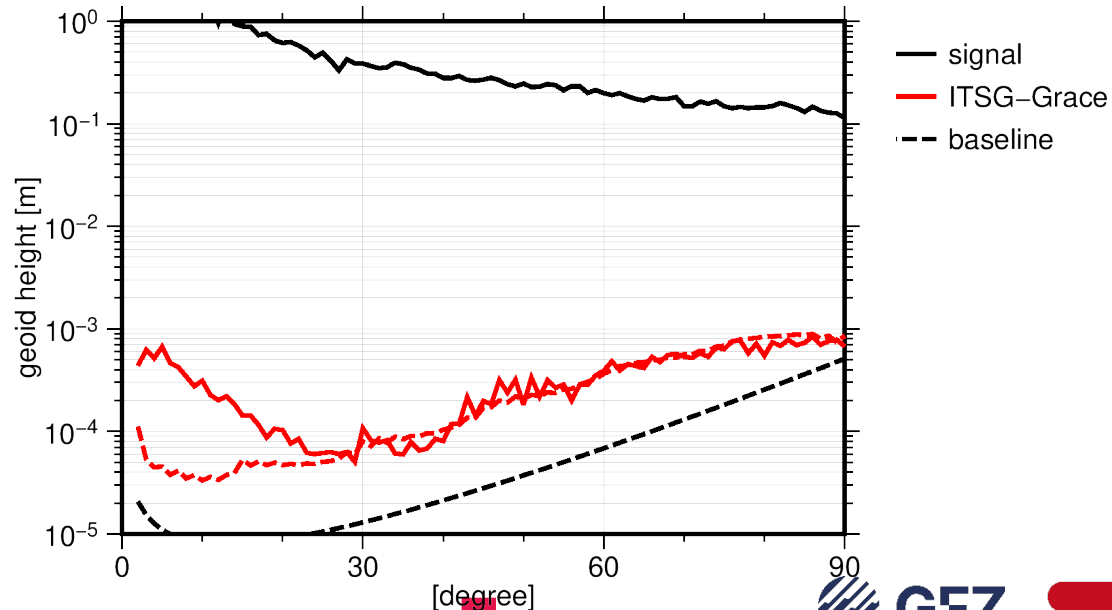


Least squares adjustment

Gaussian filter 350 km

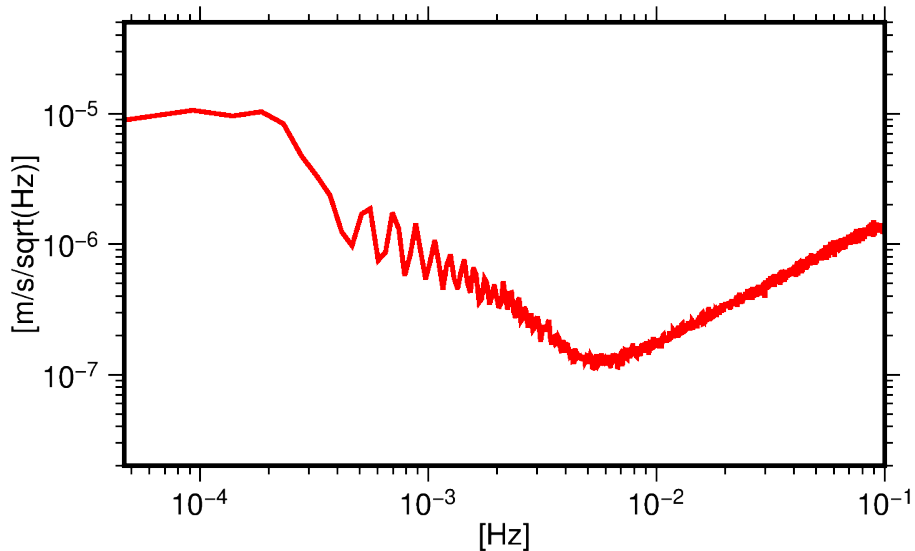


degree amplitudes (2010-02)

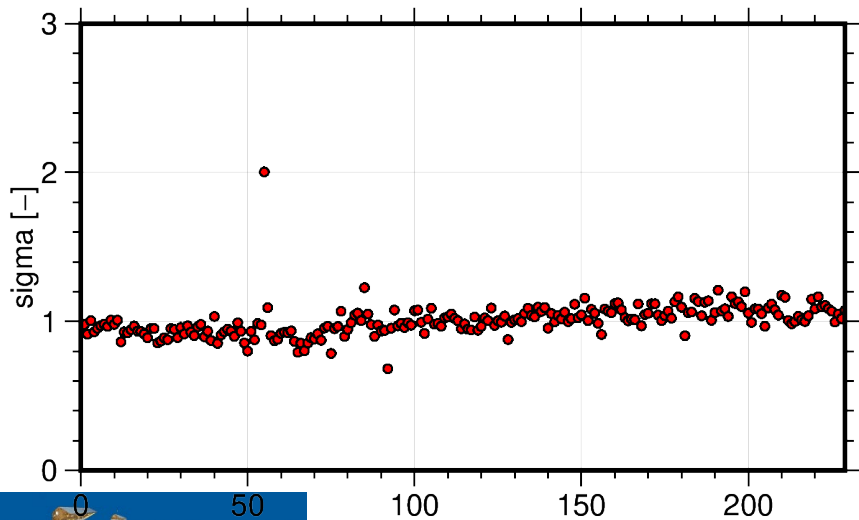


3. iteration

PSD range rate residuals (2010-02)



arc sigmas (2010-02)



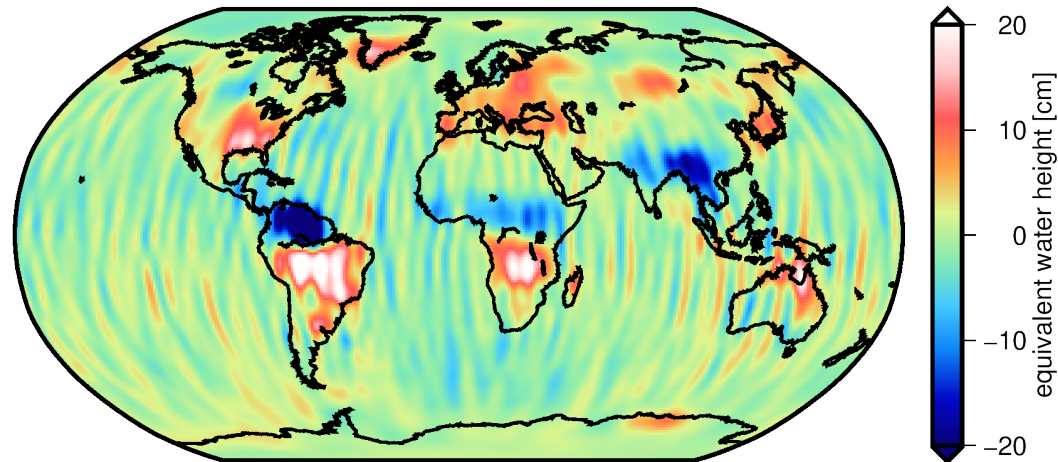
Post-fit residuals



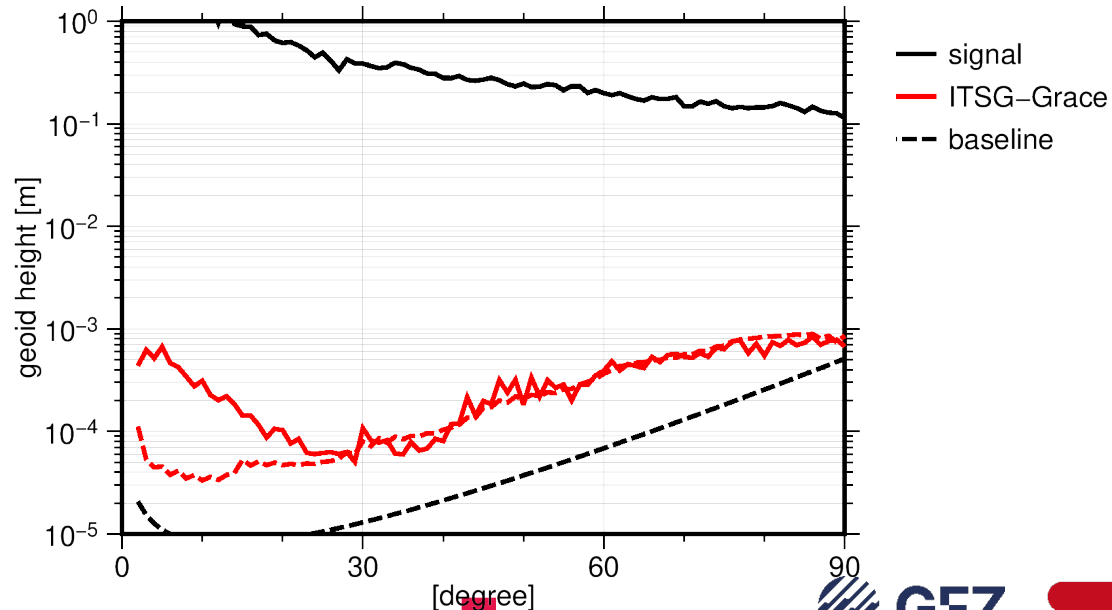
Estimate new covariance matrix

No more changes

Gaussian filter 350 km

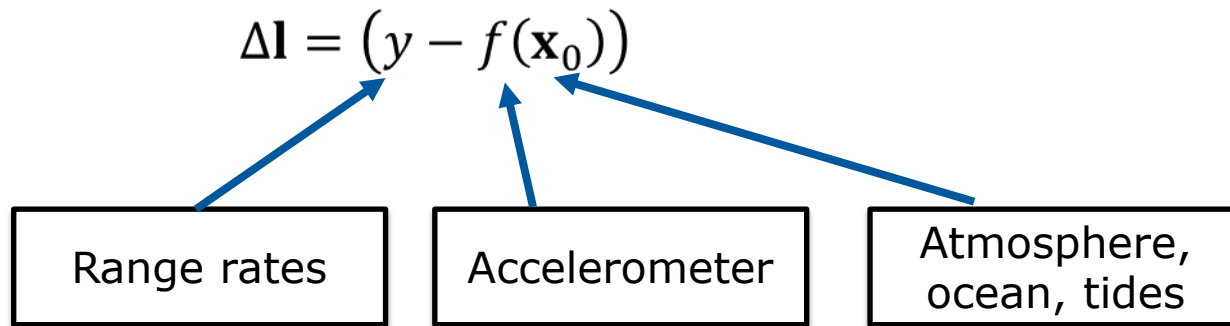


degree amplitudes (2010-02)



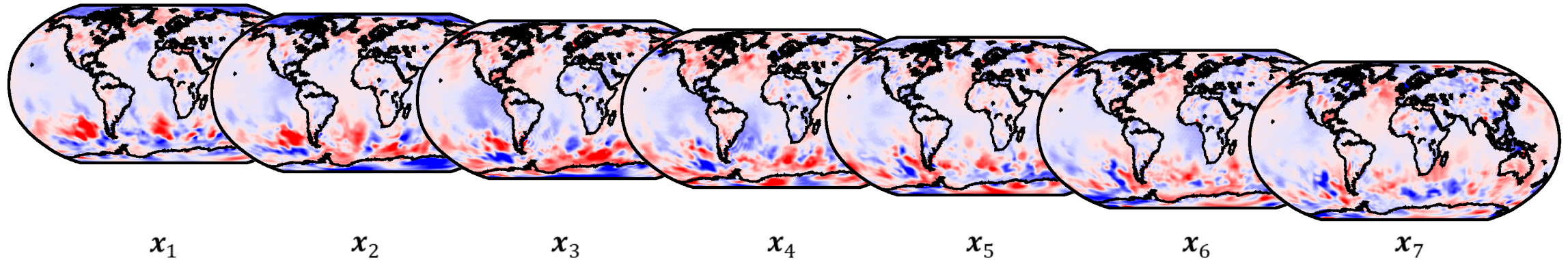
Summary of the first part

- Iterative algorithm to determine the weight matrix in least squares adjustment
 - Analysis of the post-fit residuals
 - Arcwise optimized relative weighting using variance component estimation (VCE) [Koch (1999): Parameter estimation and hypothesis testing in linear models, Springer, doi.org/10.1007/978-3-662-03976-2]
 - Ellmer (2018): Contributions to GRACE Gravity Field Recovery, doctoral thesis 2018, doi.org/10.3217/978-3-85125-646-8
 - Murböck et al. (2023): In-Orbit Performance of the GRACE Accelerometers and Microwave Ranging Instrument, Remote Sens. 2023, 15(3), 563; <https://doi.org/10.3390/rs15030563>
- Assumption: Noise time series is stationary (along the orbit)
 - This might be true for the instrument noise
 - But not for background model errors



Background model noise

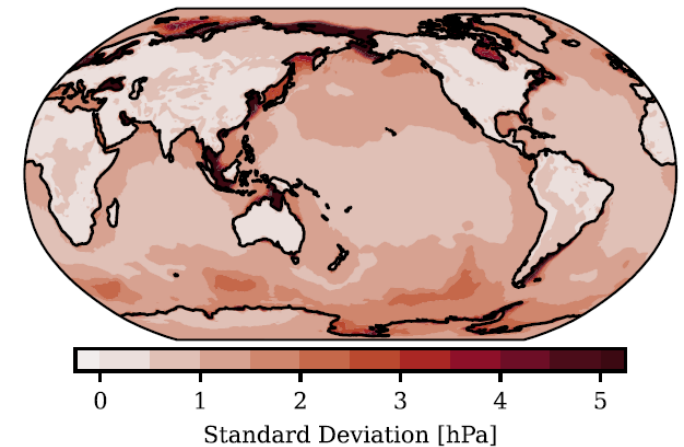
Shihora et al. (2024): Accounting for residual errors in atmosphere–ocean background models applied in satellite gravimetry, J Geod, 98:27, doi.org/10.1007/s00190-024-01832-7



Time series of vectors (SH coefficients), 26 years

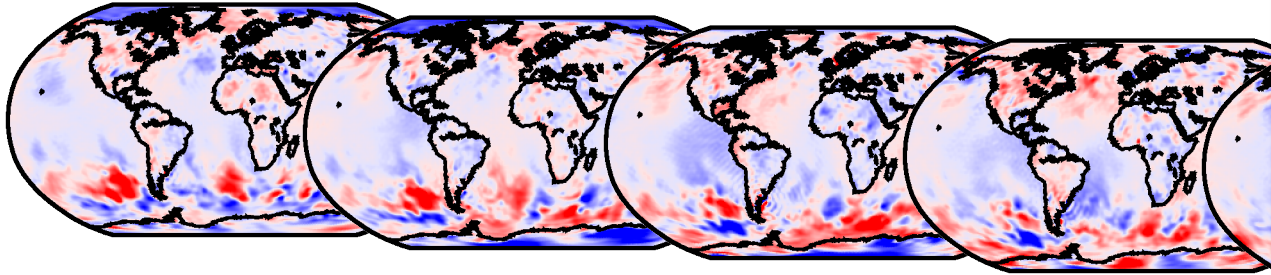
Assumption: stationary random process

$$\Sigma = \frac{1}{N} \sum_{i=0}^N \mathbf{x}_i \mathbf{x}_i^T \quad \Sigma_{\Delta 1} = \frac{1}{N} \sum_{i=0}^N \mathbf{x}_{i-1} \mathbf{x}_i^T \quad \Sigma_{\Delta 2} = \frac{1}{N} \sum_{i=0}^N \mathbf{x}_{i-2} \mathbf{x}_i^T \quad \dots$$



Background model noise

Shihora et al. (2024): Accounting for residual errors in atmosphere–ocean background models applied in satellite gravimetry, *Journal of Geodesy*, 98:27, doi.org/10.1007/s00190-024-01832-7



x_1

x_2

x_3

x_4

Time series of vectors (SH coefficients), 26 years

Assumption: stationary random process

$$\Sigma = \frac{1}{N} \sum_{i=0}^N x_i x_i^T \quad \Sigma_{\Delta 1} = \frac{1}{N} \sum_{i=0}^N x_{i-1} x_i^T \quad \Sigma_{\Delta 2} = \frac{1}{N} \sum_{i=0}^N x_{i-2} x_i^T$$

Full covariance matrix of one month
(Block Toeplitz matrix)

Day 1	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$	$\Sigma_{\Delta 4}$	$\Sigma_{\Delta 5}$
Day 2	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$	$\Sigma_{\Delta 4}$
Day 3	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$
	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$
⋮	$\Sigma_{\Delta 4}^T$	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$
Day 31	$\Sigma_{\Delta 5}^T$	$\Sigma_{\Delta 4}^T$	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ

Modeling the observation noise

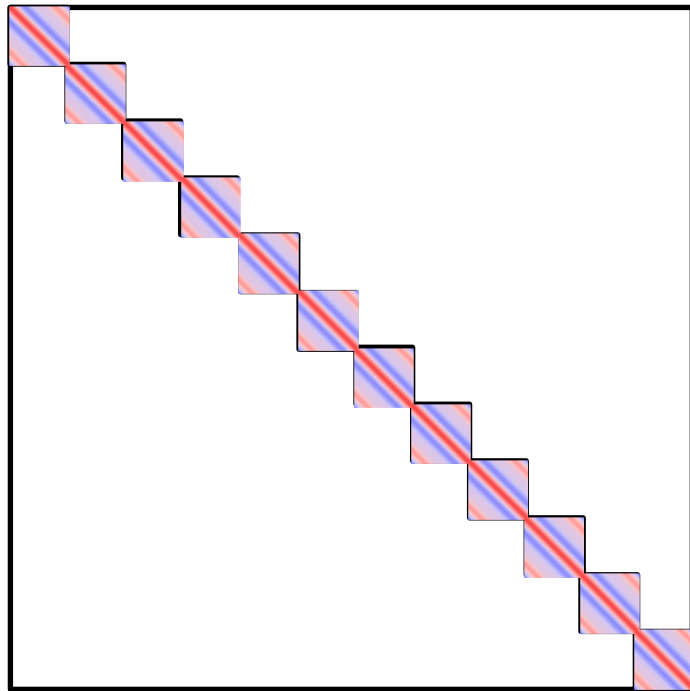
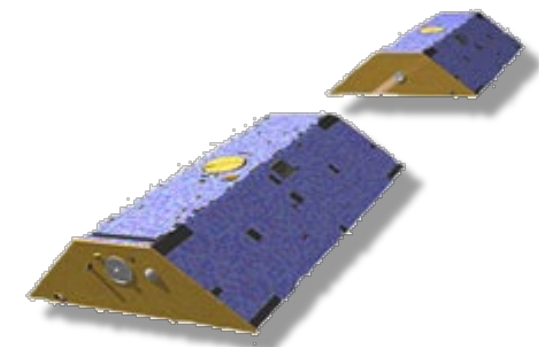
Covariance matrix of the reduced observation vector

$$\Sigma_{\Delta l} = \Sigma_{instr} + \mathbf{B}\Sigma_{model}\mathbf{B}^T$$

Variance propagation
(from spherical harmonics to range rates)

Stationary along orbit

Stationary at Earth surface



Day 1

Day 1	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$	$\Sigma_{\Delta 4}$	$\Sigma_{\Delta 5}$
Day 2	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$	$\Sigma_{\Delta 4}$
Day 3	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$	$\Sigma_{\Delta 3}$
⋮	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$	$\Sigma_{\Delta 2}$
⋮	$\Sigma_{\Delta 4}^T$	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ	$\Sigma_{\Delta 1}$
Day 31	$\Sigma_{\Delta 5}^T$	$\Sigma_{\Delta 4}^T$	$\Sigma_{\Delta 3}^T$	$\Sigma_{\Delta 2}^T$	$\Sigma_{\Delta 1}^T$	Σ

⋮

Day 31

Least squares adjustment

- Observation model

$$\Delta \mathbf{l} = \mathbf{A} \Delta \mathbf{x} + \mathbf{e} \quad \text{with} \quad \Sigma_{\mathbf{e}} = \Sigma_{instr} + \mathbf{B} \Sigma_{model} \mathbf{B}^T$$

$$\mathbf{P}_{\mathbf{e}} = (\Sigma_{instr} + \mathbf{B} \Sigma_{model} \mathbf{B}^T)^{-1}$$

Problem:
Matrix is fully occupied,
2 TB!

Least squares adjustment

- Observation model

$$\Delta \mathbf{l} = \mathbf{A} \Delta \mathbf{x} + \mathbf{e} \quad \text{with} \quad \boldsymbol{\Sigma}_{\mathbf{e}} = \boldsymbol{\Sigma}_{instr} + \mathbf{B} \boldsymbol{\Sigma}_{model} \mathbf{B}^T \quad \mathbf{P}_{\mathbf{e}} = (\boldsymbol{\Sigma}_{instr} + \mathbf{B} \boldsymbol{\Sigma}_{model} \mathbf{B}^T)^{-1}$$

- Alternative model: co-estimation of submonthly (6 hourly) signals \mathbf{y} and constraining these signals towards zero

$$\Delta \mathbf{l} = \mathbf{A} \Delta \mathbf{x} + \mathbf{B} \mathbf{y} + \mathbf{e} \quad \boldsymbol{\Sigma}_{\mathbf{e}} = \boldsymbol{\Sigma}_{instr} \quad \mathbf{P}_{\mathbf{e}} = \boldsymbol{\Sigma}_{instr}^{-1}$$

Both models are equivalent as shown in:

Kvas & Mayer-Gürr (2019): GRACE gravity field recovery with background model uncertainties. *J Geod* 93, 2543–2552. doi.org/10.1007/s00190-019-01314-1

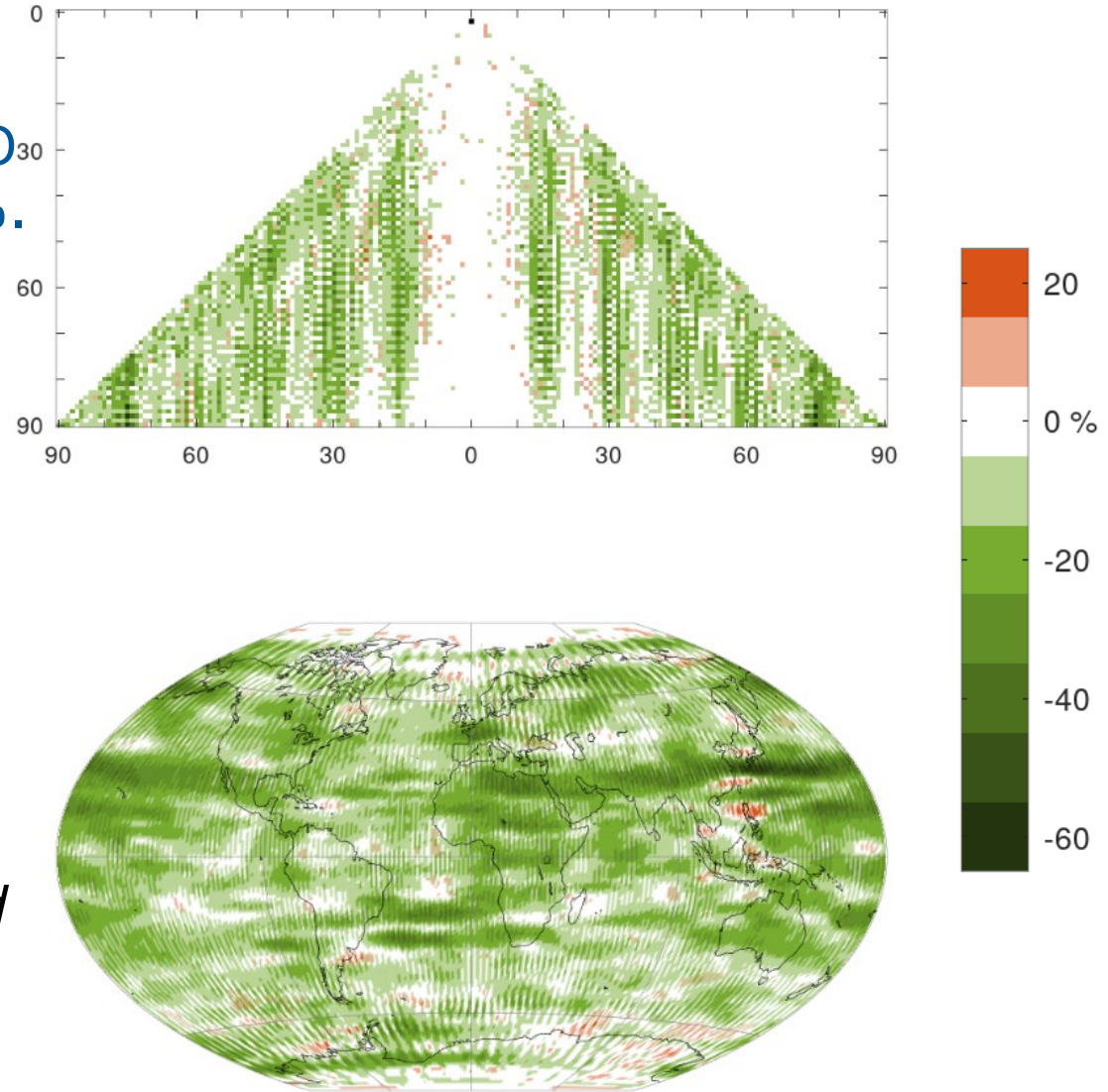
Background model noise

Stochastic modeling applied for ocean tide and non-tidal AOD models **improves GRACE/GRACE-FO gravity fields by up to 20 %.**

Hauk et al. (2023). Satellite gravity field recovery using variance-covariance information from ocean tide models. *Earth and Space Science*, 10(10), e2023EA003098.

<https://doi.org/10.1029/2023EA003098>

Wilms et al. (2025). Optimized gravity field retrieval for the MAGICmission concept using background model uncertainty information. *J Geod* 99.21. <https://doi.org/10.1007/s00190-024-01931-5>



Very short summary

- The weight matrix in least squares adjustment is important

$$\|\Delta \mathbf{l} - \mathbf{A} \cdot \Delta \mathbf{x}\|_{\mathbf{P}}^2 \rightarrow \min$$

- Analyzing the post-fit residuals helps to derive a proper weight matrix

$$\hat{\mathbf{e}} = \Delta \mathbf{l} - \mathbf{A} \Delta \hat{\mathbf{x}}$$

- This is true for almost every least squares adjustment