

GRACE fast mascons from spherical harmonics and a regularization design trade study

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Key Points:

- Computationally efficient mascons computed from GRACE Level-2 spherical harmonics are equivalent to those from Level-1B ranging data
- These mascons can be tailored to specific problems of interest and do not require special orbit determination software
- A presented trade study shows the effects of spherical expansion truncation and compares diagonal regularization to that with correlations

Abstract

Mass concentration (mascon) solutions have become a prominent medium for investigating time-variable gravity recovered by GRACE and GRACE Follow-On. While GRACE Level-2 spherical harmonic products require various post-processing techniques to eliminate correlated noise, mascon formulations employ spatial regularization strategies during the estimation step to improve signal recovery. However, mascon estimation has traditionally required large computing resources and GRACE Level-1B processing capabilities. In this study, we show that a typical mascon estimation system can be reformulated to allow for the estimation of regularized mascons from Level-2 spherical harmonics. Provided that spherical harmonic solution covariances are available, the computed mascons will be mathematically equivalent to similar mascons estimated from Level-1B observations. This method is computationally efficient, better leverages GRACE spherical harmonics than past methods, and matches the performance of typical mascon solutions without locking scientists into pre-determined regularization designs. We develop a proof-of-concept solution using ITSG-Grace2018 and compare results with traditional mascons from JPL and NASA GSFC. We then assess the effects of spherical harmonic truncation and use of regularization correlations on basin signal recovery. We find that spherical expansions to degree and order 60 provide the minimum expansion necessary to study most basins, while larger expansions help further localize signals. We also find that diagonal regularizations (i.e., regularizations that do not contain inter-mascon correlations) are adversely affected by leakage, especially across boundaries such as coastlines where signals are not highly correlated, whereas including inter-mascon correlations and regional boundaries in the regularization greatly improves signal recovery.

Plain Language Summary

This study derives a new method for producing surface mass change maps in the form of so-called “mascons” using GRACE and GRACE Follow-On data that is computationally simpler but equally as rigorous as typically used methods. Using this method, scientists no longer need specialized orbit determination and estimation software to produce these maps, and therefore this type of work is now accessible to scientists outside of the few major centers that currently produce these maps. At the same time, centers with these specialized software packages can incorporate the computational efficiencies presented here to improve their own processes. As a result, this new method can be used

to study individual problems of interest outside the scope of the globally focused solutions available today (for example, to specifically study targeted river basins), and these new studies can additionally incorporate other known information about those problems. We provide a proof-of-concept solution showcasing the new method and apply the new method to highlight key design decisions that must be made when producing mascon solutions.

1 Introduction

The Gravity Recovery and Climate Experiment (GRACE) and GRACE Follow-On (GRACE-FO) missions have enabled a record of Earth’s time-variable gravity and surface mass change approaching 20 years in length, and this record has been used to study mass changes in global ice sheets, oceans, terrestrial water storage, and more (Tapley et al., 2004, 2019; Landerer et al., 2020). Due to the nature of the primary observable of these missions, multiple steps are typically employed in producing data products for scientific research and applications. The GRACE and GRACE-FO Science Data System (SDS) team at the Jet Propulsion Lab (JPL) computes Level-1B ranging measurements from the missions’ raw inter-satellite microwave and laser ranging observations, and these data are then used to estimate a variety of user-focused products. In addition to these ranging measurements, the Level-1B products also include a number of other necessary measurements, including star tracker data, GPS orbits, and on-satellite accelerometer measures.

Level-2 spherical harmonic solutions produced by the SDS teams at JPL, the University of Texas at Austin’s Center for Space Research (CSR), and the German Research Centre for Geosciences (GFZ), and equivalent products produced at additional centers (e.g., the ITSG-Grace2018 monthly solution (Kvas et al., 2019; Mayer-Gürr et al., 2018)), are unconstrained representations of the gravity field. These solutions are estimated through a data reduction and inversion process from Level-1B data using orbit propagation and estimation software systems, requiring a great deal of computing resources and expertise (Bettadpur, 2018; Yuan, 2019). These solutions are often analyzed using a variety of post-processing techniques and filters that are required to reduce noise and systematic errors (e.g., correlated errors manifesting as vertical stripes in the solution), but scientists must take care to not introduce excessive spatial signal leakage and must attempt to quantify analysis errors due to signal attenuation in the filtering process (e.g., Wahr

et al., 1998; Swenson & Wahr, 2006). For example, one common technique for computing basin mass change from spherical harmonics is the application of a properly designed basin averaging kernel, though variations in the design of these kernels or filtering applied to the solution can greatly impact results (Swenson & Wahr, 2002).

Over the past 10 years, end user-oriented mass concentration (mascon) solutions from JPL, CSR, and NASA Goddard Space Flight Center (GSFC) have been introduced (Luthcke et al., 2013; Watkins et al., 2015; Save et al., 2016). These solutions estimate sets of surface mass cells globally and enable much simpler basin and regional analysis than with Level-2 products. Additionally, these mascon solutions are estimated directly from Level-1B observations, much like the Level-2 spherical solutions, but they do not have the same post-processing requirements as with spherical harmonic solutions. Instead, various regularization techniques are applied in the solution estimation step to improve signal recovery and suppress noise and leakage, and basin analysis with mascons is achieved with the simple summation of the mass change recovered over all mascon cells within the basin. However, while these solutions show improvements in signal recovery and ease of use, they restrict users to the specific regularization choices made in each solution and inhibit advanced users from fine tuning analyses for investigations of specific regions. Additionally, effort must be made to account for errors due to the imposed regularization during any analyses, such as by applying the resolution operator to estimate biases (Luthcke et al., 2013; Loomis et al., 2019).

While post-processing with spectral filters has generally been the dominant method of investigating the gravity field with spherical harmonic products, numerous studies have also explored the application of regularization to spherical harmonic solutions. For example, Save et al. (2012) included regularization constraints in the least squares inversion of GRACE spherical harmonic estimates, finding that such regularization reduces errors in the gravity field estimate compared with the unconstrained Level 2 solutions. This and similar efforts still required particular understanding of how to properly apply a spherical harmonic solution in investigations of time-variable gravity and surface mass change. Additionally, like the previously mentioned mascon solutions, any investigations using this or other regularized solutions are dependent on the regularization design.

Swenson and Wahr (2011) discussed a method for adding regularization to an unconstrained spherical harmonic solution as a post-processing measure that showed similar signal characteristics to a solution where regularization was included in the estimate inversion. The construction of that method was in many ways similar to the resolution operator approach used in Luthcke et al. (2013) and Loomis et al. (2019) and similarly showed that the method would enable GRACE data end users to construct their own regularization constraints and use those to help build analysis error budgets. However, while the method allows for regularization to be introduced into the estimate, the regularization is applied in post-processing and is not an exact match to that applied during an inversion from Level-1B data.

To reduce computational complexity while trying to capture the same benefits of traditional mascons, multiple studies have estimated simplified mascons from Level-2 sphericals to study mass change in various ice sheets and ice caps across the Earth (e.g., Jacob et al., 2012; Velicogna et al., 2014; Schrama et al., 2014). While most such studies have focused regionally on ice sheets, these methods can all be applied to any basin or globally. Watkins et al. (2015) notes these and similar efforts when they define three primary types of GRACE mascon solutions: those estimated directly from ranging measurements (such as the JPL mascon solution), those estimated from ranging measurements through a finite truncation of spherical partial derivatives (such as the GSFC and CSR mascon solutions), and simplified mascons fit directly from Level-2 spherical harmonics. While the first two approaches are largely equivalent methods for estimating the gravity field directly from GRACE ranging measurements, the third simplified mascon approach is a less rigorous post-processing step that does not account for any spherical harmonic error covariance information. Ran et al. (2018) improved on these simplified methods by using the law of covariance propagation to optimally estimate mascons over Greenland from sphericals and their full error covariances, but this study is still a post-processing of Level-2 data, was conducted regionally, and did not include regularization as with the more rigorous global mascon solutions.

We present a new method of regularized mascon estimation from spherical harmonics that matches traditional rigorous mascons in their solution quality. This new “fast mascon” approach applies equations from Sabaka et al. (2010) in a new way, relating monthly spherical harmonic fields and their full error covariances to a global set of mascon cells. Importantly, this method is mathematically equivalent to the approaches for comput-

ing the GSFC and CSR mascons from Level-1B data in Luthcke et al. (2013) and Save et al. (2016). As with these rigorous mascons, the fast mascon method can utilize the same tools for accounting for estimate errors (e.g., the resolution operator). Further, this method does not rely on complex orbit determination and parameter estimation systems (e.g., GEODYN) and can be implemented on most commonly used hardware using standard scientific computing packages. As such, this new approach is comparable to a traditional rigorous mascon approach from Level-1B data - rather than to the many various Level-2 post-processing approaches - while also allowing for a customizable design and providing large benefits in terms of computational complexity and cost. Mascon estimates using this approach fully incorporate all parameterization decisions made by the center that produced the source spherical harmonic solutions and normal equations, and results using this approach are therefore dependent on the parameterization choices made by that processing center. This is not a restriction of the method for the processing centers themselves, and for others this restriction is no different from any other GRACE analysis technique.

2 Development of the Fast Mascon Method

Mascon solutions from GSFC and CSR use similar formulations for the determination of least squares normal equations relating GRACE Level-1B ranging observations to mascon space. Both centers employ the same general least squares system to solve $\mathbf{d} = \mathbf{A}\mathbf{m}$ for the best estimate $\hat{\mathbf{m}} \in \mathcal{R}^{N_M \times 1}$ of N_M mascons from N_K ranging observations using a Gauss-Newton least-squares estimator whose k th step estimates an adjustment $\Delta\mathbf{m}_k$ to the mascon state $\mathbf{m}_k$,

$$\begin{cases} \Delta\hat{\mathbf{m}}_k &= (\mathbf{A}^T\mathbf{W}\mathbf{A} + \lambda\mathbf{P})^{-1} [\mathbf{A}^T\mathbf{W}(\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \lambda\mathbf{P}(\mathbf{m}_a - \mathbf{m}_k)] \\ \mathbf{m}_{k+1} &= \mathbf{m}_k + \Delta\hat{\mathbf{m}}_k \end{cases}, \quad (1)$$

where the observation vector is the difference between the ranging observations $\mathbf{d} \in \mathcal{R}^{N_K \times 1}$ and the model prediction vector $\mathbf{f}$ and contains the range rate measurement residuals, $\mathbf{m}_a$ is the preferred mascon state, $\lambda\mathbf{P} \in \mathcal{R}^{N_M \times N_M}$ is the mascon regularization matrix (i.e., $\lambda^{-1}\mathbf{P}^{-1}$ is the signal covariance), $\mathbf{W}^{-1} \in \mathcal{R}^{N_K \times N_K}$ is the data noise covariance, and $\mathbf{A} \in \mathcal{R}^{N_K \times N_M}$ contains the partial derivatives of the range rate measurements with respect to the global set of mascons. Of particular interest in this study is the formulation $\mathbf{A} \equiv \mathbf{H}\mathbf{L}$ used by both GSFC and CSR, where $\mathbf{H} \in \mathcal{R}^{N_K \times N_C}$ contains the partial derivatives of the range rate measurements with respect to the N_C differential spher-

ical harmonic coefficients and $\mathbf{L} \in \mathcal{R}^{N_C \times N_M}$ contains the partial derivatives of the differential spherical harmonic coefficients with respect to the mascon parameters (Loomis et al., 2019; Save et al., 2016).

We then apply the Woodbury Matrix Identity and simplify (see Appendix A for full derivation) to obtain a new expression for the mascon estimate in terms of the spherical harmonic normal equations and estimate as

$$\hat{\mathbf{m}} = \mathbf{P}^{-1} \mathbf{L}^T (\lambda \mathbf{N}^{-1} + \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T)^{-1} \mathbf{c}. \quad (2)$$

In other words, this equation allows us to compute mascon solutions from Level-2 spherical harmonic solutions in a single iteration that are equivalent to those computed from Level-1B ranging observations (using Equation 1) if the normal equations or solution covariances are available for the Level-2 solutions. Note that Equation 2 matches Equation 14 in Sabaka et al. (2010), which is applied in a new way here.

To verify the equivalence between the developed fast mascon technique and the traditional rigorous mascon estimation method, we estimated a single month’s solution with each method, using equivalent regularizations. For this test, we used an in-house spherical harmonic estimate that is computed alongside the traditional GSFC monthly mascons. This allows for us to know that the exact same processing was applied to each solution. We then calculated the spatial RMS of the difference between the two solutions. We found this RMS to be on the order of 1E-10 cm water equivalent height for a given month (compared to a spatial RMS of the monthly signal on the order of 10 cm w.e.), indicating that the two solutions agreed to numerical precision.

To investigate bias due to leakage in the solution, we can use the resolution operator from Loomis et al. (2019):

$$\mathbf{R} = (\mathbf{L}^T \mathbf{N} \mathbf{L} + \lambda \mathbf{P})^{-1} \mathbf{L}^T \mathbf{N} \mathbf{L}. \quad (3)$$

As before, we use the Woodbury Matrix Identity and simplify to re-write this as

$$\mathbf{R} = \mathbf{P}^{-1} \mathbf{L}^T (\lambda \mathbf{N}^{-1} + \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T)^{-1} \mathbf{L}. \quad (4)$$

As with Equation 2, the developed expression for computing the resolution operator is mathematically equivalent to one developed for solutions from Level-1B observations. This operator can then be applied to determine mascon and basin biases, as in Loomis et al. (2019) and Croteau et al. (2020).

2.1 Conservation of mass and geocenter motion

GRACE spherical harmonic solutions do not usually include degree 0 and 1 terms, as mass should be conserved globally and the GRACE measuring system is insensitive to geocenter variations. Instead, GRACE Technical Note 13 is typically used to restore surface mass change induced degree 1 signals, following Sun et al. (2016). In practice, this means that the spherical harmonic solutions and normal equations that we use for the fast mascon method omit the first four spherical harmonic coefficients (C_{00} , C_{10} , C_{11} , and S_{11}). When estimating global mascons, it is therefore important to ensure that these terms likewise remain fixed. While a direct, unconstrained transformation from spherical harmonics to mascons will maintain these characteristics without any special attention, the addition of regularization into the mascon estimate can result in the unintended introduction of artificial changes in global mass and the geocenter. Therefore, it is imperative that any regularized mascon estimation method properly account for these effects.

For the fast mascon method, conservation of mass and a fixed geocenter are achieved through the straightforward introduction of a diagonal constraint holding these terms fixed. Equations 2 and 4 use a full spherical harmonic expansion including these four terms (i.e., $N_C = 9,409$ for $N_{max} = 96$) and the Level-2 spherical harmonic solutions and normal equations (which contain only 9,405 terms) are used to populate the degree 2 and higher terms. The degree 0 and 1 terms in $\Delta \mathbf{c}$ are set to zero for all months, and non-zero constraints $\alpha \mathbf{I}$ are added into the first four diagonal terms of the normal matrix $\mathbf{N}$ to make the matrix full rank:

$$\Delta \mathbf{c} = \begin{bmatrix} \mathbf{0} \\ \Delta \mathbf{c}_{\text{Level-2}} \end{bmatrix}, \mathbf{N} = \begin{bmatrix} \alpha \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{N}_{\text{Level-2}} \end{bmatrix}. \quad (5)$$

This differs from the method used for the traditional GSFC mascons by establishing conservation of mass and fixed geocenter constraints in spherical harmonic space rather than mascon space. Assuming α is sufficiently large, the degree 0 and 1 terms will be adequately constrained to zero, ensuring that mass is conserved globally and the geocenter is held fixed in the resulting mascon estimate. We found a value of $\alpha = 1.0 \times 10^{30}$ to be sufficiently large to ensure global conservation of mass and maintain a fixed geocenter during the inversion for all GRACE and GRACE-FO months investigated in this analysis. As with the other rigorous GRACE mascon solutions, geocenter motion can then be restored to the solution post-estimation using Technical Note 13.

2.2 Regularization matrix design

Following the traditional mascon approach, the GSFC solution defines a regularization matrix in constraint space as $\mathbf{P}$ (Sabaka et al., 2010; Loomis et al., 2019). Given Equations 2 and 3, the fast mascon method instead defines the regularization matrix in covariance space as $\mathbf{P}^{-1}$. This is perhaps a more straightforward design, as the full regularization covariance matrix can be defined by expected uncertainties σ_i for each mascon i and correlations ρ_{ij} for each i, j mascon pair. Taken as a whole, the individual terms in $\mathbf{P}^{-1}$ are then defined for each row/mascon i and column/mascon j as $P_{ij} = \rho_{ij}\sigma_i\sigma_j$.

The presented regularization matrix construction is then quite flexible, and various design choices can be tested for their effects. In this study, we define correlations between mascons based on the distance between mascons (similar to the GSFC solution), rather than using model-driven correlations (like with the JPL solution). In Section 4, we present a proof of concept solution that uses the Gaussian smoothing function from Wahr et al. (1998) with a radius of 300 km to populate these ρ_{ij} values in the regularization matrix. As with the GSFC mascon solution, a regional constraint for each i, j mascon pair can be defined such that $\rho_{ij} = 0$ if mascons i and j are in different regions. Then, in Section 5, we present a trade study that in part explores this design choice, comparing results for various computed sets of ρ_{ij} values for smoothing distances from 0 km (i.e., a diagonal regularization with no correlations between mascons) to 800 km.

2.3 Notable method advantages

Before continuing, we note a few key takeaways for the developed method. First, compared with the traditional mascon formulation used by GSFC and CSR, the lower computational cost of the developed method allows for mascon estimation to be computed faster and on relatively modest hardware using standard scientific computing resources. This is both because the method allows one to start with a spherical solution and normal equations rather than with Level-1B ranging observations and also because the method benefits from the inversion in Equation 2 taking place in spherical space, rather than in mascon space as in Equation 1. For a spherical expansion to $N_{max} = 96$, the inverted matrix is $9,409 \times 9,409$, rather than a $41,168 \times 41,168$ matrix for the set of 1-arc-degree mascons used in this paper. As a simple illustration of the reduced computational cost of this method, all results in this paper were computed on a 2018 MacBook

Pro 15-inch laptop (2.6 GHz 6-Core Intel Core i7 processor, 32 GB 2400 MHz DDR4 memory) using Python’s numerical and scientific computing libraries. A computationally efficient and stable algorithm for evaluating Equation 2 is presented in [Appendix B](#).

Recalling the three types of mascons discussed in Section 1, an initial presumption might be made that the method developed here best fits the third description. However, our method should be considered more akin to the second type due to the equivalence between Equation 1 and Equation 2, and it is therefore more rigorous than past methods using spherical harmonic solutions. In fact, while our input data is a spherical product, the aforementioned mathematical equivalence means that this method provides an estimate from the same information as one from Level-1B data without the added computational costs involved in such solutions. Instead, this method leverages the Level-1B processing done in creating the input data to avoid these extra computations during the mascon estimation step. As this method results in a global solution that correctly conserves mass and handles geocenter motion, it further distinguishes itself from other less rigorous Level-2 post-processing techniques.

Finally, for a given set of converged spherical harmonics and their normal equations to a maximum degree and order N_{max} , it is possible to truncate all parts of the developed expressions to any smaller degree and order. This provides for a straightforward opportunity to explore the impact of high degree terms on mascon-based GRACE basin analyses. In the trade study in Section 5, we explore this space.

3 Data

In order to test the fast mascon methodology, we use the ITSG-Grace2018 unconstrained monthly solutions and full normal equations (referred to simply as “ITSG” from here) to degree and order 96 for 193 months, including the full duration of the GRACE mission through the first 33 months of GRACE-FO (April 2002 - April 2021) (Mayer-Gürr et al., 2018). During our investigation, we found that two months in the ITSG solution at the end of the original GRACE mission (March 2017 and June 2017) yielded particularly unstable results, and we have omitted these months from this investigation. As our method requires a spherical harmonic solution that is provided with either associated covariances or normal equations, we chose to use the ITSG solution for our tests

because that solution fits our data needs while also having a long history of being fully open and available to the general public. Recently, other spherical harmonic solutions (e.g., the GFZ solution) have begun releasing normal equations alongside their spherical harmonic estimates, and these solutions could be used in place of the ITSG solution. We use only one solution because the goal of this paper is to discuss the presented method and explore what effects different regularization decisions have on signal recovery, not to compare the impact of different data processing strategies. The ITSG solution is estimated using the same processing standards and background models as other Level 2 solutions, and in particular uses the same Atmosphere and Ocean Dealiasing (AOD) model as these solutions, meaning that results using this solution should produce similar results as would be expected with other Level 2 solutions. We note that the ITSG solution does not include non-gravitational arc parameters in their distributed normal equations. Rather, these parameters have been eliminated before accumulating the normal equations (Kvas et al., 2019), meaning that our resulting mascon estimates are properly influenced by these parameters and their errors without needing to include these parameters in the estimation itself. At the same time, this makes our solutions dependent on the parameterization decisions made during the development of the ITSG solution.

As a first order test of how well the developed method recovers signals globally, we compare our results against the GSFC RL06 v1.0 (Loomis et al., 2019) and JPL RL06M v02 (Watkins et al., 2015) global mascon solutions. We also use the GSFC 1-arc-degree mascon definitions and metadata to define the 41,168 mascons and various basins estimated in this study; the GSFC solution includes all the necessary spatial information to fully define the $\mathbf{L}$ matrix, as described in Section 2, and the comparisons between our results and the GSFC solutions are made easier by using these definitions. We compute partial derivatives of the spherical harmonics with respect to these mascons to degree and order 96 to populate the $\mathbf{L}$ matrix and match the degree and order expansions of the ITSG solution. Comparisons to the JPL mascons follow all the prescribed best practices for basin analysis with that solution, applying the CRI filter and model-based scaling factors (Watkins et al., 2015; Wiese et al., 2016).

We use additional models and data during the investigation to provide meaningful mass change result comparisons, following GRACE SDS recommended practices. Glacial Isostatic Adjustment (GIA) is corrected for using the ICE-6G_D model prior to mascon estimation (Peltier et al., 2018), Degree 1 terms are added to the resulting mascon es-

timates using Technical Note 13 as described by Sun et al. (2016), and C_{20} and C_{30} are replaced by that determined from Satellite Laser Ranging using Technical Note 14 (Loomis et al., 2020).

4 Proof of Concept

To demonstrate the fast mascon method, we first compute a monthly solution using a relatively straightforward regularization design. For this solution, we use the ITSG normal equations to the full degree and order 96 expansion. We then compare basin results with those using the GSFC and JPL mascon solutions.

An important step to regularized mascon estimation is the design of the regularization matrix $\mathbf{P}^{-1}$, which we design through a two-step approach. First, we estimate a solution using a simple weighting scheme in the regularization matrix. Then, we use the results from that first solution to build a more representative weighting scheme and estimate a new final solution. In that first step, we set σ_i values for land and inland sea locations to 20 cm (water equivalent height) and open ocean locations to 8 cm and compute correlation terms using a Gaussian smoothing radius of 300 km. We use the GSFC solution’s 11 regional boundary definitions (Listed in Appendix C) to impose regional constraints (Loomis et al., 2019). This effectively makes our regularization matrix block-diagonal, with each region fully populated by design variances and covariances and cross-region off-diagonal areas equaling zero, as described in Section 2.2. We estimate monthly solutions for 18 years of GRACE and GRACE-FO data, adjusting λ to find an over-constrained solution, greatly reducing noise while also suppressing signal. This over-constrained solution is useful because it provides information on the distribution of recovered monthly signals, from which we can build data-driven σ values for a new regularization matrix that we will use in the second step of this process. To achieve this, we compute an RMS map from the 18 years of GRACE and GRACE-FO monthly results and accordingly repopulate the regularization matrix $\mathbf{P}^{-1}$ using those RMS values for land and inland sea locations whose RMS is greater than 20 cm, capping individual mascon σ_i values at a maximum of 80 cm. This maximum encompasses 99.5% of all non-ocean mascons, and prevents the 0.5% of mascons that exceed this limit from over-influencing the solution regularization. Figure 1 shows the determined RMS map used to define the final proof-of-concept regularization σ_i values. This allows for locations with considerably larger-than-average signals to be better recovered and localized while also reducing noise glob-

ally. After defining this new regularization weighting, we can then re-estimate the 18 years
of monthly solutions for our proof of concept.

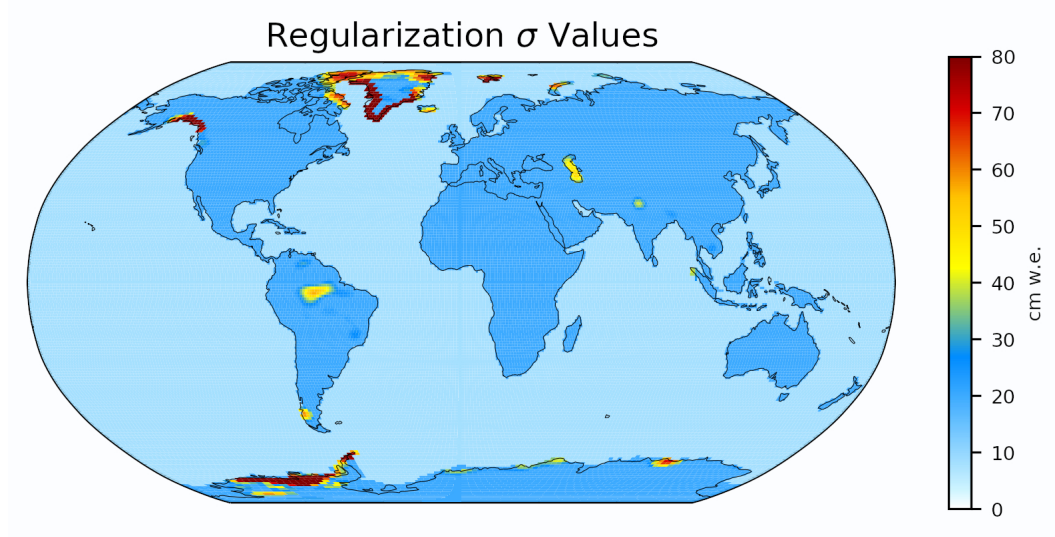


Figure 1. Spatial RMS of initially overly constrained solution, used to populate final regularization matrix σ values.

Having defined the regularization matrix, each monthly estimate needs to be individually tuned to determine the λ that produces an optimal solution for each month. While $\mathbf{P}^{-1}$ is fixed in our proof of concept, tuning λ for each month ensures that the full regularization is scaled appropriately for each month. If λ is set too small, the regularization matrix will have little effect and correlated errors will dominate the inversion; setting λ too high will result in an over-constrained solution with suppressed signal recovery. An optimal λ is therefore one where correlated noise and striping are eliminated without simultaneously over-damping real signal. For each month, we compute solutions for 16 logarithmically spaced values of λ spanning 3 orders of magnitude and then determine the optimal lambda by examining how the recovered signals change with each successively larger λ . In order to find an optimal λ for each month, we compute the 15 difference fields between the 16 successively more constrained solutions. These difference fields represent the change in signal recovery given each incremental increase in λ . For under-constrained solutions, these fields are dominated by striping that is removed as λ increases, while for over-constrained solutions these fields are dominated by surface mass signals suppressed by the regularization. To find the λ where these two effects are a combined minimum, we compute the correlation between the difference fields and the orig-

inal fields and determine the location where this correlation is at a minimum. Here, only small amounts of correlated errors remain in the solution and only small amounts of real signal are affected by the regularization. For the fast method, we found that this procedure works best using mascons that are not dominated by large trends or seasonal variability, and for this reason we compute these correlations using ocean mascons only. An example of this analysis for May 2002 is depicted in Figure 2. Further refinement of these optimal λ is likely by narrowing the search space around each determined λ and testing additional possible λ values, though actual differences in signal recovery will be small.

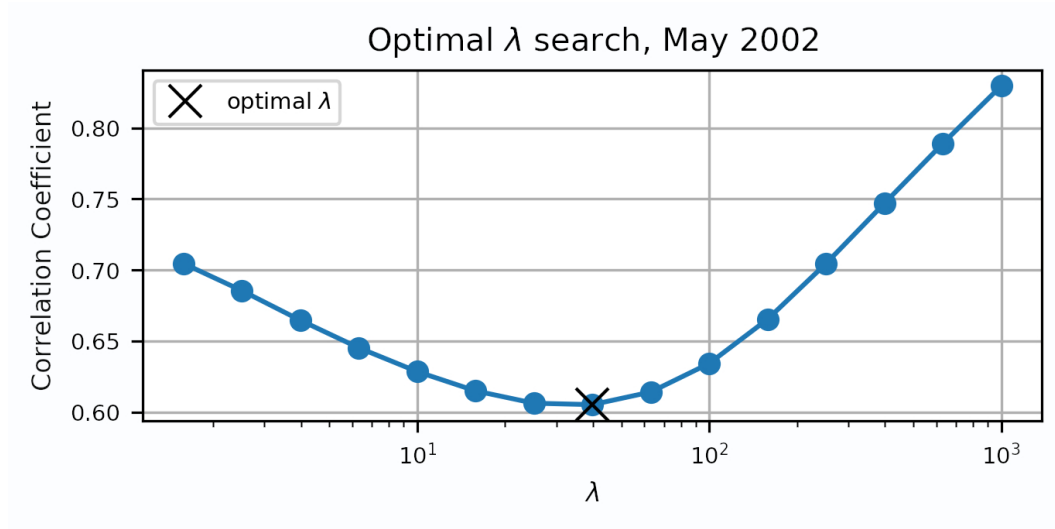


Figure 2. Results of optimal λ weight search for May 2002: Example determined λ where the correlation over the ocean between the λ -weighted solution and the difference to the successively smaller λ -weighted solution is a minimum.

To demonstrate the performance of this proof of concept, we compute basin mass averages for a number of representative basins and compare these results with those using the latest GSFC and JPL mascon solutions. Basin mass changes for eight representative basins are depicted in Figure 3. The Antarctic Ice Sheet region definition includes both grounded ice and the Ross and Ronne ice shelves, as these are constrained to the continent in both the GSFC and fast mascon solutions in the regularization design. We see strong agreement between the fast mascon solution and the others, both in terms of trends and seasonal signals as well as inter-annual variations, as demonstrated in Table 1. Note that the presented method could potentially be improved by including a monthly-varying regularization matrix $\mathbf{P}^{-1}$ designed to optimally recover expected signals for each

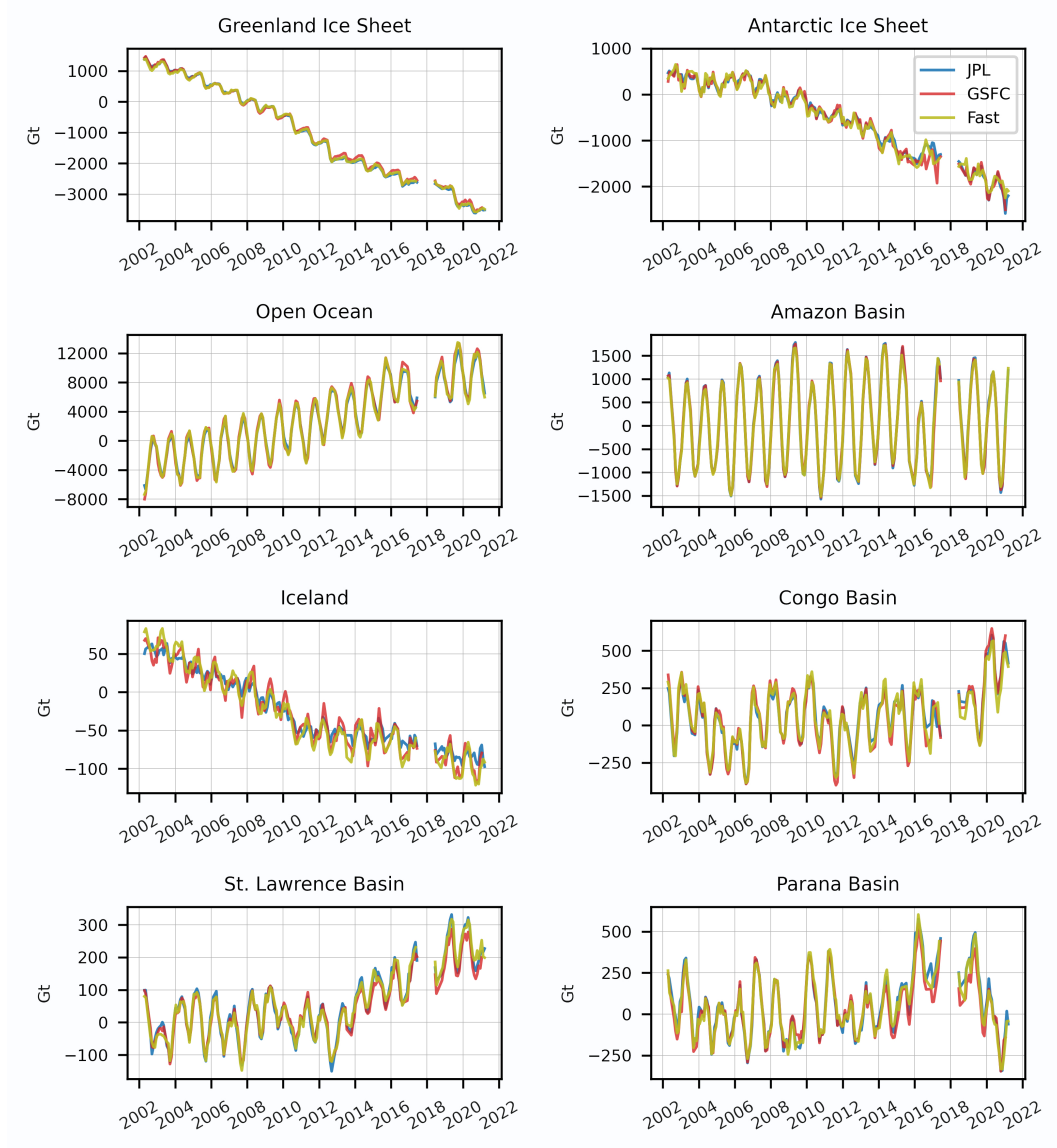


Figure 3. Basin mass averages for eight representative basins, comparing the Fast Mascon approach with the GSFC and JPL mascon solutions.

month, but we chose to use a fixed regularization matrix for this study to improve computational efficiency while reducing model-dependency of the final solution.

To determine whether the developed mascons fully capture the signal content of the original ITSG sphericals, we can compare the signal content of each solution. We map the fast mascons into spherical harmonics through the partial derivatives of sphericals with respect to mascons, $\mathbf{c} = \mathbf{L}\mathbf{m}$, then subtract the source ITSG solution from these fast mascon harmonics. We compute the residual trend of this difference and map that

Table 1. Basin comparison of fast mascons versus JPL and GSFC solutions

Basin (# mascons)	Trend (Gt / year)		Annual Amplitude (Gt)		Basin RMS (Gt)	
	Fast	GSFC	Fast	GSFC	Fast	GSFC
Antarctic Ice Sheet (1 185)	-142 ± 8	-143 ± 8	164 ± 83	152 ± 85	11 210	11 260
Greenland Ice Sheet (198)	-274 ± 13	-271 ± 10	147 ± 138	153 ± 107	21 010	20 490
Gulf of Alaska (42)	-68.2 ± 6.9	-67.1 ± 6.6	145 ± 75	147 ± 71	5 480	5 310
Iceland (13)	-9.29 ± 0.96	-8.70 ± 0.61	17.9 ± 10.3	16.8 ± 6.6	746	691
Amazon Basin (484)	14.0 ± 40.8	11.6 ± 41.7	1 178 ± 438	1 203 ± 447	12 330	12 570
Sahara (446)	-13.6 ± 0.8	-13.5 ± 1.2	20.2 ± 8.9	28.1 ± 13.1	1 196	1 246
Congo Basin (306)	10.7 ± 7.4	11.9 ± 8.5	178 ± 79	189 ± 91	2 740	2 940
Mississippi Basin (267)	14.6 ± 8.1	12.8 ± 8.2	194 ± 87	203 ± 88	2 700	2 730
Interior Australia (245)	-1.98 ± 5.02	-0.20 ± 5.46	33.8 ± 53.9	36.9 ± 58.6	1 260	1 310
Parana Basin (242)	9.12 ± 8.84	6.7 ± 7.8	161 ± 95	170 ± 84	2 610	2 410
St. Lawrence Basin (103)	14.3 ± 4.0	12.1 ± 3.4	56.4 ± 42.8	60.9 ± 36.6	1 480	1 310
Mid Atlantic USA (22)	0.39 ± 0.61	0.10 ± 0.63	17.2 ± 6.5	16.1 ± 6.8	229	206
Open Ocean (27 870)	741 ± 116	768 ± 118	3 500 ± 1 250	3 620 ± 1 260	66 400	68 300
Mediterranean (152)	0.84 ± 1.63	2.29 ± 1.69	57.4 ± 17.5	66.4 ± 18.2	942	1 024
Hudson Bay (71)	1.17 ± 0.54	-0.39 ± 0.55	7.57 ± 5.83	7.19 ± 5.92	442	463
Red Sea (43)	-0.29 ± 2.23	0.99 ± 2.25	83.7 ± 23.9	85.2 ± 24.1	873	907
Caspian Sea (37)	-28.8 ± 3.0	-29.3 ± 2.3	52.9 ± 31.6	37.4 ± 24.8	2 380	2 280
Black Sea (28)	-1.14 ± 0.70	-1.22 ± 0.73	16.1 ± 7.5	16.2 ± 7.8	351	401

Trend and annual fits computed over 2002.0-2021.0 range.

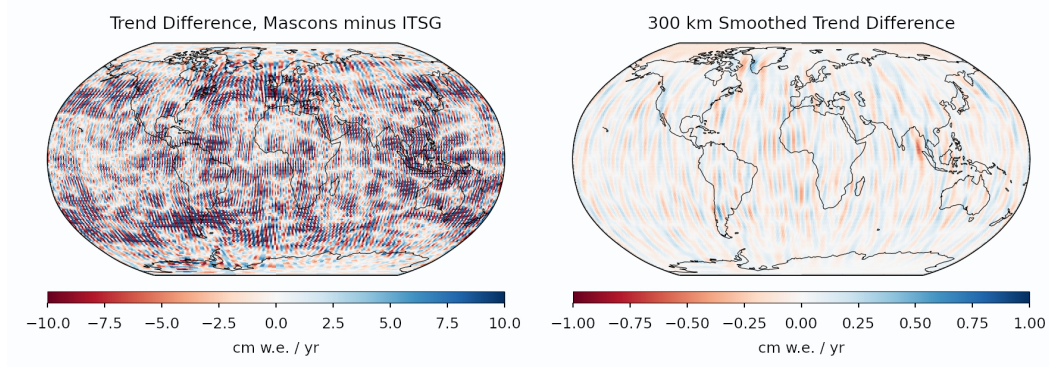


Figure 4. Maps of the trend difference between the fast mascon solution and the ITSG solution. The map on the left has no smoothing and is dominated by vertical striping, and the map on the right (with 300 km smoothing applied) has virtually no remaining signal.

residual signal in Figure 4 (left). As this difference is dominated by vertical striping, we apply 300 km Gaussian smoothing to these residuals (which matches the smoothing built into the mascon regularization) and find that there is practically no remaining residual signal (Figure 4, right). In other words, the developed fast mascons capture the full signal content of the source Level 2 spherical solution while greatly reducing the noise and correlated errors in that solution.

5 Regularization Trade Study

The three widely available mascon solutions to date (CSR, GSFC, and JPL) each use unique regularization strategies, but a straightforward comparison between these and other strategies is challenging due to processing differences between each solution center. The fast mascon method allows for many solutions to be estimated using similar processing while continuously adjusting a single parameter in the regularization design across all solutions. These solutions can then be compared to determine the impact of adjusting that parameter on solution results. The fast mascon method is particularly useful for this kind of rapid solution prototyping and trade space exploration due to the significantly lower computational costs of the method compared to traditional mascon solutions. We therefore use the developed method to conduct a trade study comparing various regularization design choices related to a few of the largest differences between the designs of the GSFC, JPL, and CSR mascons. Results from this trade study are then applicable in the design of any future mascon solutions, using either the presented fast

mascon method or one of the more traditional methods. Similarly, future regularization design studies can employ the fast mascon method to study a wide variety of other specific problems of interest.

5.1 Spherical harmonic maximum expansion

As discussed in Section 2, mascons solutions produced at CSR and GSFC and with the fast mascon method use a truncated spherical harmonic expansion in determining the least squares partial derivatives relating inter-satellite ranging measurements to surface mascon cells. This truncation means that each mascon definition includes a small amount of Gibbs effect ringing, where each discontinuous mascon is not quite perfectly represented by the finite expansion. At the same time, for any set of 1-arc-degree mascons, including the CSR and GSFC solutions, each mascon represents an area below the expected minimum resolution observable with GRACE and GRACE-FO at monthly intervals. Information contained in the spherical harmonic solutions at the highest degrees and orders are increasingly contaminated by noise and the contributions of these harmonics to a final regularized solution accordingly decrease, meaning that information recovered at the highest degrees and orders is dominated by the regularization parameterization. In the interest of minimizing computational and storage requirements, it may then be of interest to reduce the maximum degree and order to which these partial derivatives are expanded. It is therefore important to determine the extent to which lowering the expansion maximum degree and order impacts solution recovery.

We use the same regularization design as in the proof-of-concept solution described in Section 4 to investigate the dependence of the solution on the spherical harmonic truncation degree and order. We compute solutions for expansions to N_{max} values ranging from 30 to 96 and compare results for various sized basins for these multiple solutions. A least squares fit of each solution is used to determine the recovered trend and annual amplitude for each basin at each maximum expansion. We also compute the RMS of the residuals to each fit as a measure of additional variations recovered in each solution. Fits are determined for the ten year period from Jan. 2005 through Dec. 2014, chosen because this period has relatively consistent long-term signals, relatively low noise, and begins after the “deep repeat” period in 2004 that degraded the quality of all GRACE solutions for July-October of that year (Kvas et al., 2019). Figure 5 shows a comparison of results for smaller expansions relative to the degree and order 96 expansion (the max-

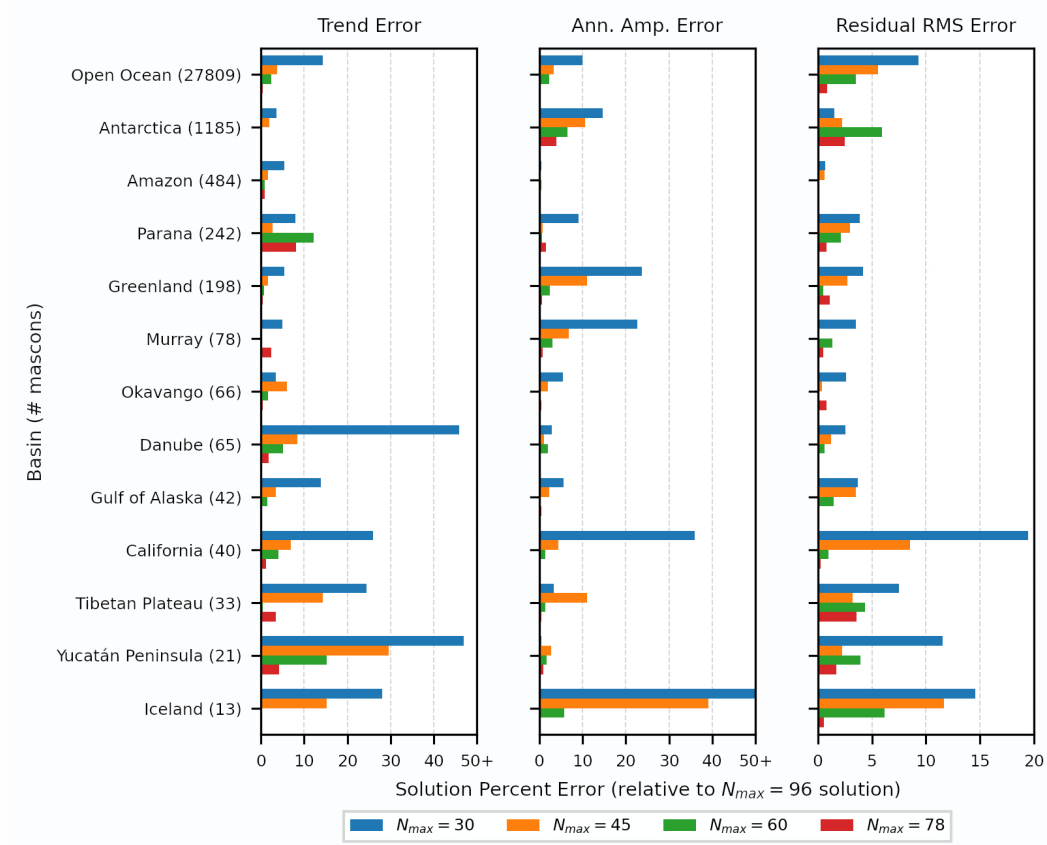


Figure 5. Comparison of basin mass recovery with different spherical harmonic expansion truncations; results are in terms of percent error relative to a degree and order 96 expansion for recovered basin trend (left), annual amplitude (center), and RMS of the residuals (right) to each trend + annual fit.

imum expansion distributed for the ITSG normal equations). Additional figures comparing the recovered trends and annual signal with each expansion are included in the Supporting Information. We find that the recovered trend, annual amplitude, and RMS signals are fairly stable for expansions at degree and order 60 and above, with differences of 10% or less for basins across many difference sizes and shapes, though smaller basins such as the Yucatan Peninsula show degraded signal recovery at $N_{max} = 60$. At $N_{max} = 78$, we find signal differences to be smaller still. Additionally, larger basins generally perform better at lower expansions than smaller basins.

Interestingly, Iceland (which at only 11 mascons is one of the smallest basins observable at monthly timescales with GRACE) generally shows comparable or better sig-

nal recovery than larger inland locations (e.g., the Tibetan Plateau) for expansions to degree and order 60 or higher but worse recovery with smaller expansions. Likewise, signal recovery in the Gulf of Alaska shows comparable performance to larger basins (such as the Danube). Both cases help illustrate a separate but notable point: the coastline boundary constraints for Iceland and regional boundary constraints for the Gulf of Alaska play a significant role in constraining mass loss if a sufficiently large expansion is used. On the other hand, if the expansion is too small to observe Iceland, the Gulf of Alaska, or any other isolated basin, then the addition of a regional constraint cannot on its own cause the basin to be fully observable.

5.2 Inter-mascon correlation distance

Unconstrained GRACE and GRACE-FO solutions contain correlated errors that manifest as vertical striping in gravity maps in addition to noise in the solution. In order to remove these errors and best recover surface mass signals, the GSFC and JPL mascon solutions include off-diagonal terms (i.e. correlations) in their mascon regularization schemes, while the CSR mascons rely on a diagonal regularization. JPL uses a model-based approach for determining constraint correlations, while GSFC uses a statistical approach based on inter-mascon distances. This second approach is similar in effect to the typical approaches applied to spherical harmonic-based studies, which use filtering to remove correlated errors. For this reason, we have used a Gaussian smoothing based method for determining regularization correlations.

We computed mascon solutions using the Gaussian smoothing radius to define correlations in the regularization matrix, testing for $r = [0, 200, 300, 400, 500, 600, 800]$ km (where a value $r = 0$ km means the regularization matrix is diagonal). Each solution was computed using a full spherical harmonic expansion to $N_{max} = 96$, and each solution used the same relatively simple regularization weighting scheme, where ocean, land and inland sea, and ice mascons were given σ_i weighting values of 4, 8, and 20 cm, respectively. As in the proof of concept and first trade study, the GSFC 11 regional boundary definitions are applied to define a block-diagonal regularization (for those cases where $r > 0$). Note that while changes to these weights will change the recovered signals in general, such changes will not significantly impact this trade study in particular because the weighting scheme is fixed for all solutions in this trade study. Recovered signal is analyzed for 12 basins of varying magnitudes by considering the recovered trends and an-

nual signals in each basin. Figure 6 shows the magnitude of these recovered trends and annual amplitude for each sample basin relative to the results for a Gaussian smoothing radius of $r = 400$ km. For this figure, we include basins that demonstrate performance in glaciated areas (e.g., Antarctica and Greenland), adjacent basins near regional boundaries (e.g., Caspian Sea and East Caspian Coast), isolated regions (e.g., Iceland and Taiwan), and other interesting individual cases.

We find that trends and annual signals recovered in large basins tend to drop off significantly for values of r smaller than 300 to 400 km. On the other hand, smaller basins tend to see less total signal recovery (in particular for recovered trends) for r values greater than 300 to 400 km, indicating that excessive smoothing results in signal leakage to outside smaller basins. Less obviously, basins of all sizes whose boundaries are built into the

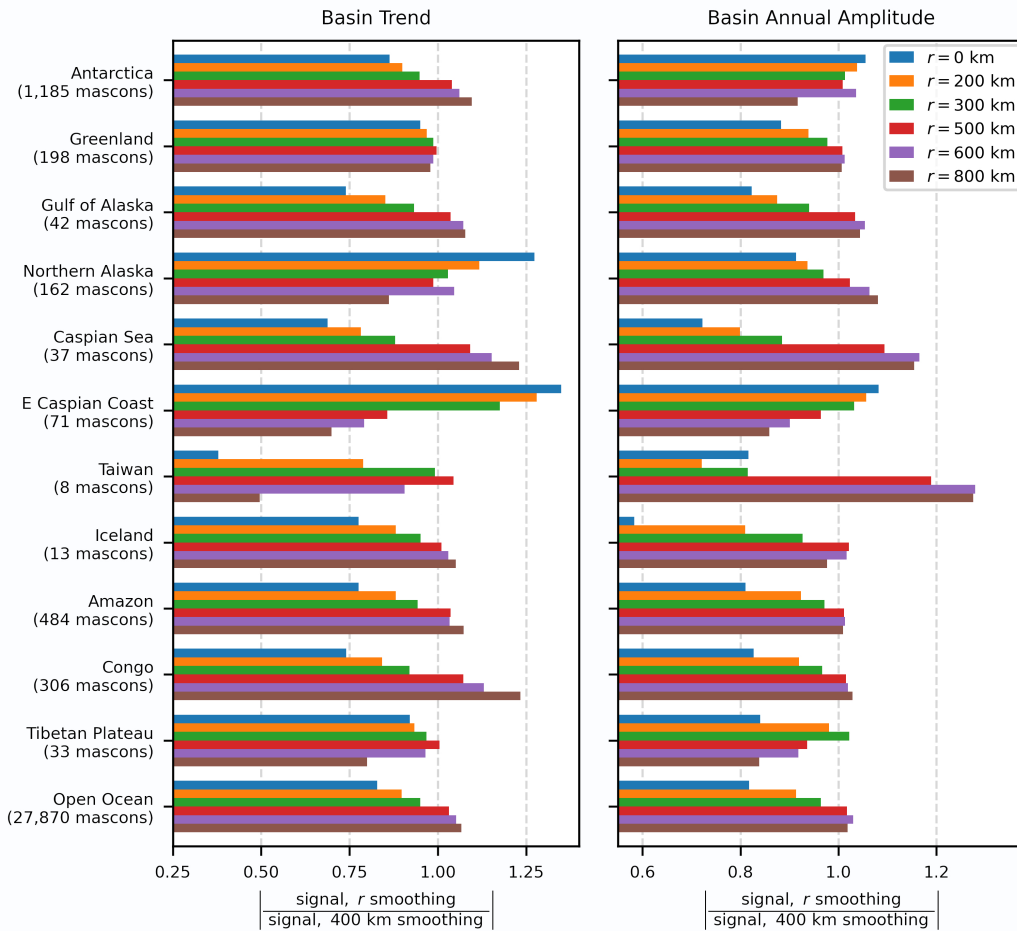


Figure 6. Comparison of basin trend and annual signal recovery with different Gaussian smoothing r built into the regularization. Results are relative to those with $r = 400$ km.

regularization matrix (such as the Ocean, Antarctica, Greenland, and Iceland) see significant decreases in signal recovery for values of r smaller than 400 km, indicating that these boundary constraints have less impact with smaller values of r . Two instances where adjacent basins are separated by regional boundary constraints demonstrate this dependence on r particularly well: 1) Gulf of Alaska and Northern Alaska, and 2) the Caspian Sea and Eastern Caspian Coast. In both cases, the results in Figure 6 show increased signal differentiation as r increases and show that signals (particularly trends) are isolated more over those areas where the regularization weighting was most relaxed (i.e., Gulf of Alaska and the Caspian Sea, see Figure 2) as r increases. This makes sense, as smaller r values lead to smaller correlations in the off-diagonal portions of the regularization matrix, reducing the effect of regional boundary cutoffs in the correlation definitions. At $r = 0$ km, the regularization becomes diagonal and boundary constraints are eliminated, leading to increased signal leakage across these boundaries. These results are consistent with findings in WCRP (2018) as part of an analysis of the global sea level budget, which found that the total recovered ocean mass trend in the CSR mascon solution, which uses a diagonal regularization, recovered a significantly smaller ocean mass trend (1.76 mm/yr) than the ensemble mean of all examined GRACE mascon and spherical harmonic solutions (2.3 mm/yr) for the period of 2005 through 2016. This underestimate almost perfectly matches the Ocean result in Figure 6 for $r = 0$ km, indicating that significant signal leakage remains between land and ocean mascons across unconstrained coastal boundaries. To further illustrate this point, maps of the recovered trends over portions of Africa, Asia, and Europe for the $r = 0$ km, $r = 400$ km, and $r = 800$ km solutions are depicted in Figure 7. The figure, which includes portions of six distinct regions defined in the regularization matrix (Land, Ocean, the Mediterranean Sea, the Black Sea, the Red Sea, and the Caspian Sea) shows clear differences between the solutions in terms of signal localization and smoothing as well as leakage across regional boundaries. This is most obvious in the case of the Caspian Sea, where signal leaks substantially beyond the borders of the Sea for the $r = 0$ km solution, as the diagonal regularization matrix prevents the inclusion of regional constraints. Additional figures comparing the recovered trends and annual signal globally for each smoothing radius are included in the Supporting Information.

Combined, these findings indicate that a global solution with $N_{max} = 96$ shows optimal signal recovery using smoothing between 300 and 400 km. Smaller regulariza-

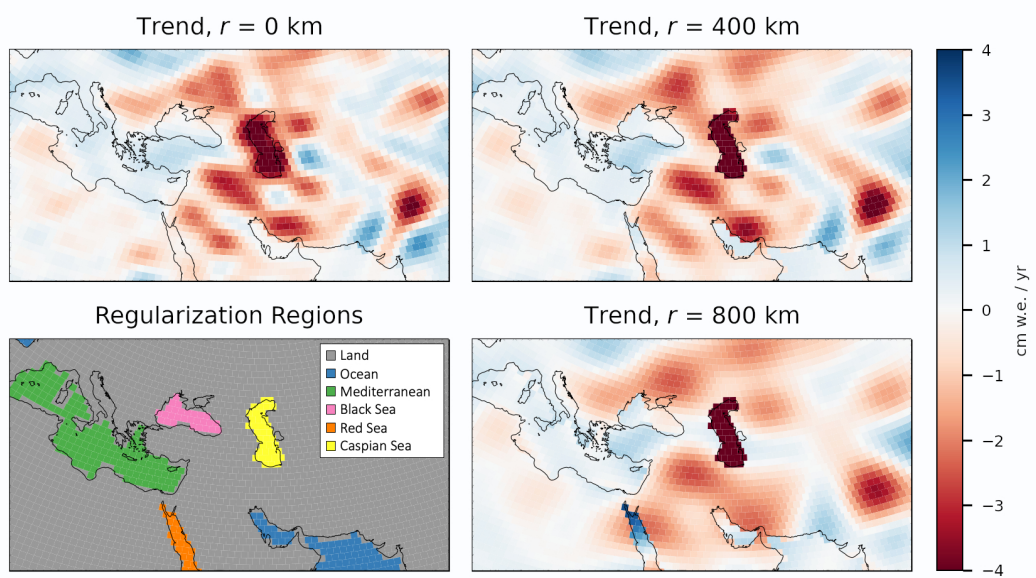


Figure 7. Recovered trends (Jan. 2005 - Dec. 2014) over parts of Europe, Central Asia, and North Africa for regularizations with Gaussian smoothing for $r = [0, 400, 800]$ km. This area includes six distinct regions defined in the regularization: Land, Ocean, the Mediterranean Sea, the Black Sea, the Red Sea, and the Caspian Sea.

tion correlations (and at the extreme, diagonal regularizations) will result in more signal leakage outside basin boundaries, especially where regional cutoffs such as coastlines can be defined. Larger correlations will cause small basins to become less observable. We note that past GRACE studies have additionally shown a significant latitudinal dependence in recovered uncertainties (Wahr et al., 2006) and achievable spatial resolutions for GRACE terrestrial water storage solutions (Croteau et al., 2020). While we have not attempted to measure this effect in this study, it is likely that an optimal solution would include a latitudinally dependent inter-mascon correlation constraint.

6 Discussion

User-focused GRACE and GRACE-FO data products are primarily delivered in one of two forms: unconstrained spherical harmonics and regularized mascons. The first requires extra care and handling in order to balance signal recovery with noise and leakage suppression, while the second handles these issues in an optimal way but locks users into the regularization decisions made in developing the solution. Both solution types are estimated from GRACE’s primary observable, Level-1B ranging measurements, but

this requires large computational resources and specialized orbit and estimation software. In this work, we reformulate the traditional mascon estimation equations to develop a method for rigorously estimating regularized mascons from unconstrained spherical harmonics. This new method does not require sophisticated orbital dynamics software or large computer resources and can be implemented to run quickly on consumer hardware with standard scientific computing tools.

The developed method can be useful for targeting specific cryospheric, hydrologic, and solid earth signals of interest that have not been a specific focus of a global product like the three main mascon solutions. A proof-of-concept estimate using the ITSG-Grace2018 spherical harmonic solution and normal equations shows excellent agreement with more traditional mascons from GSFC and JPL. Using a relatively simple regularization scheme, we show that strong signal recovery and optimal leakage control can be achieved matching the quality of the JPL and GSFC mascon solutions.

The low computational costs of this method are also useful in regularization design and development, allowing for a wide variety of regularization strategies to be rapidly tested and compared. We used this advantage to investigate two regularization parameters of interest: the maximum spherical harmonic truncation used and the scale of off-diagonal inter-mascon correlations. Findings from these studies can be applied to any future mascon studies and showcase the usefulness of the fast mascon method in exploring specific problems of interest. By using fully open datasets and carefully documenting our full methodology, this study should open the door to further investigations into more specialized regularization methods and targeted surface mass signal investigations in difficult-to-isolate basins of interest.

The developed method allows scientists to quickly estimate regularized mascons from unconstrained sphericals in a robust and rigorous way. This can be useful in targeting specific science problems or in the development cycle of a more traditional global mascon solution like those at JPL, CSR, and GSFC. Importantly, the developed fast mascon approach is mathematically equivalent to traditional methods for estimating global mascons from Level-1B observations and is superior to less rigorous Level-2 spherical harmonic post-processing methods. It is this equivalence that makes this method useful, and also highlights a further application. While this study shows the usefulness of the fast mascon technique for users that do not have Level-1B processing capabilities to construct

mascons through a single additional iteration of a Level-2 solution, the method is also useful for centers that do have Level-1B processing capabilities. A stated restriction of the technique is that it relies on the non-gravitational arc parameterization built into Level-2 solutions, but this is not a limitation for the Level-1B processing centers themselves. This means that the fast mascon technique can also be incorporated into the processing systems that develop Level-2 products from Level-1B data to construct iterative methods that combined these capabilities with the fast mascon technique.

Finally, we have demonstrated the application of the fast mascon method to an unconstrained monthly spherical harmonic solution. However, there is nothing specific to the method that would suggest this technique could not be applied to a spherical harmonic solution that already contains regularization. It is a straightforward extension of the method to develop mascons from a regularized spherical solution, where the fast mascon technique could add an additional level of regularization (for example, to build regional boundaries into a new mascon solution).

7 Conclusions

We have developed a new method for computing regularized GRACE mascons from Level-2 spherical harmonic solutions and their covariances. This fast mascon method handles leakage and correlated errors more effectively than previous spherical harmonic investigations of surface mass change, and resulting estimates are equivalent to traditional rigorous mascons estimated from Level-1B ranging observations while also being less computationally expensive. This method can be readily used by scientists to incorporate additional local knowledge into the mascon regularization scheme and develop specialized mascon solutions focused on individual problems and basins of interest. We use a proof-of-concept study to demonstrate the effectiveness and efficiency of the fast mascon method, comparing results generated using standard scientific computing tools and hardware to mascon solutions from JPL and GSFC produced using specialized software and systems. We then use the developed method in a trade study to demonstrate the importance of including cross-mascon spatial correlations in the mascon regularization and establish a minimum effective spherical harmonic expansion needed to produce rigorous scientific results. We found that basin-scale analyses are relatively consistent for any expansion above $N_{max} = 60$, but larger expansions better localize signal within basins. Testing the application of Gaussian smoothing within pre-defined regions, we found smoothing

between 300 and 400 km best balanced signal recovery and noise suppression for a set of 1-arc-degree mascons.

Appendix A Derivation of Equation 2

The traditional method for estimating rigorous mascons, as employed by GSFC and CSR, uses a Gauss-Newton least-squares estimator whose k th step estimates an adjustment $\Delta \mathbf{m}_k$ to the mascon state $\mathbf{m}_k$ (with a preferred mascon state $\mathbf{m}_a$) as

$$\begin{cases} \Delta \hat{\mathbf{m}}_k &= (\mathbf{L}^T \mathbf{H}^T \mathbf{W} \mathbf{H} \mathbf{L} + \lambda \mathbf{P})^{-1} [\mathbf{L}^T \mathbf{H}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \lambda \mathbf{P} (\mathbf{m}_a - \mathbf{m}_k)] \\ \mathbf{m}_{k+1} &= \mathbf{m}_k + \Delta \hat{\mathbf{m}}_k \end{cases} \quad (\text{A1})$$

where the observation vector is the difference between the ranging observations $\mathbf{d}$ and the model prediction vector $\mathbf{f}$.

We derive the fast mascon method from this formulation as follows. Letting $\mathbf{N} = \mathbf{H}^T \mathbf{W} \mathbf{H}$, we use the Woodbury Matrix Identity to reformulate Equation A1

$$\begin{aligned} \Delta \hat{\mathbf{m}}_k &= (\mathbf{L}^T \mathbf{N} \mathbf{L} + \lambda \mathbf{P})^{-1} [\mathbf{L}^T \mathbf{H}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \lambda \mathbf{P} (\mathbf{m}_a - \mathbf{m}_k)] \\ &= \left[\lambda^{-1} \mathbf{P}^{-1} - \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T)^{-1} \lambda^{-1} \mathbf{L} \mathbf{P}^{-1} \right] \\ &\quad [\mathbf{L}^T \mathbf{H}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \lambda \mathbf{P} (\mathbf{m}_a - \mathbf{m}_k)] \end{aligned} \quad (\text{A2})$$

Now, let $\mathbf{Z} = \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T$ and simplify:

$$\begin{aligned} \Delta \hat{\mathbf{m}}_k &= \left[\lambda^{-1} \mathbf{P}^{-1} - \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \lambda^{-1} \mathbf{L} \mathbf{P}^{-1} \right] \\ &\quad [\mathbf{L}^T \mathbf{H}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \lambda \mathbf{P} (\mathbf{m}_a - \mathbf{m}_k)] \\ &= \mathbf{m}_a - \mathbf{m}_k + \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) - \\ &\quad \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \lambda^{-1} \mathbf{Z} \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) - \\ &\quad \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \mathbf{L} (\mathbf{m}_a - \mathbf{m}_k) \\ &= \mathbf{m}_a - \mathbf{m}_k + \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T \left[\left(\mathbf{I} - (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \lambda^{-1} \mathbf{Z} \right) \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) - \right. \\ &\quad \left. (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \mathbf{L} (\mathbf{m}_a - \mathbf{m}_k) \right] \\ &= \mathbf{m}_a - \mathbf{m}_k + \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T \left[(\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \mathbf{N}^{-1} \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) - \right. \\ &\quad \left. (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} \mathbf{L} (\mathbf{m}_a - \mathbf{m}_k) \right] \\ &= \mathbf{m}_a - \mathbf{m}_k + \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} [\mathbf{N}^{-1} \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) - \mathbf{L} (\mathbf{m}_a - \mathbf{m}_k)] \end{aligned} \quad (\text{A3})$$

For the GSFC mascons, the preferred mascon state is defined as $\mathbf{m}_a = \mathbf{0}$. We can simplify the result from Equation A3 and develop a new expression for the new mascon

state $\mathbf{m}_{k+1}$ to be

$$\mathbf{m}_{k+1} = \Delta \hat{\mathbf{m}}_k + \mathbf{m}_k = \lambda^{-1} \mathbf{P}^{-1} \mathbf{L}^T (\mathbf{N}^{-1} + \lambda^{-1} \mathbf{Z})^{-1} [\mathbf{N}^{-1} \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) + \mathbf{L} \mathbf{m}_k]. \quad (\text{A4})$$

By definition,

$$\Delta \mathbf{c}_k = \mathbf{N}^{-1} \mathbf{A}^T \mathbf{W} (\mathbf{d} - \mathbf{f}(\mathbf{m}_k)) \quad (\text{A5})$$

and

$$\mathbf{c}_k = \mathbf{L} \mathbf{m}_k. \quad (\text{A6})$$

Therefore, we can finally write Equation A4 as:

$$\mathbf{m}_{k+1} = \mathbf{P}^{-1} \mathbf{L}^T (\lambda \mathbf{N}^{-1} + \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T)^{-1} [\Delta \mathbf{c}_k + \mathbf{c}_k]. \quad (\text{A7})$$

The ITSG-Grace2018 spherical harmonic solution is computed as monthly estimates relative to a time-variable background field that contains a secular trend and annual variations for each harmonic coefficient. In other words, the time-variable background model corresponds to $\mathbf{c}_k$ and the estimated monthly deviations from that model correspond to $\Delta \mathbf{c}_k$. The sum of these two pieces make up the final monthly solution, which can be expressed as

$$\mathbf{c}_{k+1} = \Delta \mathbf{c}_k + \mathbf{c}_k, \quad (\text{A8})$$

and this can be substituted into Equation A9 to get

$$\mathbf{m}_{k+1} = \mathbf{P}^{-1} \mathbf{L}^T (\lambda \mathbf{N}^{-1} + \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T)^{-1} \mathbf{c}_{k+1} \quad (\text{A9})$$

which matches Equation 2 presented in Section 2.

Here we note a few facts. First, this equation applies regardless of whether a time-variable starting model is used for determining the time-variable spherical estimate (i.e., if no starting model is used, $\mathbf{c}_k = 0$). Second, as with all other mascon solutions, the added regularization is applied to the full time-variable estimate (including the trend + annual starting model) but not the GRACE RL06 background models (e.g., the AOD or solid earth tide models). Finally, Equation A6 implies that there is a mascon solution $\mathbf{m}_k$ (as in Equation A1) that corresponds to the spherical starting model $\mathbf{c}_k$, but this method does not require ever actually determining this intermediate solution. In fact, neither $\mathbf{m}_k$ nor $\Delta \hat{\mathbf{m}}_k$ from Equation A1 are ever determined separately, and only the sum of these two components, $\mathbf{m}_{k+1}$, is ever explicitly determined.

Appendix B Computationally stable and efficient algorithm

In order to promote a stable inversion and maintain a computationally efficient mass-con estimation algorithm, we perform a Cholesky decomposition of the normal matrix $\mathbf{N}$ and simplify Equation 2. Let $\mathbf{N} = \mathbf{U}^T \mathbf{U}$ and $\mathbf{Q} = \mathbf{P}^{-1} \mathbf{L}^T$. Then,

$$\Delta \hat{\mathbf{m}} = \mathbf{Q} [\mathbf{U}^{-1} (\lambda \mathbf{I} + \mathbf{U} \mathbf{L} \mathbf{Q} \mathbf{U}^T) \mathbf{U}^{-T}]^{-1} \Delta \mathbf{c}. \quad (\text{B1})$$

Now, letting $\mathbf{K} = \mathbf{Q} \mathbf{U}^T$ and $\mathbf{M} = \mathbf{U} \mathbf{L} \mathbf{K}$,

$$\begin{aligned} \Delta \hat{\mathbf{m}} &= \mathbf{K} [\lambda \mathbf{I} + \mathbf{U} \mathbf{L} \mathbf{K}]^{-1} \mathbf{U} \Delta \mathbf{c} \\ &= \mathbf{K} [\lambda \mathbf{I} + \mathbf{M}]^{-1} \mathbf{U} \Delta \mathbf{c}. \end{aligned} \quad (\text{B2})$$

Noting that $\mathbf{M}$, and therefore $\lambda \mathbf{I} + \mathbf{M}$, is symmetric ($\mathbf{M} = \mathbf{U} \mathbf{L} \mathbf{P}^{-1} \mathbf{L}^T \mathbf{U}^T$), a symmetric linear algebra solver can be used to optimally solve for $\Delta \hat{\mathbf{m}}$. Specifically, our implementation uses SciPy's `linalg.solve` symmetric solver.

Appendix C Regional Boundaries used in Regularization Matrix

The regions included in our regularization design, from (Loomis et al., 2019), are:

- Greenland Ice Sheet, low elevations (< 2000 m)
- Greenland Ice Sheet, high elevations (> 2000 m)
- Antarctic Ice Sheet including the Ronne and Ross ice shelves
- Gulf of Alaska
- Land
- Ocean, including smaller ice shelves
- Mediterranean Sea
- Black Sea
- Red Sea
- Caspian Sea
- Hudson Bay

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The JPL RL06M v02 mascon solution and GRACE/GRACE-FO Technical Notes 13 and 14 are available from JPL's Physical Oceanography Distributed Active Archive Center (PO.DAAC), <https://podaac.jpl.nasa.gov>. The GSFC RL06 v1.0 mascon solution and associated GSFC 1-arc-degree mascon definitions are available from the GSFC Geodesy and Geophysics Science Research Portal, <https://earth.gsfc.nasa.gov/geo/data/grace-mascons>.

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