GOCE gravity field determination by means of rotational invariants: first experiences

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1. Introduction
Launched on 17 March 2009, ESA’s Gravity field and steady-state Ocean Circulation Explorer (GOCE) will revolutionize our understanding of one of Earth’s most fundamental forces – gravity. Commonly, GOCE gradiometry analysis relates the single gravitational gradients to the unknown gravity field parameters. For its application, the orientation of the gravitational tensor relative to the reference frame of gravity field modeling is of prime importance. Hence, the orientation information quality strongly influences the accuracy of the entire analysis procedure. Gravity field recovery based on the rotational invariants of the gravitational tensor avoids any orientation concerns. For this reason, the invariants representation constitutes an alternative and independent procedure for GOCE data analysis.

Within the support programs GOCE-GRAND I and II [12], the methodological fundamentals were established to apply the invariants approach to gradiometer data. Most notably, in this context, the algorithms have been implemented on high performance computing platforms and have been tested successfully within the framework of comprehensive numerical simulation studies. The major objective of this work package is the application of the existing routines to GOCE real data. The final outcome is an Earth’s gravity field solution based on the invariants representation.

In case of full tensor gradiometry all second-order derivatives of the geopotential, denoted as gravitational gradients (GGs) \( V_{ij} \), \( i, j = 1, 2, 3 \) can be derived. They are summarized in the symmetric gravitational tensor, or Eötvös tensor [3]. Due to technical reasons (ground calibration), for GOCE two of the off-diagonal elements \( V_{12} \) and \( V_{23} \) are reduced in accuracy by several orders of magnitude, hence can be considered as unobserved.

Typically, gradiometer data analysis is performed at the level of individual GGs, in particular the main diagonal elements of the gravitational tensor. This approach embraces a variety of methods commonly attributed to the space-wise or time-wise methods [10]. Here we present an alternative analysis concept. It is based on gravitational tensor rotational invariants [1].

As invariants are composed of gravitational gradients products, the alternative representation yields a non-linear least-squares minimization problem requiring iterative model parameter estimation. Moreover, invariants are composed of all individual GGs. Thus, GGs accuracies must be compatible, which is only ensured by full tensor gradiometry.

In brief, the pros and cons of the invariants representation can be summarized as follows:

Pros of the invariants representation:
- scalar-valued gravity field functionals
- independent of the gradiometer orientation in space
- independent of the orientation accuracy
- independent of reference frame rotations / parameterization

Cons of the invariants representation:
- non-linear observables
- gravitational gradients required with com-
patible accuracy (full tensor gradiometry)
- more complex stochastic model handling
- iterative parameter estimation, huge computational costs

In this contribution, we present strategies to overcome the difficulties of the invariants representation in the context of GOCE data analysis and first experiences incorporating GOCE real data. The proposed methods are a tailored combination of (i) linearization in terms of a perturbation theory approach, (ii) synthesis of GGs for full tensor gradiometry reconstruction, (iii) error propagation in order to derive the stochastic model of invariants, and (iv) implementation of the algorithms on high performance computing platforms.

2. Invariants representation
The basic observation equation in satellite gradiometry reads [9]

$$\Gamma = -V + \Omega + \Omega^2.$$  \hspace{1cm} (1)

The observation tensor $\Gamma$ is the sum of the gravitational tensor $V$ and rotational parts, i.e., the Euler tensor $\Omega$ and the centrifugal tensor $\Omega^2$. The rotational parts occur due to the rotation of the gradiometer reference frame relative to inertial space; they have to be reduced from the observation tensor prior to data analysis. For GOCE the separation is achieved by gradiometer observations (splitting the observation tensor into its symmetric and antisymmetric part) in combination with star tracker measurements. We denote the coefficient matrix of $V$ as $V=[V_{ij}]$. The properties $V_{11}+V_{22}+V_{33}=0$ and $V_{ij} = V_{ji}$ hold true, i.e., $V$ is a trace-free symmetric matrix.

A tensor itself is independent of orthogonal transformations. This does not hold for its coefficient matrix. The individual components vary according to their projection on the base coordinate axes. Scalar-valued tensor invariants, however, are independent of frame rotations and thus independent of the reference base. A second order tensor in three-dimensional Euclidean space (such as the Eötvös tensor) is characterized by three independent invariants [6], constituting a so-called complete invariants system. Invariants systems can be defined in various ways; transformation relations allow to transfer them to each other [5, 4].

The two most prominent invariants systems result from the eigenspace representation of $V$, i.e., from the solution of the general eigenvalue problem of the tensor coefficient matrix. The characteristic equation $\det(V-\lambda I) = 0$ yields the cubic polynomial

$$\lambda^3 - I_1\lambda^2 + I_2\lambda - I_3 = 0. \hspace{1cm} (2)$$

The roots of the characteristic equation are well-known as the eigenvalues $\lambda_i$, $i = 1, 2, 3$ of $V$. They constitute the complete invariants system $\{\lambda_1, \lambda_2, \lambda_3\}$. As the eigenvalues are invariants, according to Eq. (2) the polynomial coefficients $I_i$, $i=1, 2, 3$ form an invariants system too, denoted as $\{I_1, I_2, I_3\}$. As a function of the eigenvalues it reads

$$I_1 = \lambda_1 + \lambda_2 + \lambda_3, \hspace{1cm} (3)$$
$$I_2 = \lambda_2\lambda_3 + \lambda_3\lambda_1 + \lambda_1\lambda_2,$$
$$I_3 = \lambda_1\lambda_2\lambda_3.$$  \hspace{1cm} (3)

In terms of GGs (symmetric and trace-free coefficient matrix $V$) the $I_i$ become [9]

$$I_1 = \text{tr} V = 0, \hspace{1cm} (4a)$$
$$I_2 = -\frac{1}{2} \text{tr} V^2 = -\frac{1}{2} (V_{11}^2 + V_{22}^2 + V_{33}^2) - V_{12}^2 - V_{13}^2 - V_{23}^2, \hspace{1cm} (4b)$$
$$I_3 = \det V = V_{11}V_{22}V_{33} + 2V_{12}V_{23}V_{31} - V_{11}V_{23}^2 - V_{12}V_{22}^2 - V_{13}V_{33}^2. \hspace{1cm} (4c)$$

The invariant $I_1$ equals the trace and $I_3$ the determinant of the tensor coefficient matrix. $I_2$ is the sum of the coefficient matrix principal minor determinants by deleting one row and column.
In case of a nadir-pointing gradiometer of GOCE type the invariants system \( \{I_1, I_2, I_3\} \) is particularly suited for gravity field recovery. Within this contribution we restrict ourselves on the invariant \( I_2 \). The results and conclusions hold for \( I_3 \) accordingly. Analysis of the invariant \( I_1 \), yields the trivial solution, however, might be used as constraint within the parameter estimation process. The superiority of the system \( \{I_1, I_2, I_3\} \) is due to the minor effect of the (unobserved) off-diagonal tensor elements on the overall invariants computation, as will be discussed in Sect. 4.

3. Linearization

We achieved efficient linearization of the functional model (4b) by the calculation of perturbations relative to an a priori known reference solution according to

\[
\delta I_2 = I_2 - I_{2}^{\text{ref}} \tag{5}
\]

where \( I_2^{\text{ref}} \) indicate synthesized invariants from reference GGSs \( U_{ij}, i, j = 1, 2, 3 \). The \( U_{ij} \) are approximations to the real GGSs and thus \( V_i = U_{ij} + \delta V_i \) holds true with \( \delta V_i \) the (incremental) corrections to the a priori values. Neglecting all non-linear incremental correction terms, the linearized perturbation of \( I_2 \) becomes

\[
\delta I_2 = -U_{ij}\delta V_{ji} - U_{22}\delta V_{22} - U_{33}\delta V_{33} - 2(U_{12}\delta V_{12} + U_{13}\delta V_{13} + U_{23}\delta V_{23}) \tag{6}
\]

Linearization induces an iterative processing scheme. To start the iterative potential parameter estimation process, external information in terms of reference gradients \( U_{ij} \) is necessary. From the second iteration on, the actual result is used to set up the linearized functional model. The synthesis of the \( U_{ij} \) is done within the initialization phase of each iteration. In order to demonstrate the performance of the proposed procedure we conducted a series of (error-free) closed-loop simulation studies. The GOCE-like synthetic test data set consists of 518400 samples using the EGM96 gravity field model [7] up to degree and order 300. Figure 1 highlights results adopting the gravity field model OSU86F [8] as initial a priori information. In Figure 1, the invariants estimates are displayed relative to the \( V_{33} \) reference solution (deviation of invariants analysis from \( V_{33} \) analysis, hence a relative measure), i.e., the \( V_{33} \) degree-error RMS curve serves as baseline accuracy.

The iterative process can be terminated after only two iterations, demonstrating the linearization error to be small. Moreover, further experiments showed that the linearization per-
formance is insensitive towards the a priori linearization field.

4. Full tensor gradiometry reconstruction
Exemplary for an arbitrary day of GOCE data registration, Figures 2 and 3 present the invariant $l_2$ on November 2, 2009. The comparison of forward modeled invariants (based on GGs derived from an a priori reference gravity field) with real data clearly reveals the destructive impact of the inaccurate GGs $V_{12}$ and $V_{23}$ on invariants computation. Neglecting the off-diagonal elements in Eq. (4b) yields values that are close to the reference invariants. Consequently, $V_{12}$ and $V_{23}$ have a minor effect on the overall invariants computation.

The same conclusion is also supported by the power spectral densities in Figures 4 and 5. Considering the off-diagonal GGs provided by GOCE results in a noise level well above the reference invariants signal (noise is defined here as the difference between the real and reference signal). Neglecting $V_{12}$ and $V_{23}$, on the other hand, decreases the noise level below the reference signal.

For the invariant $l_3$, the similar conclusion can be drawn from Figures 6, 7, 8 and 9, i.e., $V_{12}$ and $V_{23}$ have a minor effect on the overall invariants computation and neglecting $V_{12}$ and $V_{23}$, decreases the noise level below the reference signal.

The geographical distribution of the invariant $l_2$ derived from the main diagonal GGs along the GOCE ground tracks for November and December 2009 is shown in Figure 10.

For GOCE data analysis, we propose to replace the elements $V_{12}$ and $V_{23}$ by forward modeled GGs. In each iteration step the actual estimate is used for the evaluation of $V_{12}$ and $V_{23}$. Based on these values, invariants computation is straightforward and thus the solution of the linearized observation model. To start the iterative process, initial values have to be provided in terms of external information. Since the con-
Figure 5: Invariant $I_2$. November 2009: real data, main diagonal GGs only (black dashed line); forward modeled reference invariants, all GGs (gray solid line); noise (black solid line).

Figure 6: Invariant $I_3$. November 2009: real data, all GGs (black line); forward modeled reference invariants, all GGs (gray line).

Figure 7: Invariant $I_3$. November 2009: real data, main diagonal GGs only (black line); forward modeled reference invariants, all GGs (gray dashed line).

Figure 8: Invariant $I_2$. November 2009: real data, all GGs (black dashed line); forward modeled reference invariants, all GGs (black line); noise (gray solid line).

Figure 9: Invariant $I_3$. November 2009: real data, main diagonal GGs only (black dashed line); forward modeled reference invariants, all GGs (gray solid line); noise (black solid line).

Figure 10: Global map of the Invariant $I_2$ from 02-Nov-2009 to 31-Dec-2009, in E2.
tributions of $V_{12}$ and $V_{23}$ on invariants computation are small compared to the main diagonal components, the iterative process turned out to be insensitive towards the initial values for GGs synthesis. According to Figure 11, the elements can even be neglected in the first iteration without decisive influence on the convergence behavior and final results.

5. Stochastic model

Following the formalism in [11], temporal correlations of GGs can be modeled by means of an auto-regressive moving-average (ARMA) process. It is characterized by the filters $F_{ij}$ subject to $D(V_{ij}) = (F_{ij}'F_{ij})^{-1}$ with $D(V_{ij})$ the variance-covariance matrix of element $V_{ij}$. Here we make use of these filters in order to derive a filter for the invariants by error propagation.

According to Eq.(4b), the linearized invariant $I_2$ can be expressed by

$$I_2 = c_1 \delta V_{11} + c_2 \delta V_{12} + c_3 \delta V_{13} + c_4 \delta V_{22} + c_5 \delta V_{23} + c_6 \delta V_{33}. \tag{7}$$

The linear factors $c_k$, $k=1,..,6$ are subject to the reference gradients $U_{ij}$, $i, j = 1, 2, 3$. Error propagation yields

$$D(I_2) = JD(V)J^T. \tag{8}$$

Therein, $J$ denotes the matrix of linear factors (Jacobian matrix), $D(V)$ the total GGs variance-covariance matrix, and $D(I_2)$ the invariants variance-covariance matrix. Neglecting correlations between different types of GGs results in a block-diagonal structure of $D(V)$. Consequently, $D(I_2)$ simplifies to

$$D(I_2) = JD(V_{ij})J^T_v + \cdots + J_iD(V_{33})J^T_v. \tag{9}$$

Inserting $D(V_{ij}) = (F_{ij}'F_{ij})^{-1}$ in Eq.(9) finally yields

$$D(I_2) = JJD(V_{ij}) = (F_{ij}'F_{ij})^{-1}J_iD(J^{-1}_vF_{ij})^T. \tag{10}$$

As a result, the invariants variance-covariance matrix is characterized by products between the (diagonal) matrices of linear factors and the inverse GGs filter matrices.
6. High Performance Computing

GOCE real data analysis requires the estimation of tens of thousands of unknown gravity field parameters from tens of millions of observations. The computational burden can only be tackled by a tailored parallel processing scheme. We implemented our analysis algorithms on high-performance computing platforms adopting OpenMP and MPI for parallelization. Here we present our parallelization strategies for the normal equations system inversion approach. A more comprehensive overview on least-squares solvers in the context of gravity field determination is provided in [2].

Figure 12 outlines our parallel processing scheme on shared memory systems. The design matrix is assembled block-wise (in order to reduce memory requirements) by the individual processors. Standard BLAS routines perform the necessary algebraic operations and sum up the block-wise normal equations systems. As all CPUs have access to all memory units of the system, data accessibility has not to be organized. After the assembling of the overall normal equations system, we solve it by inversion (Cholesky decomposition) using LAPACK routines.

On distributed memory systems, data accessibility has to be organized in detail, cf. Figure 13. CPU-specific data sets are inter-changed between the processors by block-cyclic distribution. PBLAS and ScaLAPACK routines allow for the assembly and inversion of the normal equations system.

Exemplary for the parallelization performance of our implementations, Table 1 summarizes achieved runtime results using up to 8 CPUs in parallel. Ranging from 88.8% to 93.8% of the total wall time, the NES computation is by far the most time-consuming part of the algorithm. With increasing number of CPUs, the NES inversion requires higher relative runtime costs. The computational effort for the design matrix assembly is less than 1%. The parallelization is performed successfully with very good speed-up results.

Table 1: Runtime results of normal equations system (NES) inversion, achieved with an SGI Altix 3700 system (shared-memory), 518400 observations, 40398 unknown parameters

<table>
<thead>
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<th>CPUs</th>
<th>1</th>
<th>4</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>total runtime (h)</td>
<td>64.46</td>
<td>17.06</td>
<td>9.06</td>
</tr>
<tr>
<td>design matrix (%)</td>
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<td>0.8</td>
<td>0.8</td>
</tr>
<tr>
<td>NES assembly (%)</td>
<td>93.8</td>
<td>92.1</td>
<td>88.8</td>
</tr>
<tr>
<td>NES inversion (%)</td>
<td>1.5</td>
<td>3.4</td>
<td>6.8</td>
</tr>
<tr>
<td>Speed-up</td>
<td>1</td>
<td>3.84</td>
<td>7.22</td>
</tr>
</tbody>
</table>

Figure 13. Implementation of normal equations system assembly and inversion on distributed memory systems.
7. Conclusions
We demonstrated the gravitational tensor invariants approach to be a viable alternative for GOCE gravity field recovery to more conventional analysis methods based on individual GGs. The alternative strategy is motivated by its independence of the gradiometer instrument orientation in space. Although rotation information in terms of angular velocities and accelerations is required to reduce the centrifugal and Euler effects, the orientation parameters themselves have not to be known.

The combination of linearization by means of perturbation theory, synthesis of unobserved GGs, error propagation for the modeling of the invariants variance-covariance information, and the parallelization of the analysis software prepare the approach for GOCE real data analysis.

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