Highlights

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- GROOPS is a software package for geodetic, geophysical, and environmental applications
- Global and regional gravity field recovery
- GNSS processing from single-station precise point positioning to large global networks
- Orbit determination of low-Earth-orbiting satellites

GROOPS: A software toolkit for gravity field recovery and GNSS processing

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ABSTRACT

The Gravity Recovery Object Oriented Programming System (GROOPS) is a software toolkit written in C++ that enables the user to perform core geodetic tasks. Key features of the software include gravity field recovery from satellite and terrestrial data, the determination of satellite orbits from global navigation satellite system (GNSS) measurements, and the computation of GNSS constellations and ground station networks. Next to raw data processing, GROOPS is capable to operate on time series and spatial data to directly analyze and visualize the computed data sets. Most tasks and algorithms are (optionally) parallelized through the Message Passing Interface, thus the software enables a smooth transition from single-CPU desktop computers to large distributed computing environments for resource intensive tasks. For an easy and intuitive setup of complex workflows, GROOPS contains a graphical user interface to create and edit configuration files. The source code of the software is freely available on GitHub (`https://github.com/groops-devs/groops`) together with documentation, a cookbook with guided examples, and step-by-step installation instructions.

Software availability

Software name GROOPS

Availability GitHub (`https://github.com/groops-devs/groops`)

Lead developer Torsten Mayer-Gürr

Program language C++

License GPL v3

Documentation Usage guide, source code documentation, cookbook with examples, and step-by-step installation instructions included in the repository

1. Introduction

The determination of Earth's geometric shape, orientation in space, and gravity field are core geodetic tasks and provide the basis for a wide range of environmental sciences. A stable geometric reference frame allows long-term observations of critical processes such as sea level rise, tectonic plate motion, and post-glacial rebound (Le Cozannet et al., 2015; Nerem et al., 2000; Blewitt et al., 2010). Earth's static gravity field is a key quantity for oceanographic and geological sciences (Bingham et al., 2014; Johannessen et al., 2003; Ebbing et al., 2018). Temporal changes in gravitational attraction can be used to infer mass changes on Earth's surface caused by, for example, the continental water cycle, ocean currents, or melting ice caps and glaciers (Chambers, 2006; Velicogna, 2009; Chen et al., 2010; Tapley et al., 2019) and provide key insights into these climate-relevant processes.

The derivation of these quantities is typically very resource intensive, that is, a vast number of measurements from different observation techniques need to be combined and processed. As a consequence, dedicated software packages, both for research and commercial purposes, have been developed (e.g., Dach et al., 2015; Böhm et al., 2018; Bertiger et al., 2020).

In this short communication we present the Gravity Recovery Object Oriented Programming System (GROOPS), a software toolkit for performing core geodetic tasks. The source code of GROOPS is publicly available on GitHub (`https://github.com/groops-devs/groops`) together with a comprehensive documentation and an installation guide. GROOPS is written in C++ and is designed to be operating system independent. It can be compiled and run on both Linux and Microsoft Windows.

While GROOPS is intended to be a standalone software package, some functionality depends on external libraries. Hard dependencies are the Expat XML parser (`https://libexpat.github.io`, last accessed 25-08-2020), routines of the International Earth Rotation and Reference Systems Service Software Collection (Petit and Luzum, 2010), the Jacchia-Bowman 2008 Empirical Thermospheric Density Model (Bowman et al., 2008), the horizontal wind model (HWM14, Drob et al., 2015), the International Geomagnetic Reference Field (IGRF, Thébault

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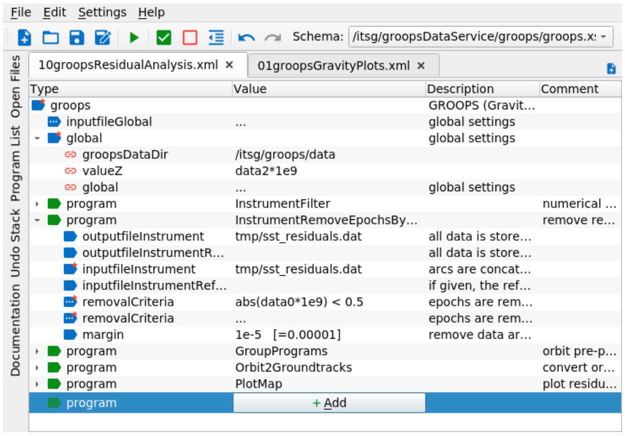

Figure 1: Screenshot of the GROOPS graphical user interface.

et al., 2015) and an implementation of the Linear Algebra Package (LAPACK, Anderson et al., 1999).

Additional libraries extend the feature set of GROOPS and can be optionally enabled at compile time. At the moment, these include NetCDF (`https://unidata.ucar.edu/software/netcdf`, last accessed 25-08-2020) for reading and writing NetCDF files, zlib (`https://zlib.net`, last accessed 25-08-2020) for reading and writing compressed files, and the Essential Routines for Fundamental Astronomy (`https://github.com/liberfa/erfa`, last accessed 25-08-2020) for high-precision Earth rotation. Another optional dependency is an implementation of the Message Passing Interface (MPI) standard. Resource intensive tasks and algorithms are designed and implemented to be optionally run in parallel on distributed systems. If an MPI implementation is available, GROOPS can be compiled as an MPI executable and either run on a local desktop machine with multiple processes or on a large high-performance computing cluster.

To enable an intuitive interaction with the software, GROOPS includes a graphical user interface (GUI). The GUI is also written in C++ and depends on the Qt toolkit (`https://qt.io`, last accessed 25-08-2020).

2. GROOPS overview

2.1. Software usage

User interaction with GROOPS is based on XML configuration files typically generated in the GUI. A configuration file represents a sequence of smaller tasks, dubbed "programs", which comprise a work flow. Programs vary in complexity, but mostly represent atomic operations on data, for example, removing trends or resampling a time series. These elementary building blocks allow the user to create flexible processing chains where individual processing steps can be added, removed, or adapted. This modular approach allows programs to be used in different contexts and applications. For example, data preprocessing and outlier removal is usually very similar for different satellite missions and also shares common steps with GNSS processing.

Figure 1 shows an example of a configuration file as depicted in the GUI. This example covers a typical workflow for data analysis. In a first step, post-fit residuals of inter-satellite ranging measurements are numerically differentiated by applying a corresponding digital filter to the time series in the program *InstrumentFilter*. Then, values below 0.5 nm s^{-2} are removed through *InstrumentRemoveEpochsByCriteria*, to only show large outliers in the data. To see if any geophysical signals are present in the remaining residuals, we want to analyze the time series in space rather than in time domain. To this end, we compute the satellite ground tracks on Earth's surface from the satellite orbit and co-locate the corresponding residual epochs in *Orbit2Groundtracks*. Finally, the now georeferenced residuals are visualized on a global map through *PlotMap*. The result of this work flow is shown in Figure 4.

Interaction between programs is file-based, that is, a program reads one or more input files, performs its designed task and generates one or more output files which can then be processed by a following program. To make batch processing of large data sets easier, configuration files also support control flow statements such as loops and conditions. Loops can be used to iterate over points in time or file lists and can involve multiple programs. Each loop type sets a number of variables which are updated in each iteration. These variables are resolved at run time and can be used to process, for example, file names with varying time stamps. With conditional execution, missing input data files or different processing requirements can be accounted for.

2.2. Extensibility

The modular structure of the GROOPS configuration files is also reflected in the source code, in that it is object oriented and designed to be easily extendable. The source code can be categorized into two parts. Low-level functionality is provided by classes in the core library, which includes, for example, matrix multiplication, file input/output, and polynomial interpolation. The second part are the programs, which combine different functionalities from the core library. They can be thought of as plugins or add-ons and are the interface between the software and user. The source code repository includes a program template which can be used as a starting point for tasks that cannot be realized with the included programs.

3. Methods and results

The feature set of GROOPS can be categorized into four parts:

- gravity field recovery from satellite and terrestrial observations
- processing of GNSS constellations and ground station networks to determine GNSS products
- orbit determination of low-Earth-orbiting (LEO) satellites
- statistical analysis of time series and spatial data sets

The methods implemented in the software are documented to a high degree in peer-reviewed articles (e.g., Pock et al., 2014; Zehentner and Mayer-Gürr, 2016; Kvas and Mayer-Gürr, 2019; Strasser et al., 2019; Ellmer and Mayer-Gürr, 2017) and theses (Ellmer, 2018; Kvas, 2020). Data sets, which are the main output of GROOPS, have been used within the scientific community (e.g., Gouweleeuw et al., 2018; Humphrey and Gudmundsson, 2019; Eicker et al., 2020; Göttl et al., 2019; Jäggi et al., 2020). This means that they have undergone not only an internal pre-publication evaluation but also independent external evaluations.

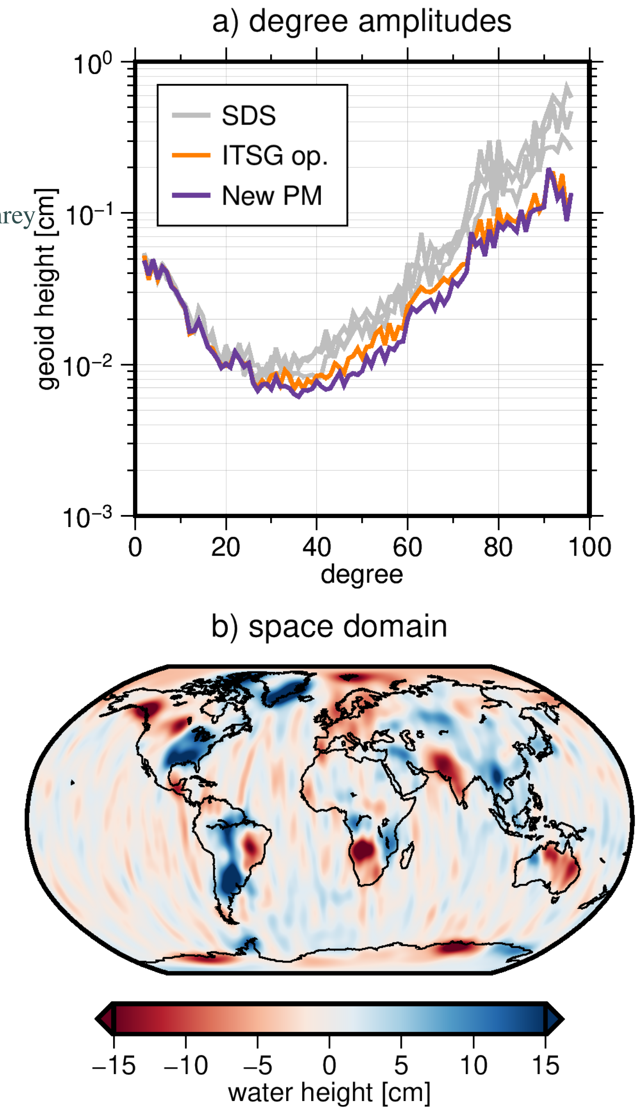

Figure 2: a) Comparison of GRACE Follow-On solutions from the official science data systems (SDS) and solutions computed with GROOPS (ITSG op., New PM) in spectral domain. b) Estimated gravity field solution in space domain expressed as equivalent water height.

3.1. Gravity field recovery

Gravity field recovery within GROOPS is based on the short-arc approach introduced by Mayer-Gürr (2006) and solves Newton's equation of motion through variational equations (Montenbruck and Gill, 2000). A detailed overview of the algorithms used on the example of the Gravity Recovery and Climate Experiment (GRACE) satellite mission can be found in Ellmer (2018, section 5).

A typical workflow starts with converting data files as well as metadata and auxiliary data into internal file formats. This has the advantage that multiple satellite missions, where data file formats in general vary drastically, can be ingested in the same fashion by the same programs. Then, the input data is quality controlled and checked for outliers. This can be done with criteria based on metadata, thresholds or robust sample statistics. In the next step, the least squares adjustment, which we use to solve for the unknown gravity field, is set up. Here, we can also determine the noise characteristics of the input data using variance component estimation. The result of this processing step is either the least squares solution of the gravity field or additionally the system of normal equations which can be stored as a file for further processing. Finally, post-processing steps such as restoring background models can be performed and the solution is converted from the internal file format to a standardized file format for publication and exchange. Optionally, the result can be visualized and evaluated through, for example, intercomparison with other solutions. Figure 2a shows an example of such an intercomparison of GRACE Follow-On (GRACE-FO) solutions in terms of degree amplitudes. Alternatively, the obtained solution can also be visualized in space domain (see Figure 2b).

GROOPS is capable of dealing with different observation types, such as orbit positions derived from raw GNSS measurements, highly-accurate intersatellite ranging observations as realized within the GRACE mission and its successor GRACE Follow-On (GRACE-FO), and gradiometer observations of the Gravity field and steady-state Ocean Circulation Explorer (GOCE). Additionally, gravity field recovery from terrestrial data is also possible and has been successfully performed for the geoid of Austria (Pock et al., 2014).

Published gravity field solutions computed with GROOPS include the ITSG-Grace time series (Kvas et al., 2019a), GOCO06s (Kvas et al., 2019b, 2020), a static gravity field model based on 1.2 billion observations from 19 satellites, and a lunar gravity field model (Wirnsberger et al., 2019). These data sets have been widely used within the geodetic and geophysical community and have undergone extensive internal and external evaluation (Bonin and Save, 2020; Göttl et al., 2019; Meyer et al., 2019; Ghobadi-Far et al., 2020). From this we can conclude that GROOPS is capable of producing state-of-the-art gravity field data products.

3.2. GNSS processing

GROOPS uses the raw observation approach (Strasser et al., 2019) to process data from multiple GNSS including the Global Positioning System (GPS), the Russian Global Navigation Satellite System (GLONASS), and the European system Galileo. Many geodetic, geophysical, and environmental applications require high-precision GNSS products

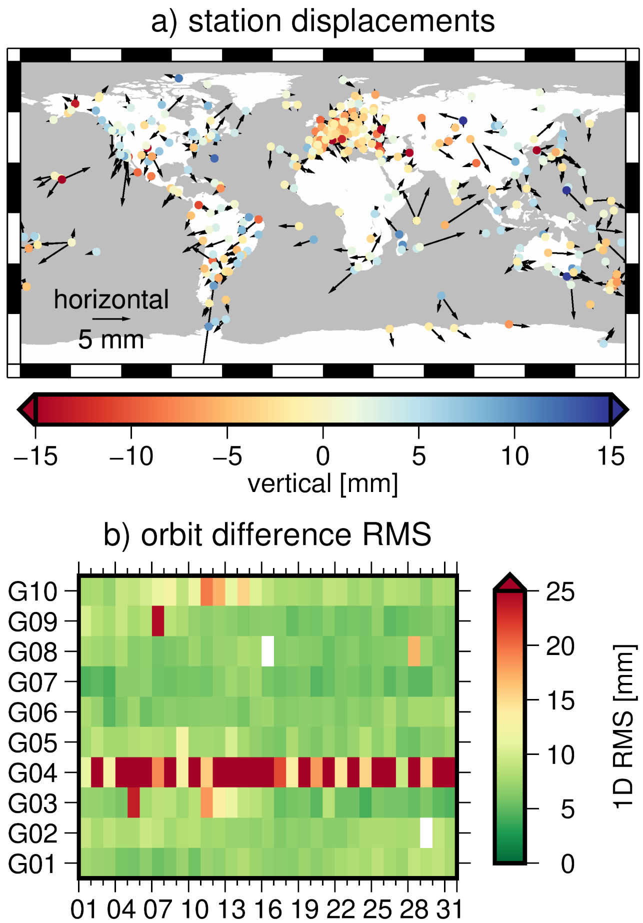

Figure 3: a) Differences of station coordinates derived by GROOPS to IGS combination for 2019-08-01 in terms of horizontal and vertical displacements. b) Root mean square (RMS) of daily GPS satellite orbit differences between GROOPS-derived and IGS combined solutions for August 2019.

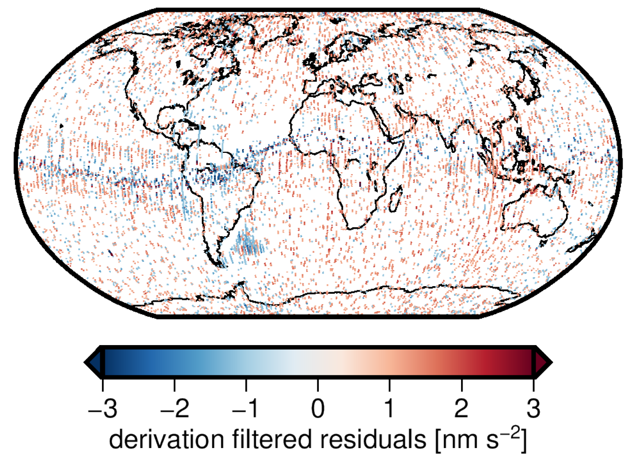

Figure 4: Derivation filtered range-rate residuals of the GRACE Follow-On laser ranging interferometer, co-located with the satellite ground track.

such as satellite orbits, satellite clocks, or station positions. They are the prerequisite for high-quality satellite orbits of many remote sensing satellites, form the basis for local and regional surveys (Harpham et al., 2016), and enable new measurement techniques (Cooper et al., 2019). Different analysis centers routinely generate such data sets by processing observations from a global GNSS station network under the umbrella of the International GNSS Service (IGS, Johnston et al., 2017).

GNSS solutions produced with GROOPS have been incorporated into the third reprocessing campaign of the IGS (repro3, Rebischung et al., 2019), which constitutes the GNSS contribution to the next International Terrestrial Reference Frame (ITRF2020, Altamimi et al., 2018). Evaluations within the reprocessing campaign show that GROOPS-derived station coordinates and satellite orbits are state of the art (Villiger and Dach, 2020). In Figure 3 we show the difference of GROOPS-derived station coordinates and satellite orbits with respect to the IGS combination. As can be seen, GROOPS-derived GNSS products fit well to the IGS combination, with differences for both stations and satellite orbits on the millimeter to low centimeter level, which is on par with solutions from other IGS analysis centers.

Next to the determination of large-scale global station networks, GROOPS also supports precise point positioning (PPP) of single receivers. PPP can be applied to a receiver on Earth's surface or on an artificial satellite in space (Zehentner and Mayer-Gürr, 2016). With GROOPS, kinematic orbits of 16 satellite missions have been computed. These data sets have been primarily used as input data for gravity field recovery (da Encarnação et al., 2020; Kvas et al., 2019b) or atmospheric research (Vielberg et al., 2018).

3.3. Data preprocessing and analysis

GROOPS has the capability to analyze and visualize both input data and computed results. This includes Fourier and wavelet transforms of time series data, filtering, computation of sample distributions through histograms, and statistical analysis of spatial and time series data.

One application of such an analysis are post-fit residuals (Goswami et al., 2018; Behzadpour et al., 2019). The example in Figure 4 shows range-rate residuals of the GRACE-FO laser ranging interferometer (LRI) to which we applied a derivation filter. For more clarity we excluded all residuals with a magnitude below 1 nm s^{-2}. Range-rate observations are originally given as a time series, however, GROOPS offers the possibility to represent the data in different domains. This allows the user to easily identify correlations or artifacts caused by different phenomena. In Figure 4 the residuals are co-located with the satellite position along the ground track at the time the corresponding measurement was taken. In this domain, we can clearly identify geophysical features such as the magnetic equator or the Argentine gyre.

Next to the analysis of observations or residuals, GROOPS also offers the possibility to visualize and analyze geophysical signals from computed gravity field solutions. One application of such an analysis are temporal water storage variations in river basins. In Figure 5 we show daily basin averages of the Danube derived from GRACE satellite data and

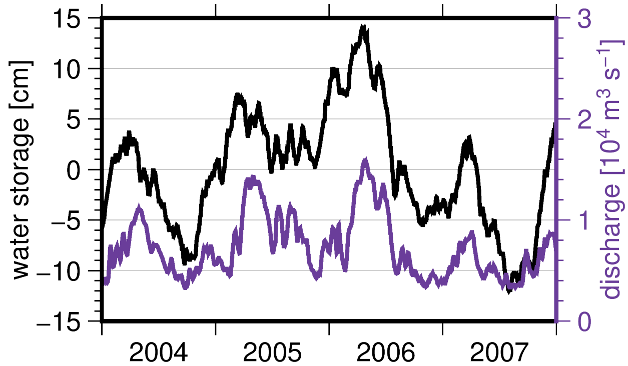

Figure 5: Time series of Danube basin averages from daily GRACE solutions and discharge data recorded at the river mouth.

compare them with in-situ discharge data which is kindly provided by the Global Runoff Data Centre (GRDC, Global Runoff Data Centre, 2007). GROOPS can not only be used to study individual river basins but also supports the analysis of global data sets. Different applications of global statistics computed and visualized with GROOPS can be found in Eicker et al. (2020).

Data visualization is realized through the Generic Mapping Tools (GMT, Wessel et al., 2019). GMT is not included in the source code, rather GROOPS generates shell or batch scripts which can be passed to the GMT executable. The information content in the different figure types is organized into layers which can be easily created and rearranged in the GUI. Next to data layers, which include line and bar graphs, scatter plots, error bars, and pseudocolor grids, additional annotations such as coast lines or text can be added as layers in the different plotting programs. This enables a flexible composition of publication-quality figures.

4. Summary

Data sets that describe Earth's geometric shape, orientation in space, and gravity field provide the basis for a broad range of applications in Earth and environmental sciences. In this short communication we presented GROOPS, a software toolkit which is capable of computing these quantities with state-of-the-art methods. The software features include gravity field recovery, GNSS constellation and ground station processing, the determination of LEO satellite orbits, and analysis of time series and spatial data sets. The source code, documentation, guided examples, and installation instructions are publicly available on GitHub (`https://github.com/groops-devs/groops`). An included graphical user interface allows an easy setup of complex work flows for core geodetic tasks and the analysis of geophysical data sets.

GROOPS offers the possibility to compute geodetic data sets from scratch and thus enables researchers to set up processing chains from raw measurement data to the scientific analysis, with full control over each step. Additionally, the publicly available software source code in conjunction with traditionally published documentation provides a comprehensive description of data sets computed with GROOPS. This makes the data generation process transparent and allows users to build upon or adapt existing processing chains to their specific needs. These two aspects make GROOPS a valuable tool for a range of potential users in different Earth and environmental science disciplines.

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Parts of GROOPS originate from developments in the Astronomical, Physical and Mathematical Geodesy Group at the University of Bonn, Germany. Since 2010 it is developed and maintained at Graz University of Technology, Austria.

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