

Adaptive Optimization of GOCE Gravity Field Modeling

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Long years of highly intensive research allowed for the realization of the satellite mission GOCE (Gravity Field and Steady-state Ocean Circulation Explorer), which in 1999 became the first mission to be adopted within the new Living Planet Programme by the European Space Agency (ESA). The primary goal of this mission is the recording of the static component of the Earth's gravity field with an unprecedented global accuracy and resolution of at least 2 cm for the geoid at a global scale of at least 100 km . With this results other geoscientific core goals will be realized. On the one hand, the Earth system with all its interacting geophysical and oceanographic processes may be modeled with much higher reliability by means of a high-precision GOCE gravity field. On the other hand, a high-precision geoid will finally enable geodesists to unify and connect the heterogeneous national height reference systems. The goal of this article is to describe an in-situ approach to determine a global Earth gravity model and its variance/covariance information on the basis of calibrated measurements from the GOCE mission. As the main characteristics of this procedure, the GOCE data are processed in situ via development of the functionals at the actual location and orientation of the gradiometer. This high-dimensional data fitting problem (spherical harmonic analysis) with irregularly distributed data can only be managed on a massive parallel computer system using tailored algorithms. The PCGMA (preconditioned conjugate gradient multiple adjustment) algorithm consists of an iterative variance component estimation to handle heterogeneous data groups, a conjugate gradient solver supported by an efficient preconditioning procedure to find the optimal solution of the huge, dense, overdetermined linear system, and a tailored pre-whitening procedure based on digital filters to decorrelate the densely sampled measurements.

1 Introduction

1.1 Overview over the satellite mission GOCE

The GOCE satellite (see Fig. 1) was launched on 17. March 2009 after decades of scientific research¹¹ and technological development as the first core mission of ESA's new Living Planet Programme⁶. The main goal of this mission is the determination of the static part of the gravitational field of the Earth, which is inhomogeneous due to mass anomalies in the Earth's interior, with the very high accuracy of at least 2 cm for geoid heights and 1 mgal ($\hat{=}10^{-5}\frac{m}{s^2}$) for gravity anomalies at a global resolution of 100 km ⁶. The GOCE spacecraft is orbiting planet Earth at a very low altitude of about 255 km and with an inclination of 96.5° (Fig. 2). The orbit is sun-synchronous to minimize thermoelastic disturbances at shadow crossings and to guarantee sufficient power supply throughout the at least one year long mission.

The main idea for reaching the unprecedented level of accuracy in global gravity field determination is the fusion of different sensors. The GOCE mission combines in particular two distinct measurement concepts, which are sensitive to the low-frequency part of the gravity field, on the one hand, and the high-frequency part, on the other hand. The low-frequency part is captured via the tracking of the low-orbit satellite using the Global Positioning System (GPS) by precisely measuring the satellite's orbit disturbances¹⁵, known

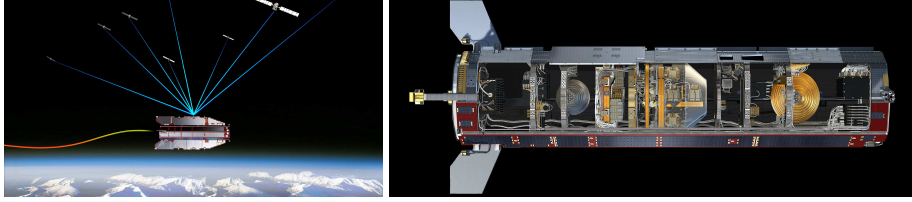


Figure 1. Two illustrations of the GOCE Satellite. Left: GPS tracking of GOCE. Right: A look at the various instruments inside the satellite, the gradiometer as the main instrument can be seen in the center. ©ESA

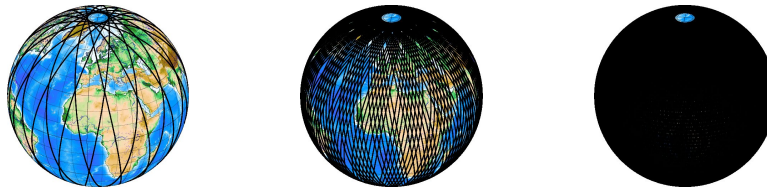


Figure 2. Ground track of the GOCE satellite after the first day, first week and first month in orbit.

as Satellite-to-Satellite Tracking (SST), see Fig. 1 left). The high-frequency part of the gravity field signal is determined by means of the innovative measurement principle of Satellite Gravity Gradiometry¹¹ (SGG). The main instrument is the gradiometer (see Fig. 1 right), which measures second derivatives \mathbf{V}_{ij} of the Earth's gravitational potential \mathbf{V} in situ. These measurements are derived from accelerations (representing the first derivatives of the gravitational potential), which are measured by six accelerometers, placed some distance (25 cm) apart the center (of mass) of the satellite, aligned along three orthogonal axes (along-track, across-track and Earth-pointing). Each accelerometer has two extremely sensitive axes. The accelerometer measurements along each axial direction are differentiated, resulting in the desired along-track, across-track and earth pointing component of the gravity tensor \mathbf{V}_{ij} . In addition, due to alignment of the sensitive axes of the accelerometers, also the mixed along-track and Earth-pointing component of the gravity tensor can be determined with high accuracy. It is essential to avoid non-gravitational nuisance accelerations such as atmospheric pressure, the satellite is maintained in a compensated drag-free fall via a feedback loop between the accelerometers and the ion thrusters⁶.

Now, in order to compute a gravity field solution from SST and SGG measurements, these two independent data groups must be merged in a common statistical model. We will, however, not focus on the SST data in this report, as their quantity and numerical characteristics do not a serious computational challenge in contrast to the SGG data; we obtained the SST data in an appropriately preprocessed model by our project partner. On the other hand, the modeling of SGG data is highly challenging due to various reasons: (1) The operational mission period of 12 months, where we use only the three most accurate gradient components (\mathbf{V}_{xx} , \mathbf{V}_{yy} and \mathbf{V}_{zz}), sampled at 1 Hz, will result in a huge number of as many as 100 million observations. (2) The SGG data with respect to each of these three components are highly auto-correlated¹³, the accommodation of which would be based on a full variance/covariance matrix with required memory of approximately 8 000 Terabyte.

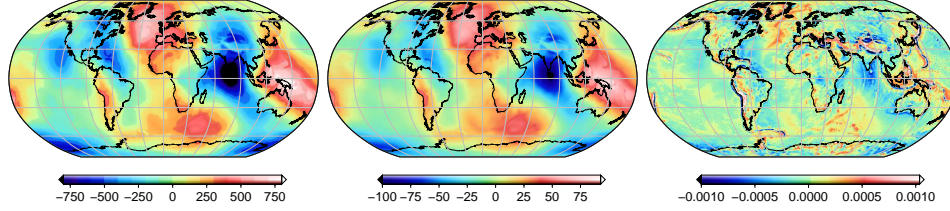


Figure 3. Functionals of the gravity field with maximum achievable resolution of GOCE (sh d/o 270). Left: potential (m^2/s^2). Center: geoid heights (m). Right: gravity anomalies (m/s^2).

A further challenge arises from the fact that the SST/SGG data combination problem is ill-posed due to data gaps over the polar regions¹⁴ (cf. Fig. 2) and the attenuation of the gravity field signal at the satellites altitude. This problem necessitates the regularization of the statistical model by introducing stochastic prior information, which may be viewed as a third independent data group (REG). Thus, the determination of the gravity field requires the solution of a highly over-determined, dense equation system with a huge dimension. For this task we developed a tailored iterative solution strategy based on the method of conjugate gradients (CG)¹².

1.2 Modeling of the Earth's gravity field

Before we explain the solution method for determining the gravity field from GOCE observations, we will outline the mathematical parameterization of global gravity field models used in our approach. The basic idea is to describe the Earth's gravitational potential as a spherical harmonic expansion up to a certain maximal degree and order (d/o) l_{\max} . Then such a potential may be written, for some evaluation point (r, θ, λ) in an Earth fixed and centered coordinate system, as⁸

$$V(r, \theta, \lambda) = \frac{GM}{a} \sum_{l=0}^{l_{\max}} \left(\frac{a}{r}\right)^{l+1} \sum_{m=0}^l (c_{lm} \cos(m\lambda) + s_{lm} \sin(m\lambda)) P_{lm}(\cos\theta), \quad (1)$$

where l and m denote the spherical harmonic degree and order, c_{lm} and s_{lm} the unknown coefficients of the spherical harmonic expansion, a the equatorial radius of the Earth reference ellipsoid, $P_{lm}(\cdot)$ the fully normalized associated Legendre functions, and GM the geocentric gravitational constant. Thus, this model comprises $m = (l_{\max} + 1)^2$ unknown coefficients, which may in turn be used to express related geometrical and physical functionals of the Earth's gravity field such as geoid heights (i.e. the metric distances between the geoid as the zero equipotential surface and an approximating ellipsoid) and gravity anomalies (i.e. the local variation of the gravity acceleration with respect to an idealized reference ellipsoid)⁸ (see Fig. 3). Using this spherical harmonics approach, all coefficients belonging to a particular degree l refer to a unique spatial resolution or frequency.

To determine the unknown gravity field parameters c_{lm} and s_{lm} from the GOCE observations (SST, SGG and REG) they are estimated by applying a linear Gauss-Markov model⁹. In this model, each observation ℓ_i , affected by an observation error v_i , is written as a (linear) function $\mathbf{A}_{i,\cdot} \mathbf{x}$ of the gravity field parameters (denoted by \mathbf{x}). This results in observation equations $\ell_i + v_i = \mathbf{A}_{i,\cdot} \mathbf{x}$, where $\mathbf{A}_{i,\cdot}$ denotes the i th row of the design matrix

A. The stochastic behaviour of the measurement errors is usually modeled by a variance/covariance matrix Σ , which contains the variances of the observations as well as the covariances between them. Minimizing the weighted squared sum of residuals $\mathbf{v}^T \Sigma^{-1} \mathbf{v}$ leads to the linear normal equation system $\mathbf{A}^T \Sigma^{-1} \mathbf{A} \mathbf{x} = \mathbf{A}^T \Sigma^{-1} \boldsymbol{\ell}$ or $\mathbf{N} \mathbf{x} = \mathbf{n}$. Here $\boldsymbol{\ell}$ comprises the three independently distributed observation groups SST, SGG and REG, thus their corresponding normal equations may be computed separately and added up subsequently. This basic property establishes the mathematical foundation for the data combination in our approach. The weighted least squares solution is then obtained as the solution of the normal equations $\mathbf{N} \mathbf{x} = \mathbf{n}$.

The SST data group is made available to us by our project partners directly in the form of preprocessed normal equations \mathbf{N}_{sst} and \mathbf{n}_{sst} . As these SST data have a relatively low resolution of d/o 90, they are related to only a small subset (≈ 8000) of the total parameter vector. Thus, they are easily handled by our solution algorithm. The processing of the regularization data (REG) does not pose a great computational challenge either as the underlying functional model is quite simple. This can be explained by the fact that the parameters are treated as directly observed unknowns with values equal to zero, the corresponding design matrix is given by the unity matrix. Furthermore, these pseudo-observations are uncorrelated and have variances according to Kaula's rule of thumb, represented by the diagonal weight matrix \mathbf{P}_{reg} .

The processing of the SGG data is, however, more intricate. To begin with, the functional model in eq. (1) is written in the Earth-fixed frame, which is transformed into the gradiometer reference frame via the application of a rotation taking into account the Earth's rotation, the satellite's orientation in space and the gradiometer's orientation within the satellite. This rotated functional model is then differentiated twice, yielding the desired SGG observation equations $\ell_{i,\text{sgg}} + v_{i,\text{sgg}} = \mathbf{A}_{1,:\text{sgg}} \mathbf{x}$. From simulations we know that these SGG data will be highly autocorrelated. Due to the huge number of observations, these correlations cannot be stored within a variance/covariance matrix. The only feasible way to take these correlations into account is to remove them from the SGG data by means of pre-whitening filters. For this purpose, we use a sequence of high-order autoregressive moving-average (ARMA) filters. The thusly decorrelated SGG observation equations read

$$\bar{\ell}_{\text{sgg}} + \bar{v}_{\text{sgg}} = \bar{\mathbf{A}}_{\text{sgg}} \mathbf{x}. \quad (2)$$

Now, the combined normal equations are established by computing the sum of the three individual normal equations, each weighted by unknown factors ω_i :

$$(\omega_{\text{sgg}} \bar{\mathbf{A}}_{\text{sgg}}^T \bar{\mathbf{A}}_{\text{sgg}} + \omega_{\text{sst}} \mathbf{N}_{\text{sst}} + \omega_{\text{reg}} \mathbf{P}_{\text{reg}}) \mathbf{x} = \omega_{\text{sgg}} \bar{\mathbf{A}}_{\text{sgg}}^T \bar{\ell}_{\text{sgg}} + \omega_{\text{sst}} \mathbf{n}_{\text{sst}} + \omega_{\text{reg}} \mathbf{n}_{\text{reg}}. \quad (3)$$

2 PCGMA algorithm

To solve the equation system (3) for the unknown spherical harmonic coefficients, we make use of a tailored version of the conjugate gradient (CG) algorithm denoted as PCGMA¹² (preconditioned conjugate gradient multiple adjustment). This algorithm extends the standard CG algorithm with (a) a data-adaptive preconditioning step, (b) the combination of the various (independent) GOCE data types (given as either observation equations or normal equations respectively) and (c) determination of the weights $\omega_i = \frac{1}{\sigma_0^2}$ via variance component estimation (VCE)¹⁰ using Monte Carlo methods^{1,5}. To give some insight

into this computational scheme⁴, recall that the CG algorithm is based on the residuals $\mathbf{r}^{(\nu)} = \mathbf{N}\mathbf{x}^{(\nu)} - \mathbf{n}$ of a symmetric equation system $\mathbf{N}\mathbf{x}^{(\nu)} = \mathbf{n}$ which are used as a search direction for finding the minimum L_2 -norm solution.

Substituting the combined GOCE normal equation system and some initial parameter values $\mathbf{x}^{(0)}$ leads to initial residuals

$$\begin{aligned} \mathbf{r}^{(0)} &= \mathbf{N}\mathbf{x}^{(0)} - \mathbf{n} \\ &= (\omega_{\text{sgg}}\bar{\mathbf{A}}_{\text{sgg}}^T\bar{\mathbf{A}}_{\text{sgg}} + \omega_{\text{sst}}\mathbf{N}_{\text{sst}} + \omega_{\text{reg}}\mathbf{P}_{\text{reg}})\mathbf{x}^{(0)} - (\omega_{\text{sgg}}\bar{\mathbf{A}}_{\text{sgg}}^T\bar{\boldsymbol{\ell}}_{\text{sgg}} + \omega_{\text{sst}}\mathbf{n}_{\text{sst}} + \omega_{\text{reg}}\mathbf{n}_{\text{reg}}) \\ &= \omega_{\text{sgg}}\left(\bar{\mathbf{A}}_{\text{sgg}}^T\left(\bar{\mathbf{A}}_{\text{sgg}}\mathbf{x}^{(0)} - \bar{\boldsymbol{\ell}}_{\text{sgg}}\right)\right) + \omega_{\text{sst}}\left(\mathbf{N}_{\text{sst}}\mathbf{x}^{(0)} - \mathbf{n}_{\text{sst}}\right) + \omega_{\text{reg}}\left(\mathbf{P}_{\text{reg}}\mathbf{x}^{(0)} - \mathbf{n}_{\text{reg}}\right) \\ &= \omega_{\text{sgg}}\left(\bar{\mathbf{A}}_{\text{sgg}}^T\mathbf{v}_{\text{sgg}}^{(0)}\right) + \omega_{\text{sst}}\left(\mathbf{N}_{\text{sst}}\mathbf{x}^{(0)} - \mathbf{n}_{\text{sst}}\right) + \omega_{\text{reg}}\left(\mathbf{P}_{\text{reg}}\mathbf{x}^{(0)} - \mathbf{n}_{\text{reg}}\right) \\ &= \omega_{\text{sgg}}\mathbf{r}_{\text{sgg}}^{(0)} + \omega_{\text{sst}}\mathbf{r}_{\text{sst}}^{(0)} + \omega_{\text{reg}}\mathbf{r}_{\text{reg}}^{(0)}. \end{aligned}$$

This iterative CG approach has the great benefit that it avoids computation of the joint normal equation matrix \mathbf{N} , and especially of the high-dimensional product $\mathbf{N}_{\text{sgg}} = \bar{\mathbf{A}}_{\text{sgg}}^T\bar{\mathbf{A}}_{\text{sgg}}$ in view of the facts that (a) $\bar{\mathbf{A}}_{\text{sgg}}$ could be of dimension $70\,000 \times 100\,000\,000$ or larger and (b) this matrix-matrix product is replaced by two far less expensive matrix-vector multiplications $\mathbf{v}_{\text{sgg}}^{(0)} = \bar{\mathbf{A}}_{\text{sgg}}\mathbf{x}^{(0)} - \bar{\boldsymbol{\ell}}_{\text{sgg}}$ and $\mathbf{r}_{\text{sgg}}^{(0)} = \bar{\mathbf{A}}_{\text{sgg}}^T\mathbf{v}_{\text{sgg}}^{(0)}$. Based on these initial residuals eq. (3) is solved using the standard preconditioned CG algorithm⁷ using \mathbf{N}_{\oplus} as the data-adaptive preconditioning matrix (cf. Sect. 3)^{2,3}.

PCGMA has been implemented on a computer cluster to distribute the computational workload. As already mentioned above, it is crucial to parallelize the processing of the huge number of SGG data. This is done by distributed row-wise assembling of the design matrix \mathbf{A}_{sgg} . Then the individual parts of the design matrix and the observation vector are transformed by means of digital ARMA filters in order to remove the autocorrelations present in each SGG component. Subsequently, the SGG residuals \mathbf{r}_{sgg} are computed in parallel, whereas the remaining CG operations are computed in serial mode on the master node, after an append-receive operation of the distributed residuals. The residuals with respect to the REG and SST groups are computed in serial mode, as \mathbf{P}_{reg} is only a diagonal matrix and \mathbf{N}_{sst} contains only a relatively small block of non-zero elements (of size less than $10\,000 \times 10\,000$). The serial CG operations have been implemented based on fast level 3 BLAS routines.

3 Computational aspects

The two parts of the whole PCGMA algorithm of main computational interest are (a) the design of the preconditioner and (b) the assembling and filtering of the SGG observation equations for the purpose of their decorrelation. In this contribution we will concentrate on the choice of a tailored data-adaptive preconditioner for the GOCE observations. The preconditioning matrix serves as an approximation of the joint normal equation matrix for the purpose of accelerating the convergence of the CG algorithm and of stabilizing the numerical procedure.

To obtain the dominant structure of the combined normal equations \mathbf{N} (3) as a sparse, and thus easy-to-handle, approximation, one exploits the properties of the spherical harmonic base functions. These functions satisfy certain orthogonality relations⁸. Conse-

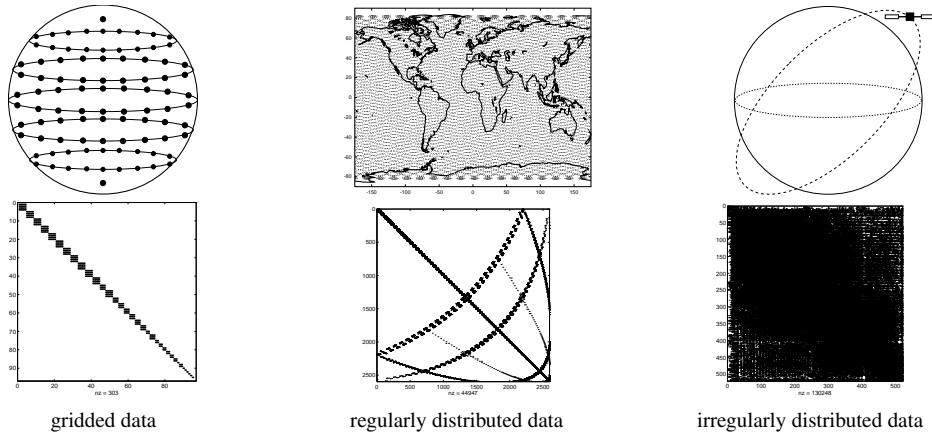


Figure 4. Resulting structure of normal equations for different scenarios of data coverage.

quently, if the data are globally distributed on the sphere with equidistance along the parallels, only coefficients of the same order are correlated and lead to non-zero elements in the normal equations. If such parallels are even symmetric with respect to the equator, then also the coefficients with odd degrees within each order are independent from the corresponding even coefficients. If the coefficients are then arranged or numbered order-wise within the parameter vector \mathbf{x} , the normal equation matrix takes a block-diagonal structure as shown in Fig. 4 (left). If some sufficiently dense and global data distribution on symmetric parallels is disturbed by slightly shifting the locations, then the resulting normal equation matrix remains nearly block-diagonal (Fig. 4 center). This matrix loses its block-diagonal structure and becomes increasingly fully populated the more the data coverage differs from a regular distribution (Fig. 4 right).

In GOCE data processing, the task is to choose a numbering scheme concerning the parameters such that it allows for a sparse approximation for the combined normal equation matrix. Analyzing the structures of the individual normal equations with respect to the three observation groups, we find three key properties: (a) The SGG data are regularly distributed over the sphere except for the polar regions. With an order-wise numbering, the resulting SGG normal equations are then nearly block-diagonal; therefore, a sparse preconditioning matrix should preserve this property. (b) The REG normal equation matrix is a diagonal matrix, which is naturally sparse and may thus be simply added to the preconditioning matrix. (c) The SST normal equation matrix should be added to the preconditioner as a whole and without using an approximation. Its numbering must be chosen such that the entire populated block remains as coherent as possible. These three desired properties hold when the free kite numbering scheme^{2,3} is applied. To understand this kite scheme it is useful to represent the spherical harmonic coefficients c_{lm} and s_{lm} as a triangle in the following way (Fig.5, left): The ordinate is defined by the degree l , which increases from top to bottom, and the abscissa by the order m , with the cosine coefficients c_{lm} to the left and the sine coefficients s_{lm} to the right.

We may now classify the parameters according to the three zones FULL (modeling the full correlations in the sparse preconditioner), INDEPENDENT (parameters where only

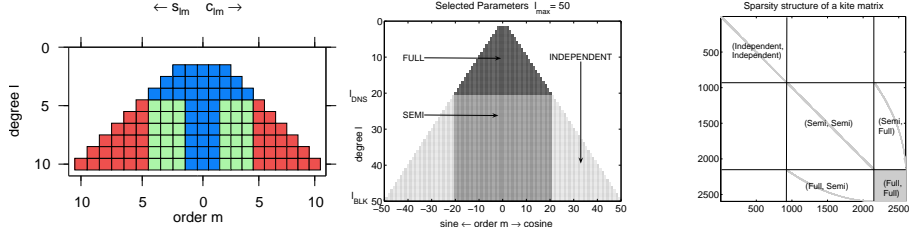


Figure 5. Coefficient triangle with the correlation zones for the free kite numbering scheme and the resulting structure of the sparse preconditioner.

the order-wise correlations are modeled) and SEMI (all the parameters of order m for which some degrees are present in the FULL zone). Then, all of the parameters first within the INDEPENDENT, then within the SEMI, and finally within the FULL zone, are numbered order-wise. From this numbering scheme follows directly the population scheme of the desired preconditioning matrix (Fig. 5 right). Such a matrix has the great advantage, that no fill-in values arise when it is reduced via Cholesky's algorithm², used in the preconditioning step within PCGMA for solving $\mathbf{N}_{\oplus}\boldsymbol{\rho} = \mathbf{r}$. As far as the SGG data are concerned, all the elements $\mathbf{N}_{\oplus,i,j} = \bar{\mathbf{A}}_{sgg,i,:}^T \bar{\mathbf{A}}_{sgg,:,j}$ are computed rigorously according to determined populations scheme. The normal equation matrices concerning the SST and REG groups are then simply added to the matrix \mathbf{N}_{\oplus} using weights ω_i .

The free kite numbering scheme has some interesting additional properties. The more parameters are assigned to the FULL zone, the faster the PCGMA algorithm converges but the larger the size of the preconditioning matrix becomes. The size of the preconditioner used in a typical GOCE simulation is about 1.0 – 2.0GB, which constitutes a good compromise between a fast convergence rate and memory requirements. The fact that the spectral radius is ≈ 0.1 demonstrates the efficiency of this preconditioner. Thus the PCGMA algorithm converges within 20 – 30 iterations, allowing for a very efficient solution of the dense normal equation system with 70 000 unknowns. In addition, the SGG part of the preconditioner may be computed in parallel, with each node processing parts of the SGG data (in which case the preconditioning matrix must be stored in memory of each of these nodes). The individual parts are collected via a global reduce operation on the master node.

4 Summary and outlook

The spherical harmonic analysis is a standard procedure to determine the gravitational potential from gravity data. In the context of the GOCE application, the processing of a high-resolution gravity field from the huge number of highly correlated, heterogeneous GOCE measurements, requires both a huge computational effort and large amount of memory. For this purpose, a tailored solution strategy was developed, which can handle heterogeneous data, avoid the expensive computation of the normal equations, allow for a sequential processing of highly correlated measurements, and which uses stochastic trace estimators to overcome the computational burden of VCE. After two decades of research PCGMA has

finally been implemented in fully operational mode and used in numerous simulations on the JUMP cluster (128–256 processors) at Forschungszentrum Jülich. Currently, the research community awaits the GOCE real data, expected to be available in the beginning of October 2009. The results derived from the GOCE real data analysis are expected to revolutionize the understanding of dynamic processes within the Earth system.

Acknowledgments

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