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Verified Quadrature in Determining Newton's Constant of Gravitation

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Abstract: This paper describes the use of interval arithmetic to bound errors in an experiment for determining Newton's constant of gravitation. Using verified Gaussian quadrature we were able to assess the numerical errors as well as the effect of several tolerances in the physical experiment.

Key Words: Constant of gravitation, Gaussian quadrature, validated numerics

1 Introduction

Of all the basic physical constants, Newton's constant of gravitation G is known to the least precision. In fact, even the relative precision of 10^{-4} that is claimed for some measurements seems dubious (note that the intervals 6.67_{17}^{35}, 6.66_{49}^{63}, and 6.71_{48}^{60} corresponding to the data from [Tab. 1] are pairwise disjoint).

The large uncertainty in the individual values is due to the fact that even if some quantities involving G can be measured to rather high precision, (e.g., the period of revolution of celestial bodies around their central mass), there is always some other quantity involved that is known to much lower precision (e.g., the mass of the central body). As the values differ by more than the error bounds, some of the measurements must contain systematic errors that are not yet fully assessed.

$G\left[10^{-11}\cdot\frac{\mathrm{m}^3}{\mathrm{kg}\cdot\mathrm{s}^2}\right]$	Uncertainty [ppm]	Source
6.6726	128	value recommended 1986 by CODATA (Committee on Data for Science and Technology of the International Council of Scientific Unions) [Cohen and Taylor (1987)]
6.6656	95	Measurements Standards Laboratory, Lower Hutt, New Zealand, 1994 [Fitzgerald *et al.* (1994)]
6.7154	83	Physikalisch-Technische Bundesanstalt, Braunschweig, Germany, 1994 [Michaelis *et al.* (1997)]

Table 1: Values and bounds for the relative error (in parts per million) for the Newtonian constant of gravitation.

One of the experiments for measuring G takes place at Wuppertal University. Its current goal is to achieve a relative precision of 10^{-4}, with hope for an additional factor of ten in the future. As explained above, attaining this accuracy requires a thorough assessment of all the systematic errors in the experiment.

In [Section 2] we briefly describe the principle of the experiment. The gravitational constant G is obtained by measuring a certain displacement Δb and equating it with a value that can be computed by numerical integration, as explained in [Section 3]. At the time being the attainable precision in G is limited mainly by tolerances in the geometry of the experiment and by their influence on the estimated value Δb, see [Section 4]. In [Section 5] we discuss interval versions of Gaussian quadrature that was used to bound the effects of some of these tolerances as well as the numerical errors inherent in the evaluation of the integrals. Finally, some numerical results are given in [Section 6].

2 The Experiment

The main components of the experiment used in Wuppertal are two heavy cylinders M_1 and M_2 (*field masses*) and a pair of pendulums whose bodies m_1 and m_2 are positioned midway between the field masses, see [Fig. 1]. All four bodies are aligned on a common axis of symmetry (horizontal line in [Fig. 1]), and the field masses can be moved along this axis.

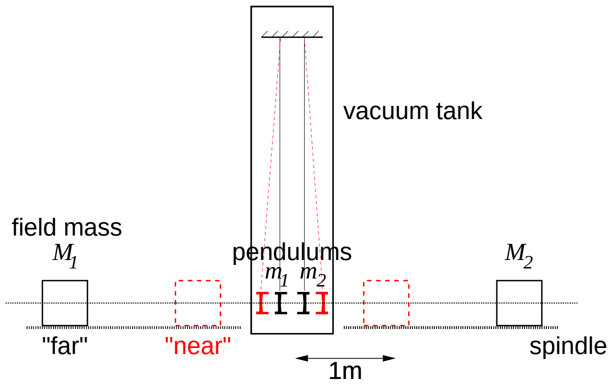

Figure 1: Principle of the experiment.

As the distance from m_1 to field mass M_1 is smaller than its distance to M_2, the first pendulum is slightly deflected from its resting position towards M_1. Analogously, m_2 is deflected towards M_2. When the field masses are moved from the "far" position to the "near" position, this effect becomes more pronounced, and the distance b between the pendulums again increases by a small amount $\Delta b \approx 12\text{nm}$.

To be able to measure Δb, the inner surfaces of the pendulums are spherical mirrors, which together work as a microwave resonator. By carefully monitoring its spectrum of resonance it is possible to determine Δb to a rather high relative precision $\varepsilon_{\Delta b} \lesssim 10^{-5}$. The sought constant of gravitation is then obtained by equating the measured value Δb with an estimate that can be computed as described in the following Section.

3 Estimating Δb

Let F_{ij} denote the (directed) attractive force on pendulum m_i due to field mass M_j. Thus a total force

$$F_i = F_{i1} + F_{i2}$$

acts on pendulum m_i, displacing it by

$$\Delta z_i = \frac{F_i^z}{m_i \omega_i^2}$$

along the z axis, which is the common axis of symmetry. Here, F_i^z denotes the z component of the force, and ω_i is the pendulum's natural frequency. Therefore, placing the field masses near to the pendulums increases their distance by the amount

$$\Delta b(\text{“near”}) = \Delta z_2 - \Delta z_1$$

as compared to having no field masses at all. In practice the field masses are moved from the "far" position to the "near" position, thus reducing the movement of the pendulums to

$$\Delta b = \Delta b(\text{“near”}) - \Delta b(\text{“far”}) \ .$$

From the above it follows that *eight* forces F_{ij} must be determined to compute Δb. Each of these eight values may be obtained as follows. Newton's law states that a point mass M at position p_M exerts the force

$$F_{mM} = G \cdot \frac{mM}{\|d\|^2} \cdot \frac{d}{\|d\|}$$

on a second point mass m at position p_m, where $d = p_M - p_m$ is the distance between the masses and G is the constant of gravitation. Integrating over the mass distributions of the pendulum and the field mass yields

$$F_{ij} = \int\limits_{\text{pendulum}_\text{i}} \int\limits_{\text{field mass}_\text{j}} G \cdot \frac{dm_i \, dM_j \cdot d}{\|d\|^3} \ .$$

To facilitate the integration we subdivide the pendulum into six segments S_{i_k} as shown in [Fig. 2] and, making use of the common axis of symmetry, introduce cylindrical coordinates for the segments and the field mass, see [Fig. 3]:

$$S_{i_k} = \{(r_i \cos\varphi_i, r_i \sin\varphi_i, z_i) \ : \ r_i \in [\underline{r}_{i_k}, \overline{r}_{i_k}], \varphi_i \in [0, 2\pi], z_i \in [\underline{z}_{i_k}, \overline{z}_{i_k}]\}$$
$$\text{field mass}_\text{j} = \{(r_j \cos\varphi_j, r_j \sin\varphi_j, z_j) \ : \ r_j \in [0, \overline{r}_j], \varphi_j \in [0, 2\pi], z_j \in [\underline{z}_j, \overline{z}_j]\}$$

Thus we have

$$F_{ij} = \sum_{k=1}^{6} F_{i_k j} \ ,$$

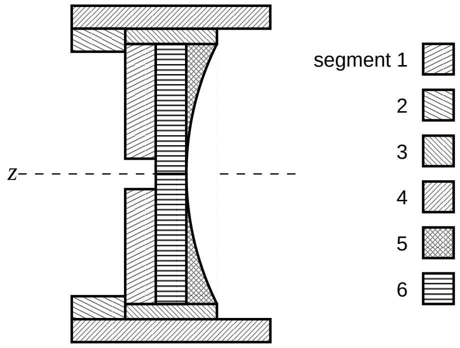

Figure 2: Decomposition of the pendulum's body into six segments.

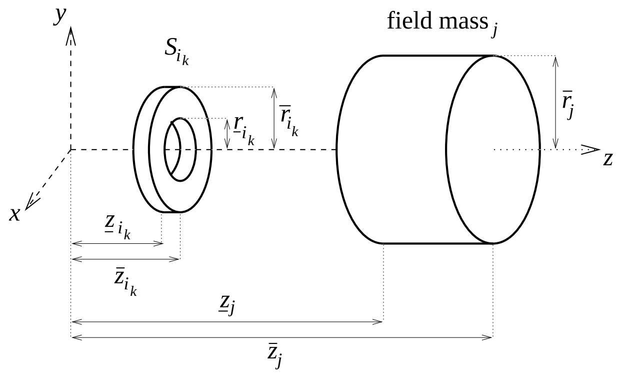

Figure 3: Coordinate system used in the integration.

where

$$F_{i_k j} = \int\limits_{S_{i_k}} \int\limits_{\text{field mass}_j} G \cdot \frac{\rho_i dV_i \cdot \rho_j dV_j \cdot d}{\|d\|^3}$$

$$= G\rho_i \int\limits_{\underline{r}_{i_k}}^{\overline{r}_{i_k}} r_i \int\limits_{0}^{2\pi} \int\limits_{\underline{z}_{i_k}}^{\overline{z}_{i_k}} \int\limits_{0}^{\overline{r}_j} \rho_j r_j \int\limits_{0}^{2\pi} \int\limits_{\underline{z}_j}^{\overline{z}_j} \frac{d}{\|d\|^3}\, dz_j\, d\varphi_j\, dr_j\, dz_i\, d\varphi_i\, dr_i \ .$$

Here we have assumed that the density ρ_i is constant within each pendulum and that the field masses have radial density profiles $\rho_j = \rho_j(r_j)$. These assumptions are justified by the respective production processes. (The field masses are made of cast and rolled brass, whereas the copper pendulums are diamond-cut after casting.)

If all the pendulums and field masses are perfectly aligned along the common axis of symmetry then three of the six integrals can be evaluated analytically, see [Holzmann *et al.* (1996)]. In this paper, however, we will only consider geometrical tolerances that destroy this symmetry and thus require numerical evaluation of the sextuple integrals.

4 Factors Limiting the Attainable Precision

As pointed out in the Introduction, the displacement Δb can be measured with a rather small relative error $\lesssim 10^{-5}$. Therefore the precision obtainable for G is presently limited by the error that is made in estimating Δb. This error consists of two components:

- approximation and rounding errors in evaluating the integrals, and
- tolerances in the geometry of the experiment (e.g., deviations from the perfect alignment on a common axis of symmetry). For example, the pendulums may be rotated or twisted or offset from the z axis, the field masses may be tilted, etc.

The tolerances are easily accounted for by suitable transformations of the local variables and/or the limits of the integrations. Combining these modifications with using a verified version of Gaussian quadrature gives guaranteed bounds for the overall effects of both types of errors.

5 Verified Gaussian Quadrature

In this Section we briefly describe some variants of Gaussian quadrature with result verification. These methods were used to enclose the multiple integrals from [Section 3]. We will only consider product formulas for Gauss-Legendre quadrature, i.e., for the evaluation of an integral

$$I := \int_Q f(x)\, dx$$

over the box $Q = [-1,1] \times \cdots \times [-1,1]$.

5.1 Enclosures for Multiple Integrals

For n-point Gaussian quadrature in one dimension we have [Stroud (1971)]

$$I = \int_{-1}^{1} f(x)\, dx = A^{(n)} + R^{(n)} \tag{1}$$

with the approximation

$$A^{(n)} = \sum_{i=1}^{n} \omega_i^{(n)} f(x_i^{(n)})$$

and the remainder term

$$R^{(n)} = e^{(n)} \cdot \frac{f^{(2n)}(\xi)}{(2n)!} \qquad \text{for some } \xi \in (-1,1)\ ,$$

provided that $f \in C^{2n}[a,b]$. (There are other representations of the remainder term; these will not be considered in the following.) The nodes $x_i^{(n)} \in (-1,1)$ and the positive weights $\omega_i^{(n)}$ can be determined by solving a suitable symmetric tridiagonal eigenvalue problem. For increasing n, the factor

$$e^{(n)} = \frac{2^{2n+1}}{2n+1} \cdot \binom{2n}{n}^{-2}$$

in the remainder term is rapidly decreasing.

From (1) we readily obtain an enclosure for the integral:

$$I \in [I] = [A^{(n)}] + [R^{(n)}] \ ,$$

where

$$[A^{(n)}] = \sum_{i=1}^{n} [\omega_i^{(n)}] \ f([x_i^{(n)}])$$

and

$$[R^{(n)}] = e^{(n)} \cdot \frac{f^{(2n)}([-1,1])}{(2n)!}$$

are enclosures of the approximation and the remainder term, resp. Very narrow intervals $[x_i^{(n)}]$ and $[\omega_i^{(n)}]$ enclosing the nodes and weights can be precomputed as described in [Storck (1993)]. An enclosure $f^{(2n)}([-1,1])/(2n)!$ for the range of the $2n$-th Taylor coefficient over the interval $[-1,1]$ is easily obtained using automatic differentiation techniques [Storck (1995)].

To evaluate multiple integrals of moderate dimension one usually employs an appropriate product of one-dimensional Gaussian quadrature formulas. In k dimensions, the $(n_1 \times \cdots \times n_k)$-point product formula is given by

$$A^{(n_1,\ldots,n_k)} = \sum_{i_1=1}^{n_1} \cdots \sum_{i_k=1}^{n_k} \omega_{i_1}^{(n_1)} \cdots \omega_{i_k}^{(n_k)} \ f(x_{i_1}^{(n_1)}, \ldots, x_{i_k}^{(n_k)}) \ ,$$

where the j-th components $x_i^{(n_j)}$ of the nodes and the factors $\omega_i^{(n_j)}$ are the nodes and weights, resp., of the n_j-point one-dimensional formula. Here we have

$$I = \int_{-1}^{1} \cdots \int_{-1}^{1} f(x_1, \ldots, x_k) \ dx_1 \cdots dx_k = A^{(n_1,\ldots,n_k)} + R^{(n_1,\ldots,n_k)}$$

with the remainder term fulfilling

$$|R^{(n_1,\ldots,n_k)}| \le 2^{k-1} \cdot \sum_{j=1}^{k} e^{(n_j)} \cdot \max_Q \left| \frac{1}{(2n_j)!} \cdot \frac{\partial^{2n_j} f}{\partial x_j^{2n_j}} \right| \ .$$

As in the one-dimensional case, an enclosure $[I]$ for the integral is obtained by substituting enclosing intervals for the nodes, weights and partial derivatives.

If the intervals $[x_i^{(n_j)}]$ and $[\omega_i^{(n_j)}]$ are very narrow and the total number of nodes is not too large then $[A^{(n_1,\cdots,n_k)}]$ is a narrow interval, too, and the diameter of $[I]$ is determined mainly by the diameter of the interval $[R^{(n_1,\cdots,n_k)}]$ enclosing the remainder term.

5.2 Static and Adaptive Subdivision

Unfortunately it is not always possible to reduce the diameter of the remainder interval to a given threshold by simply increasing the number of nodes in the formula, as might be hoped from the fact that the factors $e^{(n)}$ are rapidly decreasing. This approach may be impracticable either because the overall number of nodes becomes prohibitively large or because growth of the Taylor coefficients prevents the diameter of the remainder term from decreasing. One way to overcome these difficulties is to subdivide the domain of integration and then apply suitable product formulas to the subdomains.

We first tried a very simple static subdivision strategy named $\mathsf{Iso}(m,n)$ [Holzmann (1996)]. Here, the integration domain was subdivided into m subintervals along each axis, resulting in m^k subboxes of identical size. Then we applied the same $(n \times n \times \cdots \times n)$-point product formula to all the subboxes, see [Fig. 4]. This strategy proved successful for integrals of dimension up to four, cf. the results reported in [Holzmann *et al.* (1996)]. The enclosures computed with $\mathsf{Iso}(2,7)$ were sufficiently narrow to guarantee a relative error $\lesssim 10^{-6}$ in the estimate of Δb.

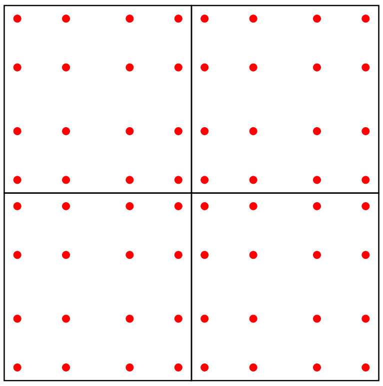

Figure 4: Subdomains and nodes for the two-dimensional static subdivision $\mathsf{Iso}(2,4)$.

For higher dimensions, the $\mathsf{Iso}(2,7)$ scheme became impracticable because it required an excessive number of function evaluations. (The estimated time for computing one Δb value via 48 sextuple integrations was 51 days!)

Therefore an adaptive subdivision strategy was developed. Here we first check if a single formula for the whole domain can give the desired accuracy. To this end, we choose $n_j \in \{1, \ldots, n_{\max}\}$, $j = 1, \ldots, k$, such that

$$d_j^{(n_j)} := e^{(n_j)} \cdot \max_Q \left| \frac{1}{(2n_j)!} \cdot \frac{\partial^{2n_j} f}{\partial x_j^{2n_j}} \right| \leq \frac{1}{k \cdot 2^{k-1}} \cdot \delta \ , \tag{2}$$

where $n_{\max}$ is a given upper bound for the number of points in each direction and δ is a prescribed bound for the radius of the remainder interval. In case of ambiguity the minimal value n_j fulfilling (2) is chosen. If at least one of the n_j values cannot be chosen according to (2) then the integration domain is bisected along the coordinate x_j featuring the largest "best case error" $d_j^{(\min)} = \min\{d_j^{(1)}, \ldots, d_j^{(n_{\max})}\}$, and the same procedure is applied to the two resulting subboxes, with the threshold replaced by $\delta' = \delta/2$.

Our first experiences with this adaptive technique were rather disappointing because it took even longer to achieve a prescribed precision than the static schemes had done. A closer look revealed that the integration domain was recursively subdivided until even a $(1 \times 1 \times \cdots \times 1)$-point formula was able to produce sufficiently narrow remainder intervals. In contrast to the static subdivision scheme, where virtually all the time was spent in function evaluations for computing the integral approximations, now the vast majority of the time was required for evaluating the Taylor coefficients.

The extremely fine subdivision of the integration domain was caused by a severe overestimation of the range of the Taylor coefficients. To overcome this problem we determined narrower enclosures for the Taylor coefficients by splitting their argument range. (Up to now this splitting is fixed a priori; we plan to develop an algorithm that is able to determine the necessary subdivisions adaptively.)

This modification led to a much lower recursion level and allowed using higher-order Gaussian formulas. As a result, our adaptive algorithm is well-balanced in the sense that the approximation of the integrals and the computation of the remainder terms each consume roughly one half of the overall time. With this technique the time for computing Δb via sextuple integrals could be reduced to below three days.

6 Numerical Results

The numerical experiments were performed on a Sun ULTRA workstation using Pascal-XSC [Klatte *et al.* (1992)]. Here we focus on the effects of two particular geometrical tolerances: offset of the pendulums from the z axis and rotation of the whole resonator around the y axis. Both deviations from the ideal coaxial geometry were handled by numerical evaluation of sextuple integrals (see [Holzmann *et al.* (1996)] for a discussion of other types of geometric errors that allow some of the six integrals to be solved analytically).

First we investigated how offsets τ of the pendulums from the z axis affect the estimated value of Δb (left picture in [Fig. 5]). The position of the pendulums is known to within 1mm. This precision is sufficient to guarantee that the relative errors due to the offsets are well below 10^{-5} (dashed horizontal lines in the picture).

The angular position of the resonator with respect to the y axis is known to within 0.1 degrees, which is again sufficient to guarantee that this kind of geometrical error cannot introduce a relative error $> 10^{-5}$ in Δb (right picture in [Fig. 5]).

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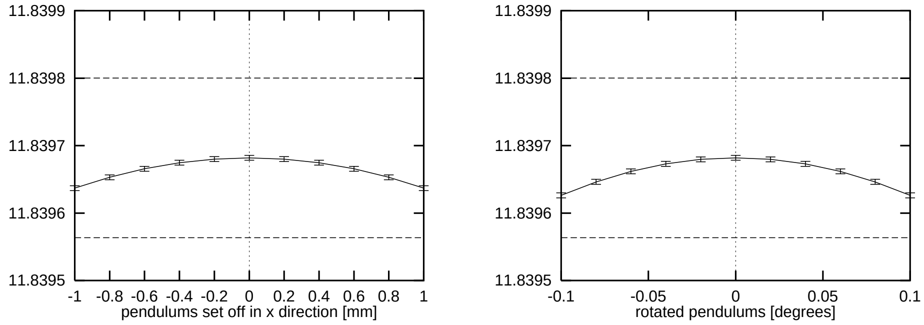

Figure 5: Influence of the tolerances on the estimate for Δb. The error bars show the resulting intervals for the eleven equidistant values that were considered for each tolerance τ. The line connecting the midpoints of the intervals *approximates* the (seemingly quadratic) functional dependence of Δb on τ.

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