Determination of optimized frequency and frequency ratio values from over-determined sets of clock comparison data

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Abstract. We summarize a recently developed method for analyzing over-determined sets of clock frequency comparison data to derive optimized values for the frequency ratios between each of the contributing standards. This least-squares adjustment procedure, based on the approach used by CODATA to derive a self-consistent set of values for the fundamental physical constants, is used to deduce optimized frequency and frequency ratio values from the international body of clock comparison data available in September 2015.

1. Introduction

The stability and accuracy of the most advanced optical atomic clocks now significantly surpass the performance of the best caesium primary frequency standards [1, 2] and a future redefinition of the SI second by the International Committee for Weights and Measures (CIPM) is anticipated [3, 4]. As a first step in this direction, seven optical clocks can already be used as secondary representations of the second, with recommended frequencies and uncertainties assigned by the Frequency Standards Working Group (WGFS) of the Consultative Committee for Time and Frequency (CCTF) and the Consultative Committee for Length (CCL). These recommended frequency values and uncertainties are periodically reviewed, updated and published on the website of the International Bureau of Weights and Measures (BIPM) [5].

Prior to 2015, almost all the data considered by the WGFS came from absolute frequency measurements made either relative to caesium fountain primary frequency standards or, if such standards were not available in the laboratory concerned, relative to International Atomic Time (TAI). The sole exception was a directly measured optical frequency ratio between the clock transitions in $^{27}Al^+$ and $^{199}Hg^+$ [6], which was used to derive a second absolute frequency value for $^{27}Al^+$ with much lower uncertainty than the directly measured absolute frequency value [7].

At the most recent meeting of the WGFS, held in September 2015, the situation was rather different (figure 1). Not only were a number of new absolute frequency measurements submitted for consideration, five new direct optical frequency ratio measurements were also reported. These included one measurement each of the ratios between the clock transitions in $^{40}Ca^+$ and ^{87}Sr [8], between the E2 and E3 transitions in $^{171}Yb^+$ [9] and between the clock transitions in ^{87}Sr and ^{199}Hg [10], and two independent measurements of the ratio between the clock transitions in ^{171}Yb and ^{87}Sr [11, 12, 13]. The complete body of data was thus over-determined, by which we mean that some frequency ratios can be deduced from the results of more than one experiment.

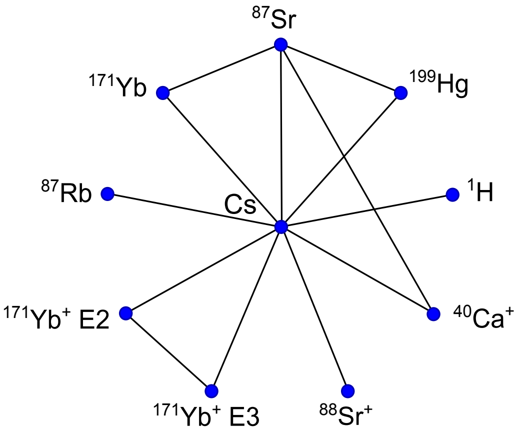

Figure 1. (*Colour online.*) New frequency ratio measurements considered by the WGFS in September 2015. Most were absolute frequency measurements, i.e. frequency ratios involving the caesium primary standard, but four optical frequency ratios had also been measured directly (in one case by two independent groups).

For example, the ratio between the E2 and E3 transitions in $^{171}Yb^{+}$ can be determined by combining the results of recent absolute frequency measurements of the two transitions made at NPL [9] and PTB [14, 15], but it has also been measured directly at NPL with comparable uncertainty [9]. These multiple routes to deriving this frequency ratio mean that it is no longer possible to treat the two clock transitions in isolation when considering the available data. The same is true of the ^{171}Yb, ^{87}Sr, ^{199}Hg and $^{40}Ca^{+}$ standards, which are similarly coupled by direct optical frequency ratio measurements.

2. Analysis procedure

We have recently developed a method for handling such over-determined sets of clock frequency comparison data in order to derive optimized values for the frequency ratios between each contributing standard [16]. This is a least-squares adjustment procedure (figure 2), based on the well-established approach used by CODATA to derive a self-consistent set of values for the fundamental physical constants [17].

The input data to the least-squares adjustment are a set of N frequency ratio measurements between clocks based on N_S different reference transitions with frequencies $\nu_1, \ldots \nu_{N_S}$, together with the variances and covariances of these frequency ratio measurements. All input data is treated in a similar way, with absolute frequency measurements simply being a special case of frequency ratios involving the caesium primary standard. The measured frequency ratios are expressed as a function of one or more of a set of $M = N_S - 1$ adjusted frequency ratios z_j, yielding a set of N equations that are, in general, nonlinear. A necessary condition is that no adjusted frequency ratio may be expressed as a function of the others. We choose the set $z_j = \nu_j/\nu_{j+1}$ where $j = 1, \ldots N_S - 1$, and it is the values of these adjusted frequency ratios that are optimized in the least-squares adjustment.

The equations relating the measured frequency ratios to the adjusted frequency ratios are linearized prior to the least-squares adjustment by using a Taylor expansion around initial estimates of the adjusted frequency ratios. This enables linear matrix methods to be applied to yield best estimates for the values of the adjusted frequency ratios, their variances and covariances. Because a linear approximation has been made, this solution will not be exact. However the improved values of the adjusted frequency ratios obtained from the least-squares adjustment can be used as starting values for a new linear approximation and a second least-squares adjustment performed. This process is repeated until the new values of the adjusted frequency ratios obtained from the least-squares adjustment are sufficiently close to the values obtained in the previous iteration. Once this condition has been satisfied, any other frequency ratio of interest (and its uncertainty) can then be calculated from the adjusted frequency ratios and their covariance matrix. Self-consistency checks are also performed on the body of data to

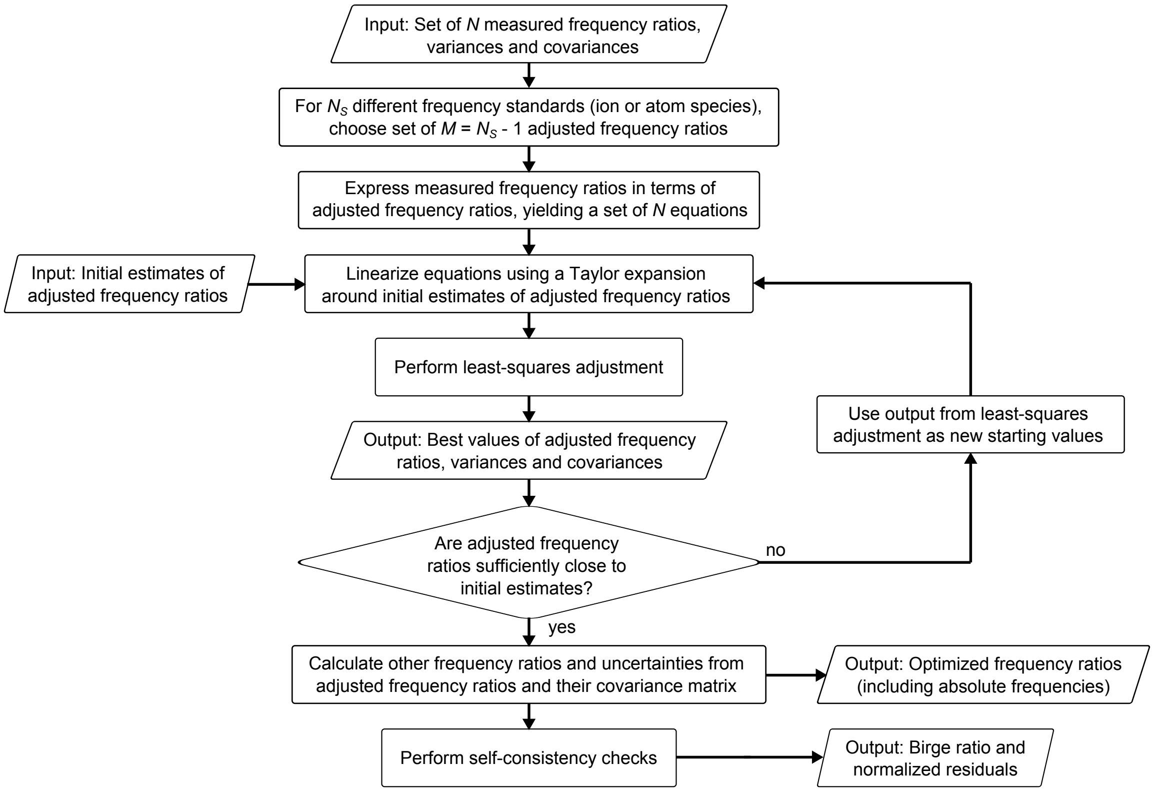

Figure 2. Least-squares analysis procedure used to derive a self-consistent set of optimized frequency and frequency ratio values from an over-determined set of clock comparison data [16].

identify any issues with the uncertainty evaluations for each individual clock comparison.

Our software algorithms, implemented in Matlab, have been shown to reproduce the 2013 CIPM recommended frequency values, when using the same input data employed by the WGFS to derive those values [16]. The uncertainties determined from our least-squares analysis, however, are smaller than those assigned to the CIPM values. The reason for this is that measurements of a particular frequency ratio have usually only been made by a few independent research groups, or in some cases only one. This leads the WGFS to take a conservative approach to uncertainty estimation, typically multiplying the relative standard uncertainty on the weighted mean of a set of frequency values by a factor of two or three.

3. Analysis of data available in September 2015

A number of new frequency comparison results were reported to the WGFS in advance of their September 2015 meeting (figure 1). As well as the five direct optical frequency ratio measurements already discussed, these included 16 new absolute frequency measurements: one each of the 1S–2S transition in ^{1}H [18], the optical clock transitions in ^{171}Yb [19] and ^{88}Sr^{+} [20] and the ground state hyperfine transition in ^{87}Rb [21], two each of the E2 [9, 14] and E3 [9, 15] transitions in ^{171}Yb^{+} and the reference transition in ^{40}Ca^{+} [22], and six of the optical clock transition in ^{87}Sr [23, 24, 25, 26, 27, 28]. In addition, a correction [29] was submitted to a previously-used absolute frquency measurement of the optical clock transition in ^{199}Hg [30] and one earlier absolute frequency measurement of the reference transition in ^{40}Ca^{+} [31] was withdrawn as new data from the same group suggested that the systematic frequency shifts may have been underestimated in this measurement [22].

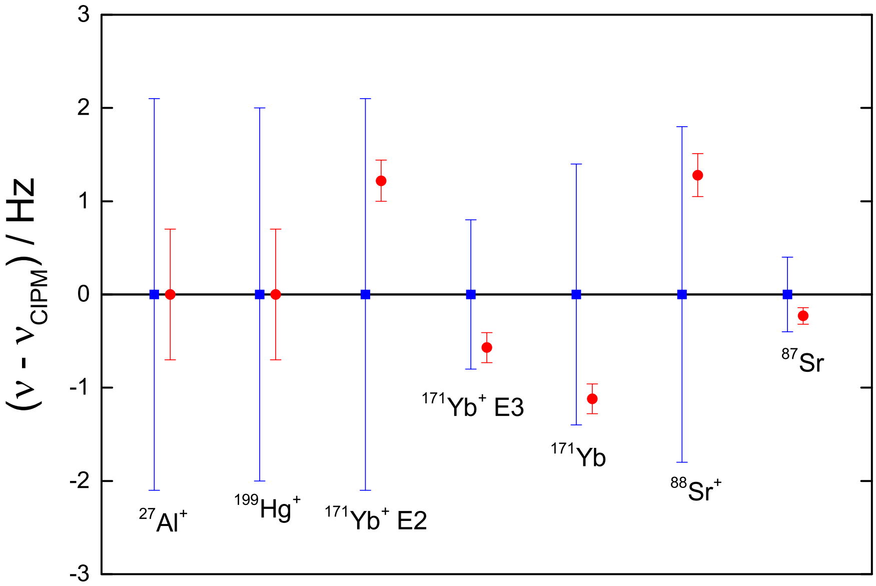

Figure 3. (*Colour online.*) Optimized frequency values obtained for the seven optical secondary representations of the second using all clock comparison data available in September 2015 (red circles) compared to the 2013 CIPM recommended frequency values and uncertainties (blue squares). The uncertainties shown for the new results are those emerging from the least-squares adjustment, not the final uncertainty assigned by the WGFS.

The effects on the optimized frequency values obtained for the optical secondary representations of the second of including this new data in the least-squares analysis are shown in figure 3. Here correlations between the input data are ignored, with the exception of the recent measurements involving the $^{171}Yb^+$ standards at NPL [9]. In this case the absolute frequency measurements of the E2 and E3 transitions were performed during the same campaign as the measurement of the direct optical frequency ratio between them, leading to non-negligible correlations between the three values. For example, part of the data from the caesium fountain primary frequency standard is common to the two absolute frequency measurements, leading to correlations from both the statistical fluctuations of the caesium standard and its systematic uncertainty. Similarly, correlations between the E3:E2 ratio measurement and the E2 absolute frequency measurement arise from the statistical and systematic uncertainties associated with the E2 clock transition. The correlation coefficients were thus calculated based on the periods of overlap between the three measurements and the estimated statistical and systematic uncertainties of the three standards ($^{171}Yb^+$ E2, $^{171}Yb^+$ E3 and Cs fountain).

It is clear from figure 3 that including the new data in the least-squares analysis leads to significant shifts in the optimized frequency values, demonstrating that the conservative approach to uncertainty estimation employed by the WGFS may indeed be a wise one. We emphasize that the uncertainties of the new optimized frequency values shown in figure 3 are the uncertainties determined from the least-squares adjustment, rather than the uncertainties finally assigned by the WGFS. Indeed, much of the discussion during the recent WGFS meeting centred around the magnitude of these uncertainties and whether (and if so, by how much) they should be expanded. For example, the least-squares adjustment yields an uncertainty of

2×10^{-16} for the frequency of the $5s^2\,{}^1S_0$–$5s5p\,{}^3P_0$ transition in ^{87}Sr, which is lower than the uncertainties of the caesium primary frequency standards used as the references for the best absolute frequency measurements of this transition. Since no secondary representation of the second can have a frequency uncertainty lower than that of the best primary frequency standards, the WGFS expanded this uncertainty in updating the list of recommended frequency values. In other cases such as the $^{171}Yb^+$, $^{88}Sr^+$ and ^{199}Hg standards, the optimized frequency values were based on input data from only one or two research groups, and so the WGFS again considered it prudent to expand the uncertainty emerging from the least-squares adjustment.

4. Conclusions and future perspectives

Our analysis procedure allows a self-consistent set of optimized frequency ratio values between high accuracy frequency standards (both optical and microwave) to be derived, based on data from a set of clock comparison experiments, and taking proper account of any correlations among the data. Although the matrix of frequency comparison data available worldwide is currently quite sparsely populated, it is already over-determined. As a consequence the WGFS used our software algorithms in preparing an updated list of recommended frequency values in September 2015, enabling full benefit to be derived from the experimental data available at the time.

The methods developed will become increasingly important as the number of direct optical frequency ratio measurements increases, and will enable valuable information to be derived about the relative performance of different candidates for an optical redefinition of the second. They can also be used to determine optimized values and uncertainties for the absolute frequencies of each optical standard relative to the current definition of the second, maximizing the potential contribution of optical clocks to international timescales prior to a redefinition.

However, in future it is likely that correlations between the input data will become more significant, as increasing numbers of high accuracy clocks are compared in measurement campaigns involving multiple institutions. For example, within the EMRP-funded ITOC project [32] a collection of optical and caesium fountain clocks were simultaneously operated at INRIM, LNE-SYRTE, NPL and PTB for a direct remote comparison via satellite links over a 26-day period. Several local optical frequency ratio measurements were also performed during this campaign. Potentially quite significant correlations can therefore be expected between some of the frequency ratio values resulting from this campaign, even though none of the clocks operated with 100% duty cycle. We therefore expect that it will be increasingly important for the WGFS to gather information about the correlations between the input data to future least-squares adjustments, to avoid biassing the optimized frequency values and underestimating their uncertainties. Such information is not usually readily extracted from publications and so will have to be sought from the research groups that performed the measurements. In addition to this requirement to calculate the correlation coefficients for the input data, it will also be necessary to study in detail the extent to which each input datum contributes to the determination of the optimized frequency ratios as well as to look at the effects of omitting inconsistent or inconsequential data from the least-squares adjustment. The task facing the WGFS is thus likely to increase in complexity over the next few years as the worldwide body of high accuracy clock comparison data continues to grow.

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