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Robust Optical Clocks for International Timescales

Guidelines on the evaluation and reporting of correlation coefficients between frequency ratio measurements, including a recommended reporting template and worked examples

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Guidelines on the evaluation and reporting of correlation coefficients between frequency ratio measurements

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Abstract

The recommended frequency values and uncertainties of secondary representations of the second are derived from the worldwide body of clock frequency comparison data, including both absolute frequency measurements and direct frequency ratio measurements that do not involve a caesium primary standard. To ensure that the recommended frequency values are unbiassed, and their uncertainties are properly estimated, account must be taken of any correlations between the measurements. We discuss ways in which such correlations may arise, and describe how they can be quantified. Worked examples are presented based on measurement data available in the published literature. These include several examples of very significant correlations which were neglected in the last update to the list of CIPM recommended frequency values in 2017. We therefore present some suggestions on how the necessary information about correlations might be gathered from the groups performing such measurements, to enable future updates to the list to be underpinned by a more robust analysis of the available data.

1 Introduction

It has long been realised that clocks based on optical transition frequencies in laser-cooled trapped ions or atoms offer the prospect of superseding the current generation of caesium microwave primary frequency standards. Indeed, in terms of both fractional frequency instability [1, 2] and estimated systematic frequency uncertainty [3–5], the optical clocks have already demonstrated superior performance, although in most cases their robustness and reliability currently lag behind that of the microwave standards. A future redefinition of the second in terms of an optical transition frequency is thus widely anticipated [6–8], once certain key milestones have been met [9].

As an intermediate step towards a redefinition, the International Committee for Weights and Measures (CIPM) introduced the concept of secondary representations of the second. These are frequency standards that can be used to realise the second, albeit with uncertainty no better than that of the best caesium primary standards. So far, nine frequency standards have been adopted as secondary representations of the second – eight based on optical transitions, and one based on a microwave transition. Recommended frequency values and uncertainties for these secondary representations of the second are assigned by the Frequency Standards Working Group (WGFS) of the Consultative Committee for Time and Frequency (CCTF) and the Consultative Committee for Length (CCL), with periodic updates being published as part of the CIPM list of recommended frequency values on the website of the International Bureau of Weights and Measures (BIPM) [10].

The WGFS derives these recommended frequency values from the results of high accuracy clock comparison experiments performed in laboratories around the world. Clock comparison experiments essentially determine the frequency ratios between pairs of standards, with the result of an absolute frequency measurement relative to a caesium primary frequency standard being a special case of such a frequency ratio. For a collection of frequency standards based on N_S different reference transitions with frequencies ν_k (k=1,2,..., N_S), a total of $N_S(N_S-1)/2$ different frequency ratios can be measured. This means that analysis procedures capable of handling over-determined datasets are required to derive optimised frequency ratio values and uncertainties. Two alternative approaches to this data analysis have been developed. The first is a least-squares adjustment procedure [11] similar to the one used by CODATA to derive a self-consistent set of values for the fundamental physical constants [12]. This approach was first used to update the list of recommended frequency values in September 2015 [13]. The second approach is based on an analysis of closed loops in a graph theory representation of the data [14]. During the June 2017 update to the list both methods were demonstrated to yield the same results at the relevant level of accuracy. The discussion in this document is framed in terms of the least-squares analysis procedure, but similar ideas apply to the alternative graph theory approach.

A set of frequency comparison experiments results in a set of N measured frequency ratio values q_i. In deriving optimised values of the frequency ratios between the N_S different reference transitions, it is important to know not only the standard uncertainties u_i or variances u_i^2 of these measured frequency ratios, but also the covariances $u_{ij} = u_{ji}$ which account for correlations between the different measurements. Failure to identify or to properly account for such correlations will in general lead to biased frequency values and incorrectly estimated uncertainties [11, 13]. Typically these uncertainties will be underestimated. For example, if four absolute frequency measurements of a particular optical clock were performed against the same Cs fountain primary frequency standard, then if correlations due to the systematic uncertainty of the fountain were neglected, the uncertainty of the frequency would be underestimated as $u/\sqrt{4} = u/2$ due to (incorrect) averaging of the systematic uncertainty in addition to the statistical uncertainty. In some circumstances, however, neglecting correlations may lead to uncertainties being overestimated [15]. For example, if two frequency ratios f_A/f_B and f_B/f_C between clocks A, B and C are measured then accounting for correlations due to the systematic uncertainty of clock B reduces the uncertainty of the ratio f_A/f_C.

The challenge faced by the WGFS is that most publications describing the results of frequency comparison experiments contain insufficient information for the correlation coefficients to be extracted. For this reason, very few correlation coefficients have so far been included in the least-squares analyses performed by the WGFS. However this neglect of correlations will become increasingly problematic as more and more optical clocks are compared in large-scale measurement campaigns involving multiple institutions [16, 17].

In this document we provide some examples of how correlations between frequency comparison measurements may arise and describe how these correlations can be quantified. The mathematical formalism for describing correlations is outlined in section 2, after which we consider in turn correlations arising from systematic corrections (section 3), correlations arising from common data (section 4) and correlations arising from data aggregation (section 5). We conclude in section 6 with some recommendations for how information about correlations might be reported to the WGFS, for use in future updates to the CIPM list of recommended frequency values.

2 Formalism

We consider a set of N measured frequency ratios q_i, each of which can be expressed as a function of a set of input quantities x_i:

$$q_i = f_i(x_1, x_2, \ldots, x_m) \tag{1}$$

or, in matrix notation,

$$\vec{Q} = \vec{f}(\vec{X}) \tag{2}$$

where $\vec{Q}$ is a column matrix with N elements, $\vec{f}$ is a rectangular matrix with N rows and m columns, and $\vec{X}$ is a column matrix with m elements. In general, any particular function $f_i(\vec{X})$ will depend on only a subset of the elements x_j of $\vec{X}$.

Correlations between individual frequency ratio measurements arise when they depend on common input quantities, and are quantified using the $N \times N$ *covariance matrix*

$$\vec{U}_q = \begin{bmatrix} u(q_1,q_1) & \dots & u(q_1,q_N) \\ \vdots & \ddots & \vdots \\ u(q_N,q_1) & \dots & u(q_N,q_N) \end{bmatrix}, \tag{3}$$

where $\mathrm{cov}(q_i,q_i) = u(q_i,q_i) = u^2(q_i)$ and $\mathrm{cov}(q_i,q_j) = u(q_i,q_j) = u(q_j,q_i)$. Following the "Guide to the expression of uncertainty in measurement" (GUM) [18, 19], this covariance matrix is computed using the formula

$$\vec{U}_q = \vec{C}_x \vec{U}_x \vec{C}_x^{\,T} \tag{4}$$

where $\vec{C}_x$ is the $N \times m$ matrix

$$\vec{C}_x = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \dots & \frac{\partial f_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \dots & \frac{\partial f_N}{\partial x_m} \end{bmatrix}, \tag{5}$$

and $\vec{U}_x$ is the diagonal $m \times m$ matrix

$$\vec{U}_x = \begin{bmatrix} u^2(x_1) & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & u^2(x_m) \end{bmatrix}. \tag{6}$$

The degree of correlation between q_i and q_j is characterised by the *correlation coefficient*

$$r(q_i,q_j) = r(q_j,q_i) = \frac{u(q_i,q_j)}{u(q_i)u(q_j)}, \tag{7}$$

where $-1 \leq r(q_i,q_j) \leq +1$. If q_i and q_j are uncorrelated, then $r(q_i,q_j) = 0$. The $N \times N$ matrix $\vec{R}_q$ of correlation coefficients is termed the *correlation matrix*:

$$\vec{R}_q = \begin{bmatrix} 1 & \dots & r(q_1,q_N) \\ \vdots & \ddots & \vdots \\ r(q_N,q_1) & \dots & 1 \end{bmatrix}. \tag{8}$$

Example

Consider the simple case of two frequency ratio measurements q_1 and q_2 that depend on three independent input quantities x_1, x_2 and x_2 as follows:

$$q_1 = x_1 + x_2, \quad q_2 = x_1 + x_3. \tag{9}$$

Applying equations (4)–(6), we find that the covariance matrix for this pair of frequency ratio measurements is

$$\vec{U}_q = \begin{bmatrix} u^2(x_1) + u^2(x_2) & u^2(x_1) \\ u^2(x_1) & u^2(x_1) + u^2(x_3) \end{bmatrix}, \tag{10}$$

and the correlation coefficient between measurements q_1 and q_2 is

$$r(q_1,q_2) = \frac{u^2(x_1)}{\{u^2(x_1)+u^2(x_2)\}^{1/2}\{u^2(x_1)+u^2(x_3)\}^{1/2}}. \tag{11}$$

3 Correlations from systematic corrections

There are several different ways in which correlations can arise from systematic effects. Such correlations can be grouped into three categories:

1. Correlations between clocks based on the same atomic transition;
2. Correlations between different measurements involving the same clock;
3. Correlations between different clocks in the same laboratory.

In cases 1 and 3, the correlation coefficients are relatively straightforward to calculate, because the necessary information is usually given in the publications reporting the measurement results. In contrast, this is often not the case for category 2, and in such cases interaction with the scientists who performed the measurement is likely to be required before the correlation coefficients can be determined. The three cases are considered in turn in sections 3.1–3.3.

3.1 Correlations between clocks based on the same atomic transition

The first scenario we consider is where correlations may arise between measurements involving any clocks that are based on the same atomic transition. Such correlations would arise, for example, if two groups used the same theoretical or experimental values of coefficients necessary to correct for certain systematic frequency shifts such as the Zeeman shift or Stark shifts. This is usually a fairly straightforward type of situation to consider, because the information required to calculate the relevant correlation coefficients is usually provided in the publications describing the results of these measurements.

Example 3.1a: Early absolute frequency measurements of Sr lattice clocks

Early measurements of optical clocks made use of blackbody radiation coefficients calculated theoretically. Given the high uncertainty of these coefficients, they dominated the blackbody radiation shift uncertainty and correlate measurements made by different groups. For example the absolute frequency measurements of the Sr clocks in Refs. [20–24] used a theoretical blackbody radiation coefficient [25] that introduced an uncertainty of 8×10^{-17} for each measurement. The resulting correlation matrix between the five absolute frequency measurements can be calculated using the formalism of section 2 as

$$\vec{R}_q = \begin{bmatrix} 1 & 0.003 & 0.001 & 0.002 & 0.001 \\ 0.003 & 1 & 0.003 & 0.006 & 0.002 \\ 0.001 & 0.003 & 1 & 0.002 & 0.001 \\ 0.002 & 0.006 & 0.002 & 1 & 0.002 \\ 0.001 & 0.002 & 0.001 & 0.002 & 1 \end{bmatrix}. \tag{12}$$

In this case correlations are low (<1 %), because of the large total uncertainty of each measurement (1×10^{-15}). However the example serves to illustrate the point that correlations may exist between measurements performed in different laboratories at different times.

Example 3.1b: Yb^+ measurements at NPL and PTB

In a measurement campaign performed at NPL [26], during which the frequency ratio between the E3 and E2 optical clock transitions in $^{171}Yb^+$ was measured as well as the absolute frequencies of the two transitions, the blackbody radiation shifts were calculated using experimental values for the differential polarizabilities of the atomic states for each transition determined at PTB [27, 28]. Since the blackbody shift uncertainties are dominated by the uncertainty in the polarizability coefficients, leading to an uncertainty of 1×10^{-16} for the E2 transition and 4.5×10^{-17} for the E3 transition, this means that the NPL measurements are correlated with the absolute frequency measurements of the two transitions performed at PTB [27, 29].

For the E3 optical clock transition the common uncertainty in the BBR shift is 4.5×10^{-17}. The resulting correlation coefficient between the absolute frequency measurements of this transition performed at PTB [27] and NPL [26], which have uncertainties of 8.1×10^{-16} and 5.8×10^{-16} respectively, is therefore 0.004. The correlation coefficient between PTB's E3 absolute frequency measurement and NPL's frequency ratio measurement between the two optical clock transitions is slightly more significant at 0.007. This is due to the slightly lower uncertainty of the optical frequency ratio measurement (3.4×10^{-16}).

Correlations between the measurements involving the E2 transition are larger, due to the larger common uncertainty of 1×10^{-16}. The correlation coefficient between the absolute frequency measurements of the E2 transition performed at PTB [29] and NPL [26], which have uncertainties of 5.2×10^{-16} and 6.1×10^{-16} respectively, is 0.03. Again, the correlation coefficient between PTB's absolute frequency measurement of the E2 transition [29] and NPL's optical frequency ratio measurement between the E3 and E2 transitions is larger at 0.06.

3.2 Correlations between different measurements involving the same clock

The second scenario we consider is that of correlations between measurements involving the same clock, performed at different times. This is more complex than the first case considered because the correlations depend on the physics package and experimental procedures, and the information necessary to calculate the correlation coefficients does not always appear in the publications reporting the measurements. Quantification of the correlations is therefore likely to require the involvement of the scientists who performed the measurements.

Example 3.2a: Blackbody radiation shift in optical lattice clocks

In general the systematic frequency shifts for a given clock are correlated in time. For example, the blackbody radiation shift in several optical lattice clocks has been evaluated by assuming a rectangular temperature probability distribution between limits set by the hottest and the coldest spots on the vacuum chamber surrounding the atoms [23, 30, 31]. For a specific physics package geometry, this uncertainty is systematic and probably dominates over statistical contributions such as those from sensor readings. The total blackbody radiation shift (coefficient plus temperature) should therefore be considered correlated in time, unless changes to the physics package of the experiment are made (e.g., as noted in [30]).

For example, two absolute frequency measurements involving the INRIM Yb optical lattice clock have been reported [31, 32]. The physics package of the experiment was the same for both measurements and the temperature evaluation followed a similar strategy in both cases. This means that the blackbody radiation shift for the two measurements is totally correlated, contributing uncertainties of 2.5×10^{-17} and 1.2×10^{-17}. Since the total uncertainty of the two measurements is 5.9×10^{-16} and 2.6×10^{-16} respectively, and there are no other significant sources of correlation (other systematic shifts were calculated differently and the two measurements involved different Cs fountain primary frequency standards), the correlation coefficient between these two measurements is 0.002.

Example 3.2b: Correlations arising from Cs fountain primary frequency standards

Correlations between measurements performed at different points in time may also arise from the Cs fountain primary frequency standard used as a local reference. In the algorithm used to compute International Atomic Time (TAI) the systematic frequency uncertainty of a particular Cs fountain is considered to be correlated in time, unless a complete re-evaluation of the standard has taken place [33]. If we take the same approach, then we can calculate the correlation between different absolute frequency measurements performed at different times but involving the same Cs fountain.

As an example, we consider absolute frequency measurements of the ^{87}Sr optical lattice clock performed at LNE-SYRTE during the periods October 2010 to July 2011 [34] and October 2014 to June 2015 [35], with respect to their ensemble of Cs fountains. Both measurements were dominated by the comparison with the best fountain SYRTE-FO2, which introduced systematic uncertainties of 2.6×10^{-16} and 2.4×10^{-16} The total uncertainties of the two measurements made with respect to SYRTE-FO2 were 3.6×10^{-16} and 2.8×10^{-16}, and hence we estimate a correlation coefficient of 0.72 from the SYRTE-FO2 systematics. It should, however, be noted that the results reported in the two papers were averages of measurements performed with respect to the different fountains at LNE-SYRTE. A more accurate estimation of the correlation coefficient for the two ensemble results is 0.54.

3.3 Correlations between clocks in the same laboratory

Correlations associated with systematic corrections may also arise between measurements involving clocks that are based on different atomic transitions, but that are located within the same institution. Most obviously, we have the case of the gravitational redshift correction to a remote clock comparison.

To take a specific example, we consider the (hypothetical) example of two optical frequency ratio measurements, the first between the Yb^+ optical clock at NPL and the Yb optical lattice clock at INRIM, and the second between the Sr optical lattice clock at NPL and the Hg optical lattice clock at LNE-SYRTE. These two measurements would be correlated because the gravitational redshift correction applied to the two optical clocks at NPL is almost perfectly correlated. As a result of a dedicated campaign to improve our knowledge of the gravity potential at clock sites around Europe, the uncertainty in their gravitational redshift corrections has been reduced to 2.4×10^{-18} [17, 36]. If the two optical frequency ratios were each to be determined with a total uncertainty of 1×10^{-17}, the correlation coefficient between them would therefore be 0.058, and as the measurement uncertainty reduces further the correlation will increase.

This source of correlation is straightforward to calculate because the necessary information is generally provided in the papers describing the measurements.

4 Correlations from common data

Significant correlations can arise if a particular clock is used to determine more than one frequency ratio at the same time. Consider a measurement campaign involving three clocks: a Cs fountain primary standard (frequency ν_{C}), an optical lattice clock (frequency ν_{L}) and a trapped ion optical clock (frequency ν_{I}). Three frequency ratio measurements can be computed:

$$q_1 = \frac{\nu_{\mathrm{L}}}{\nu_{\mathrm{C}}}, \quad q_2 = \frac{\nu_{\mathrm{I}}}{\nu_{\mathrm{C}}} \quad \text{and} \quad \mathrm{q}_3 = \frac{\nu_{\mathrm{I}}}{\nu_{\mathrm{L}}}. \tag{13}$$

The three measurements are correlated by both the systematic and the statistical uncertainties of the clocks.

Following the formalism of section 2, it can be shown that the systematic uncertainties of the three clocks contribute to the covaraiance matrix of the three frequency ratio measurements as follows:

$$\vec{U}_q = \begin{bmatrix} u_{\mathrm{C}}^2 + u_{\mathrm{L}}^2 & u_{\mathrm{C}}^2 & -u_{\mathrm{L}}^2 \\ u_{\mathrm{C}}^2 & u_{\mathrm{C}}^2 + u_{\mathrm{I}}^2 & u_{\mathrm{I}}^2 \\ -u_{\mathrm{L}}^2 & u_{\mathrm{I}}^2 & u_{\mathrm{I}}^2 + u_{\mathrm{L}}^2 \end{bmatrix}, \tag{14}$$

Clock	u	$\sigma(\tau = 1\,\mathrm{s})$
Cs Fountain	1×10^{-16}	1×10^{-14}
Lattice	1×10^{-17}	1×10^{-16}
Ion	1×10^{-18}	1×10^{-15}

Table 1. Clock uncertainties assumed for the hypothetical measurement campaign of section 4.1. The clock instabilities are assumed to scale as $\tau^{-1/2}$, where τ is the averaging time.

where u_C, u_L and u_I are the systematic uncertainties of the Cs fountain, the lattice clock, the ion clock respectively. All uncertainties and covariances are expressed here in fractional terms. (Note that if q_3 is taken as $\nu_\mathrm{L}/\nu_\mathrm{I}$ rather than $\nu_\mathrm{I}/\nu_\mathrm{L}$, then the sign of some of the off-diagonal components of the matrix changes.)

4.1 Measurement campaigns without dead time

We start by assuming that all three clocks operate continuously for the entire duration of the measurement campaign. In this case the instability of the three clocks contributes a similar matrix:

$$\vec{S}_q = \begin{bmatrix} \sigma_\mathrm{C}^2(\tau) + \sigma_\mathrm{L}^2(\tau) & \sigma_\mathrm{C}^2(\tau) & -\sigma_\mathrm{L}^2(\tau) \\ \sigma_\mathrm{C}^2(\tau) & \sigma_\mathrm{C}^2(\tau) + \sigma_\mathrm{I}^2(\tau) & \sigma_\mathrm{I}^2(\tau) \\ -\sigma_\mathrm{L}^2(\tau) & \sigma_\mathrm{I}^2(\tau) & \sigma_\mathrm{I}^2(\tau) + \sigma_\mathrm{L}^2(\tau) \end{bmatrix}, \tag{15}$$

where σ_C, σ_L and σ_I are the fractional instabilities of the Cs fountain, the lattice clock and the ion clock respectively and τ is the averaging time. Note that, the instabilities $\sigma_C(\tau)$, $\sigma_L(\tau)$ and $\sigma_I(\tau)$ are not usually available directly, as experimentally only the combined uncertainties of the comparisons can be measured. However, the individual instabilities can often be deduced by other means.

The covariance matrix for the three frequency ratio measurements is the sum of the matrices given by equations 14 and 15:

$$\vec{C}_q = \vec{U}_q + \vec{S}_q. \tag{16}$$

With the assumed uncertainties listed in table 1, for an averaging time of $\tau = 2 \times 10^4$ s, we can use the above equations to calculate the correlation matrix for this campaign:

$$\vec{R}_q = \begin{bmatrix} 1 & 0.995 & -0.066 \\ 0.995 & 1 & 0.034 \\ -0.066 & 0.034 & 1 \end{bmatrix}. \tag{17}$$

As expected, the two absolute frequency measurements q_1 and q_2 are seen to be strongly correlated, because their uncertainty is dominated by the uncertainty of the Cs fountain.

Example 4.1a: Absolute frequency measurements at PTB

As a specific example of two published absolute frequency values that are highly correlated, we consider two absolute frequency measurements performed at PTB: a measurement of the E3 optical clock transition in $^{171}\mathrm{Yb}^+$ [37] and a measurement of the optical clock transition in $^{87}\mathrm{Sr}$ [30]. Although the period during which the $^{171}\mathrm{Yb}^+$ measurement was made is not specified in reference [37], it is clear from the details presented in reference [30] that both measurements were performed during the same period and thus use the same data from the PTB Cs fountains CSF1 and CSF2. From the figures presented, we see that the uncertainty arising from the Cs fountains (3.88×10^{-16} statistical and systematic combined) completely dominates over the systematic uncertainty of either optical clock (5.0×10^{-17} for $^{171}\mathrm{Yb}^+$ and 5.2×10^{-17} for $^{87}\mathrm{Sr}$). From these figures we calculate the correlation coefficient between the two absolute frequency measurements to be 0.981.

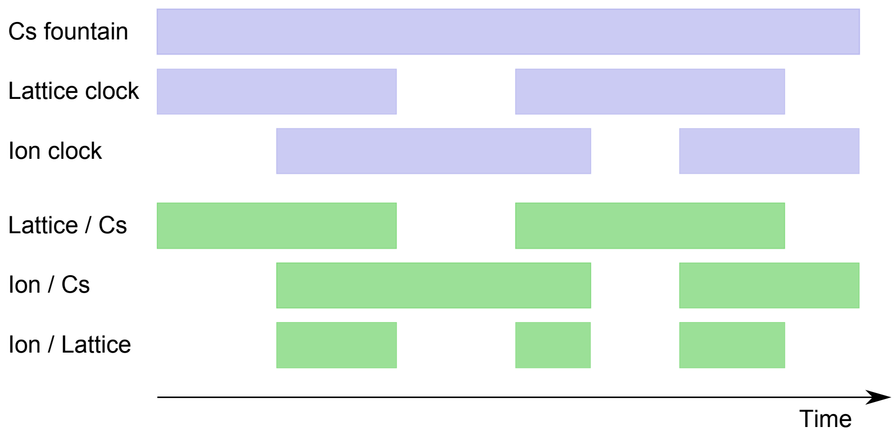

Figure 1. Hypothetical measurement campaign discussed in section 4.2 involving three different clocks which operate for different periods of time. The top half of the figure shows the periods during which each clock operates, while the lower half shows which frequency ratios can be deduced from the data collected at any particular time.

4.2 Measurement campaigns including dead time

We now consider the case of a measurement campaign in which the Cs fountain, optical lattice clock and trapped ion optical clock operate for different periods, but with substantial periods of overlap, as indicated in figure 1. The three different frequency ratios $q_1 = \nu_\mathrm{L}/\nu_\mathrm{C}$, $q_2 = \nu_\mathrm{I}/\nu_\mathrm{C}$ and $q_3 = \nu_\mathrm{I}/\nu_\mathrm{L}$ can thus be deduced from the data collected during different parts of the measurement campaign, and the three correlation coefficients between these different frequency ratio measurements are non-zero.

For simplicity we consider the case where each ratio is determined using only data where both clocks involved are operating, i.e. there is no extrapolation over periods of dead time. We assume that the caesium fountain operates for the whole campaign, without any dead time, while the lattice clock and trapped ion clock operate for total periods T_L and T_I respectively, with a period of overlap T_overlap. If all other sources of uncertainty are negligible compared to the statistical uncertainty of the caesium fountain (calculated assuming white frequency noise), then the three correlation coefficients can be calculated using the following formulae:

$$r(q_1,q_2) = \sqrt{\frac{T^2_\mathrm{overlap}}{T_\mathrm{L}T_\mathrm{I}}}, \quad r(q_1,q_3) = \sqrt{\frac{T_\mathrm{overlap}}{\mathrm{T_L}}}, \quad r(q_2,q_3) = \sqrt{\frac{T_\mathrm{overlap}}{\mathrm{T_I}}}. \tag{18}$$

For example, if $T_\mathrm{L} = T_\mathrm{I} = 2T_\mathrm{overlap}$ then $r(q_1,q_2) = 0.5$ and $r(q_1,q_3) = r(q_2,q_3) = 1/\sqrt{2} \approx 0.707$. In general, however, if averaging times are sufficiently long then it will also be necessary to consider other sources of correlation. For example, the systematic uncertainty of the caesium fountain is also common to the measurements q_1 and q_2 and will cause an increase in the correlation coefficient $r(q_1,q_2)$. Similarly, the statistical and systematic uncertainties of the optical lattice clock and trapped ion optical clock contribute to $r(q_1,q_3)$ and $r(q_2,q_3)$ respectively.

A more complicated (but still hypothetical) example involving four clocks, six measured frequency ratios involving these clocks, and twelve non-zero correlation coefficients, is given in reference [11].

Example 4.2a: Measurements involving the Yb$^+$ optical clock at NPL

In 2014, the absolute frequencies $q_1 = \nu_{E2}/\nu_{Cs}$ and $q_2 = \nu_{E3}/\nu_{Cs}$ of the two optical clock transitions in ^{171}Yb$^+$ were measured at NPL in the same campaign as the direct optical frequency ratio between them, $q_3 = \nu_{E2}/\nu_{E3}$ [26]. In this case it is clear from ref. [26] that the three measurements are correlated, but not all the information required to estimate the correlation coefficients appears in the publication.

Correlation between the two absolute frequency measurements q_1 and q_2 arises from both systematic and statistical uncertainties. From table II of reference [26], we see that there are several common sources of systematic uncertainty, specifically the gravitational redshift, the second-order Doppler effect, Cs fountain systematics and uncertainties associated with the frequency comb, rf distribution and frequency synthesis. These common sources of systematic frequency shifts contribute an uncertainty of $u_{\text{common}} = 2.16 \times 10^{-16}$ to each measurement, out of total uncertainties $u_{\text{tot1}} = 6.13 \times 10^{-16}$ for q_1 and $u_{\text{tot2}} = 5.79 \times 10^{-16}$ for q_2. To estimate the statistical contribution to the correlation coefficient, we need to know not only the times T_1 and T_2 for which each clock transition was measured, as well as their period of overlap T_{overlap}, but also the statistical uncertainties σ_{Cs1} and σ_{Cs2} associated with the Cs fountain for the two periods T_1 and T_2. From [26], it is clear that $T_1 = 105$ hours, $T_2 = 81$ hours and $T_{\text{overlap}} = 72$ hours. However the statistical uncertainties listed for the two absolute frequency measurements include contributions from both the Cs fountain and the ytterbium ion optical clock. Strictly, additional information is therefore required to determine σ_{Cs1} and σ_{Cs2}, although in this case the statistical uncertainty is dominated by the Cs fountain. The correlation coefficient between the two measurements can be calculated from the formula

$$r(q_1, q_2) = \frac{u_{\text{common}}^2 + \sigma_{\text{Cs1}}\sigma_{\text{Cs2}} \left(T_{\text{overlap}}^2 / T_1 T_2\right)^{1/2}}{u_{\text{tot1}} u_{\text{tot2}}} \tag{19}$$

and is found to be 0.680 in this case.

The optical frequency ratio measurement is correlated with the two absolute frequency measurements due to the statistical and systematic uncertainties associated with the two ytterbium ion transitions. The corresponding correlation coefficients can be calculated using the formulae

$$r(q_1, q_3) = \frac{u_{\text{E2}}^2 + \sigma_{\text{E2\_1}}\sigma_{\text{E2\_3}} \left(T_{\text{overlap}} / T_1\right)^{1/2}}{u_{\text{tot1}} u_{\text{tot3}}} \tag{20}$$

and

$$r(q_2, q_3) = -\frac{u_{\text{E3}}^2 + \sigma_{\text{E3\_2}}\sigma_{\text{E3\_3}} \left(T_{\text{overlap}} / T_2\right)^{1/2}}{u_{\text{tot2}} u_{\text{tot3}}}, \tag{21}$$

where $\sigma_{\text{E2\_1,3}}$ and $\sigma_{\text{E3\_2,3}}$ are the statistical uncertainties associated with the $^{171}\text{Yb}^+$ E2 and E3 optical clock transitions for the relevant measurement periods, u_{E2} and u_{E3} are their systematic frequency uncertainties and u_{tot3} is the total uncertainty of the optical frequency ratio measurement q_3.

Although the instability of the optical frequency ratio is stated in reference [26] to be $\sim 3.6 \times 10^{-14} \tau^{-1/2}$ for averaging times τ greater than the 15 minute measurement cycle employed in this campaign, the relative contributions of the two transitions are not stated. Additional information from the group that performed the measurements indicates that the E2 transition contributes approximately twice as much to the instability as does the E3 transition. Based on this additional unpublished information, we calculate the correlation coefficients to be $r_{q_1,q_3} = 0.507$ and $r_{q_2,q_3} = -0.018$.

Example 4.2b: Measurements performed during June 2015

An unusually large number of frequency comparisons were performed during October 2014 and June 2015, due to a large-scale coordinated effort between INRIM, LNE-SYRTE, NPL and PTB within the EMRP International Timescales with Optical Clocks (ITOC) project. The main aim of the coordinated measurement campaign was to investigate the potential of a broadband version of the standard two-way satellite time and frequency transfer technique for high accuracy remote clock comparisons [17]; however since almost all optical clocks and fountains in these four labs were running during the campaign, many local comparisons were also performed at the same time.

At LNE-SYRTE, six different frequency ratios were measured during this period, involving their ^{199}Hg and ^{87}Sr optical lattice clock (frequencies ν_{Hg} and ν_{Sr}) and their Rb and Cs fountains (frequencies ν_{Rb} and ν_{Cs}). These measured frequency ratios are reported in several different papers: $q_1 = \nu_{\mathrm{Hg}}/\nu_{\mathrm{Cs}}$, $q_2 = \nu_{\mathrm{Hg}}/\nu_{\mathrm{Rb}}$ and $q_3 = \nu_{\mathrm{Hg}}/\nu_{\mathrm{Sr}}$ in reference [38], $q_4 = \nu_{\mathrm{Sr}}/\nu_{\mathrm{Cs}}$ and $q_5 = \nu_{\mathrm{Sr}}/\nu_{\mathrm{Rb}}$ in reference [35], and $q_6 = \nu_{\mathrm{Rb}}/\nu_{\mathrm{Cs}}$ in reference [39]. Clearly many of these frequency ratios are correlated at some level, but the papers do not contain sufficient information for most of the correlations to be properly quantified; indeed, reference [38] does not even specify the dates on which the measurements were made. Nevertheless we can estimate some of the correlation coefficients from information provided in the papers. For example, measurements q_1, q_2 and q_3 are correlated through the uncertainties (both statistical and systematic) associated with the mercury optical lattice clock, and if we assume that the Cs and Rb fountains operate for the whole time that the mercury optical lattice clock is running, then we find that $r(q_1,q_2) \approx 0.02$ while $r(q_1,q_3) \approx r(q_2,q_3) \approx 0.04$. On the other hand, q_2 and q_5 are, as a minimum, correlated through the systematic uncertainty associated with the Rb fountain. There may also be a contribution from the statistical uncertainty, as it is likely that the measurement periods overlap, though the extent of this overlap cannot be determined from the publications. If we consider only the systematic contribution, the correlation coefficient is calculated to be $r(q_2,q_5) = 0.681$, but the statistical correlations can be expected to increase this.

There are also correlations between this set of measurements performed at LNE-SYRTE and measurements performed in other laboratories. To take one example, atomic fountains at LNE-SYRTE and PTB were being compared over a fibre link during June 2015, and the published report describing this comparison [39] includes an absolute frequency measurement of the Rb fountain at SYRTE against the Cs fountain ensemble, which included two at LNE-SYRTE and two at PTB. The ratio q_6 is therefore correlated with another absolute frequency measurement $q_7 = \nu_{\mathrm{Sr}}/\nu_{\mathrm{Cs}}$ performed at PTB during October 2014 and June 2015, which used their local fountains as the reference [40]. However to quantify the degree of correlation, more detailed information about the actual period of overlap is required. Further correlations will also exist with the remotely measured optical frequency ratios reported in [17], though again the published information is insufficient to quantify these correlations.

4.3 Dead time extrapolation

When the optical clock data is intermittent, as in figure 1, it is common when making absolute frequency measurements to extrapolate over dead times using a hydrogen maser as a flywheel [40, 41]. The longer averaging time this provides compensates for the additional uncertainty introduced by the extrapolation, which is usually quantified by numerical simulation of the maser noise. When the extrapolation for two absolute frequency measurements involves the same maser and overlapping measurement periods, then the extrapolation may introduce correlations that should be accounted for in the numerical simulations. In the example shown in figure 1, the extrapolation from the lattice clock uptime to the total measurement time and the extrapolation from the ion clock uptime to the total measurement time are negatively correlated.

The exact calculation depends on the maser noise characteristics but can be understood from a simple model. Consider the case of no overlap between the ion and lattice clock. Let T_{I} be the uptime of the ion clock only, and T_{L} the uptime of the lattice clock only. The extrapolation to $T = T_{\mathrm{I}} + T_{\mathrm{L}} + T_0$, where T_0 is the period in which neither optical clock operates, are quantified by the uncertainty in the ratios:

$$e_{\mathrm{I}}=\frac{f(T_{\mathrm{I}})}{f(T)},\quad e_{\mathrm{L}}=\frac{f(T_{\mathrm{L}})}{f(T)},\quad e_{0}=\frac{f(T_{0})}{f(T)},\tag{22}$$

where $f(T)$ is the maser average frequency measured in the period T. For definition of average frequency then:

$$f(T)=\frac{f(T_{\mathrm{I}})T_{\mathrm{I}}+f(T_{\mathrm{L}})T_{\mathrm{L}}+f(T_{0})T_{0}}{T},\tag{23}$$

so that

$$e_{\mathrm{L}}T_{\mathrm{L}}+e_{\mathrm{I}}T_{\mathrm{I}}+e_{0}T_{0}=T.\tag{24}$$

This is a closure relation that can be satisfied only if the covariance matrix of the e_j contains correlation terms, as the law of propagation of uncertainties (equation 4) prescribes

$$u^2(e_{\mathrm{L}})T_{\mathrm{L}}^2=u^2(e_{\mathrm{I}})T_{\mathrm{I}}^2+u^2(e_0)T_0^2+2u(e_{\mathrm{I}},e_0)T_{\mathrm{I}}T_0,\tag{25}$$

and similar by permutation of the indices. If for example sake we assume $u_{e_L}=u_{e_I}=u_{e_0}$, $T_{\mathrm{L}}=T_{\mathrm{I}}=T_0$ then it can be shown that:

$$r(e_{\mathrm{I}},e_{\mathrm{L}})=-0.5.\tag{26}$$

5 Correlations from data aggregation (TAI)

Although the most direct way of measuring the absolute frequency of an optical standard is to use a caesium fountain primary standard, which provides a local realisation of the SI second, an alternative approach is to use a frequency link to International Atomic Time (TAI). In recent years, this approach has been used for a number of high accuracy absolute frequency measurements [32, 42–49]. Making measurements in this way can lead to additional sources of correlation.

Most straightforwardly, if two groups make absolute frequency measurements of two different clocks during the same period, using TAI as a reference, there will be a non-zero correlation coefficient between them resulting from the uncertainty in the offset between the scale interval of TAI and the SI second. There may also be other "hidden" sources of correlation, for example if common satellite-based time and frequency links enter the computation of the offsets of the two local UTC(k) timescales from UTC.

However, even if the two measurements are not made simultaneously, they may still be correlated, because there are correlations in TAI between different months. Such correlations may be introduced, for example, by the fact that very often the same Cs fountain primary standards contribute to TAI month after month.

Finally, the situation is further complicated by the fact that, since November 2018, a few optical clocks have contributed data to the BIPM for use in the computation of TAI, and have been used along with Cs primary standards and the Rb secondary standard at LNE-SYRTE to determine steering corrections. This means that absolute frequency measurements performed using TAI as a reference will be influenced to some degree by the results of earlier absolute frequency measurements used to determine the CIPM recommended frequency values that are used for steering.

Quantifying the correlation coefficients associated with these effects would be best approached in cooperation with the BIPM staff responsible for the computation of TAI. However they may be estimated from the published weights of the primary standards contributing to each Circular T [50].

Measurement	
Value	
Uncertainty	
Reference	
Comments	Please give shortly pertinent details for the experiment and results here. In particular if you estimate that there are any correlations involved in the measurements that ought to be considered in the evaluation of the recommended frequency list please mention that here.

Table 2. Template that was used in 2017 for reporting the results of absolute frequency measurements or direct frequency ratio measurements to the WGFS.

6 Conclusions and recommended reporting template

From the examples presented in this document, it is clear that significant correlations can arise between frequency measurements performed at different times and/or in different institutions. Most of these correlations were neglected in the analysis underpinning the most recent update to the CIPM list of recommended frequency values, without the possible bias to those values being fully understood.

As the worldwide body of frequency comparison data continues to expand, the number of potentially significant correlations is likely to increase. Continuing to neglect these correlations in the analysis runs an increasing risk of biasing the recommended frequency values and incorrectly estimating their uncertainties. Of particular concern are correlations arising from the systematic uncertainties of caesium fountain primary frequency standards. Although the systematic uncertainties of different fountains are largely uncorrelated, the systematic uncertainty of any particular fountain will in general be correlated over time, unless a significant re-evaluation of its uncertainty budget has been undertaken. This may lead to significant correlations between absolute frequency measurements performed in a particular institution at different points in time. However it can also lead to correlations with measurements performed in different institutions using TAI to provide the link to the SI second. Significant correlations may also arise from the uncertainties of clocks that participate in more than one frequency comparison simultaneously, while the possibility that the systematic uncertainty of clocks (other than fountains) may be correlated over time must also be considered. Other potential sources of correlation include the use of the same atomic coefficients to correct for certain systematic frequency shifts or the gravitational redshift correction which is almost completely correlated for all clocks within a particular laboratory.

The published papers reporting the results of frequency comparison experiments do not normally discuss how they are correlated with other measurements, and in some cases the papers will not contain sufficient information for the correlation coefficients to be calculated. Hence if the WGFS are to account for correlations in the analysis performed to inform updates to the list of recommended frequency values, the necessary information will need to be gathered by other means.

The normal practice of the WGFS is to circulate a questionnaire to NMIs and DIs, asking whether their institutes and/or any other laboratories in their country have made new or additional absolute frequency measurements or direct frequency ratio measurements since the list of recommended frequency values was last updated. This questionnaire includes a template for reporting the results of each measurement; the template used in 2017 is shown in table 2. Although respondents were asked to comment on correlations they considered ought to be considered, only a few included any mention of correlations in their response, and none identified all possible sources of correlation, with some of the most significant correlations being overlooked. To ensure that all relevant information is reported, we therefore consider that further guidance and a more detailed template is required.

Measurement	
Value	
Uncertainty	
Reference	
Identification of the frequency standard(s) involved	For standards contributing to TAI, this should be the name used in TAI reports.
Period(s) of the measurement	MJD range(s)
Link to the SI second (for absolute frequency measurements)	For example, whether this is directly to one or more primary frequency standards, or through TAI or TT(BIPM). For measurements relative to primary standards, please include the names of these standards, their weights, their systematic uncertainties, and the date on which the last significant re-evaluation of the systematic uncertainty took place. For measurements relative to TAI or TT(BIPM), please make it clear which Circular T periods are involved, and the weights of each.
Atomic coefficients	If you have used theoretical values of atomic coefficients to correct for systematic frequency shifts, or experimental values from other groups, please give details.
Comments	Please comment on any other potential sources of correlation between this and other measurements. For example, is it correlated with previous measurements involving the same clock(s) because the systematic uncertainty has not been re-evaluated?

Table 3. Recommended reporting template for reporting the results of absolute frequency measurements and direct frequency ratio measurements to the WGFS, that would enable a proper assessment of correlations within the worldwide body of clock comparison data.

Our proposal for such a template is shown in table 3. This recommends requesting further information as follows:

- The frequency standard or standards involved in the measurement should be unambiguously identified, since a number of laboratories operate more than one clock based on the same atomic transition. If the standard contributes to TAI, then the standard should be identified by the name used in TAI reports.

- The period or periods over which the measurement was performed.

- For absolute frequency measurements, the traceability route to the SI second should be identified. If this is via a direct link to one or more primary frequency standards, then these primary standards should be identified, and the relative weights of these fountains as well as their systematic uncertainties should be provided, together with the date on which the last significant re-evaluation of the uncertainty took place. If, on the other hand, the measurement was performed relative to TAI or TT(BIPM), then it should be clear which Circular T periods were involved, and the relative weights of each.

- The source of atomic coefficients used to correct for systematic frequency shifts should be considered, and comments included if these originate from other groups.

- An assessment should be made as to whether the measurement is correlated with previous measurements involving the same clock, for example because the systematic uncertainty has not been re-evaluated, or because only some contributions to the systematic uncertainty budget have been re-evaluated.

Where possible, respondents should be encouraged to calculate the correlation coefficients between measurements that they know are correlated. In particular, if several absolute frequency measurements and/or frequency ratio measurements are reported by the same group, the provision of a correlation matrix for this subset of measurements would greatly assist the work of the WGFS. The worked examples provided in this document provide guidance on how to calculate such a correlation matrix, and will hopefully prove useful to researchers carrying out frequency comparison measurements, both within the ROCIT consortium and beyond. This guidance and our recommendations will be shared with the WGFS in order to raise awareness of the potential significance of correlations when updating the CIPM list of recommended frequency values, and to promote discussion on a possible approach to gathering the information necessary to allow these correlations to be quantified. This should allow a more robust analysis to be performed to underpin future updates to the list.

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