

Geochronology Discuss., author comment AC2  
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## Reply on RC2

Pieter Vermeesch

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Author comment on "An algorithm for U–Pb geochronology by secondary ion mass spectrometry" by Pieter Vermeesch, Geochronology Discuss.,  
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I am sorry that Dr. Rayner was unable to import her own .pd and .op files into 'simplex'. This reflects the fact that Cameca side of 'simplex' has undergone more rigorous testing than the SHRIMP side. The reviewer kindly shared the problematic .pd and .op files with me, and the issue was quickly fixed: it turns out that these files contained some comments, which were absent from the Geoscience Australia files that I had previously used to test 'simplex'.

The improved robustness of the data import function also addresses the reviewer's concern that it 'simplex' is not able to 'clear' the existing data. Whenever a new dataset is loaded, it replaces the previous data and resets the calculations. I have also fulfilled Dr. Rayner's request for "better tracking of what is being processed". The latest version provides the user with a lot more status updates, which is especially useful when loading large SHRIMP .pd files.

Although the reviewer is correct that 'simplex' was, first and foremost, created as a vehicle to test and demonstrate the algorithms presented in the GChron manuscript, I do hope that it will be used for actual isotope geoscience research in the future. I have posted a request for further feedback on Facebook's 'SHRIMP Fan Club' page. Hopefully, this feedback will iron out any remaining bugs and issues.

The reviewer points out two simplifications in the new algorithm, which are only briefly mentioned in the original manuscript:

1. The assertion that mass-dependent fractionation of the Pb-isotopes can be safely ignored in most cases.
2. The assumption that  $^{204}\text{Pb}$  is measured accurately, i.e. is free of isobaric interferences (' $^{204}\text{Pb}$  overcounts') and has been adequately peak-centred.

The manuscript already mentions these issues, and suggests solutions to them. Mass dependent fractionation can already be corrected using the stable isotope functionality of 'simplex' (see line 385 of the original manuscript). Possible issues with the  $^{204}\text{Pb}$  measurements can be corrected by manually specifying a session blank that brings the common-Pb corrected  $^{207}\text{Pb}/^{206}\text{Pb}$  ratios into alignment with reference values (line 170 of the manuscript).

These solutions are quite straightforward to implement from the command line, but not with a GUI. In anticipation of a user-friendly implementation of these fixes, I will be more upfront about simplex' existing simplifications in the revised manuscript. I will add a paragraph to the introduction and/or conclusions explaining (to quote the reviewer) "what simplex CAN do (today) and CANNOT do (today)."

Dr. Rayner asks for an example where covariance matrices of isotopic data improve the accuracy and/or precision of geochronological data. I think that an error weighted mean (as in Section 13 of Vermeesch, 2015, doi:10.1016/j.chemgeo.2015.05.004) would be a good way to satisfy this request.

Her other comments are all minor and easy to address. I will document the corresponding changes in the cover letter of the revised manuscript. There are just two points where I have decided not to follow the reviewer's suggestions:

1. A review of the 'conventional approach' to drift and dead time correction. First, I am not sure if there actually is a 'conventional' way to do these calculations that applies to all instruments and labs. Second, the current practice to apply a dead-time correction to the data before the drift correction turns integer counts into real numbers, which are incompatible with the Poisson distribution. To reduce the reviewer's confusion, I will try to explain the rationale behind Sections 8 and 9 more clearly. However, I would prefer not to dedicate too much space to describing existing procedures that are, in my opinion, suboptimal.

2. Plotting the synthetic data of Table 1 on Figure 2. First, the data of Table 1 are raw measurements, which do not have a 1-to-1 match with the isochron surfaces of Figure 2. Second, the example of Table 1 would produce a tightly clustered set of points in Figure 2, without uncertainties. I am concerned that this would confuse rather than illuminate the reader. Third, the addition of data points to Figure 2 would make it less 'pretty', and less universally applicable.

On a related note, I have completely redrafted Figure 2, because it had some mistakes in it. These mistakes happened because I made the original version of this plot many years ago, and have since used it in several presentations, research proposals etc. The figure was changed numerous times (fonts, orientation, colours), and somewhere down the line the scales were messed up (Reviewer 1 pointed out one of the errors). The landing page of the simplex website contains a fresh version of this crucial figure, which will be also used in the revised manuscript.