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Standard Grant PROPOSAL

Document Status: With Council
NERC Reference: NE/T001518/1

Standard Grant JAN19
Panel A

Organisation where the Grant would be held

Organisation	University College London	Research Organisation Reference:	2466184
Division or Department	Earth Sciences		

Project Title [up to 150 chars]

Beyond Isoplot: new software for better geochronology.

Start Date and Duration

a. Proposed start date	01 January 2020	b. Duration of the grant (months)	36

Applicants

Role	Name	Organisation	Division or Department	How many hours a week will the investigator work on the project?
Principal Investigator	Dr Pieter Vermeesch	University College London	Earth Sciences	11.25

Technology

Is this project technology-led? Yes

Describe the type of technology being developed and its application to NERC science; an indicator of the level of maturity of the technology should be included (up to 500 characters).

The proposed research will develop a new suite of software to process mass spectrometer data and calculate isotopic ratios and ages whilst keeping track of all sources of correlated uncertainty. The software builds on existing components and aims to integrate these with new programs to ensure internal consistency. Mass spectrometry and geochronology benefit a wide range of NERC-supported research, including palaeobiology, geology, environmental geochemistry and geomorphology

Collaborative Centres

Please check the the appropriate button if this proposal is being submitted under the auspices of either NCAS or NCEO, and has been explicitly agreed with the centre administrator.

NCAS	
NCEO	
Neither	Yes

Objectives

List the main objectives of the proposed research in order of priority [up to 4000 chars]

The proposed research aims to develop an integrated suite of software for geochronological data processing that keeps track of correlated uncertainties between samples, and between chronometers. Preliminary results indicate that this has a first order effect on the precision and accuracy of geochronological dates. The new software ecosystem will require the modification of existing codes and the creation of entirely new programs. This new software will be applied to five high impact case studies. Specific objectives are to:

1. update the PI's IsoplotR software to accommodate inter-sample error correlations;
2. develop an 'IsoplotR4Excel' add-in that will allow users to access the full functionality of IsoplotR within a familiar spreadsheet environment;
3. 'fork' shiny, which is a widely used interface package between R and Javascript, and release a lightweight version of it under the name 'shinylight'; to use this new software to improve IsoplotR's existing browser-based graphical user interface;
4. implement a data exchange format to allow IsoplotR to import and combine datasets generated by lower level data processing programs such as ET_Redux (U-Pb) and Ar-Ar_Redux (40Ar/39Ar), including inter-sample error correlations;
5. modify the 'Pychron' program for 40Ar/39Ar data acquisition and processing for compatibility with logratio statistics, which provides the mathematical framework that ensures the greatest accuracy and precision;
6. formulate a new approach to 'time zero' regression in noble gas mass spectrometry, following a physics-based approach developed by Project Partner Chris Hall (U. of Michigan);
7. implement the new regression algorithm in a general purpose noble gas mass spectrometer data reduction code called 'timezero', and incorporate its code into Ar-Ar_Redux and Pychron;
8. release all the source code for free, and carefully document the corresponding application programming interfaces (APIs) to facilitate the creation of third party extensions;
9. use the new software to recalculate the age of the Solar System;
10. re-determine the timing of the most notorious mass extinction event in Earth's history, at the Cretaceous-Palaeogene boundary;
11. date tufa deposits above and below the Taung Child discovery site (South Africa) using the U-Pb method, in order to bracket the age of one of the world's most famous hominin fossils;
12. refine the time-temperature history of lower crustal rutile from NW Canada by updating an inverse modelling code for U-Pb depth profiling;
13. fit Arrhenius-style diffusion experiments for noble gas thermochronology and I-Xe dating of achondritic meteorites;
14. (begin to) recalibrate the geologic time scale, determine the (non-radiogenic) isotopic abundances of the elements, and intercalibrate the decay constants of long-lived radioactive isotopes.

Summary

Describe the proposed research in simple terms in a way that could be publicised to a general audience [up to 4000 chars]

The development of radiometric geochronology is one of the greatest triumphs of 20th century geoscience. Geochronology underpins the study of Earth history and puts fundamental constraints on the rate of biological evolution. Tremendous resources are invested in the development of sophisticated mass spectrometers capable of measuring isotopic ratios with ever increasing resolution and sensitivity. Unfortunately, the statistical treatment of mass spectrometer data has not kept up with these hardware developments and this undermines the reliability of radiometric geochronology.

This proposal aims to create a 'software revolution' in geochronology, by building an internally consistent ecosystem of computer programs to account for inter-sample error correlations. These have a first order effect on the precision and accuracy of geochronology but are largely ignored by current geochronological data processing protocols. The proposed software will modify existing data reduction platforms and create entirely new ones. It will implement a data exchange format to combine datasets from multiple chronometers together whilst keeping track of the correlated uncertainties between them. The new algorithms will be applied to five important geological problems.

1. The age of the Solar System is presently constrained to 4567.30 +/- 0.16 Ma using primitive meteorites. The meteorite data are 'underdispersed' with respect to the analytical uncertainties. The presence of strong inter-sample error correlations is one likely culprit for this underdispersion. Accounting for these correlations will significantly improve the accuracy and precision of this iconic age estimate.
2. The Cretaceous-Palaeogene boundary marks the disappearance of the dinosaurs in the most notorious mass extinction of Earth history. We will re-evaluate the timing of critical events around this boundary using high precision 40Ar/39Ar geochronology. Preliminary results from other samples show that 40Ar/39Ar data are prone to strong (r^2 > 0.9) inter-sample error correlations, and that these have a first order effect on the precision and accuracy of weighted mean age estimates. A sensitivity test indicates that this may change the timing of the mass extinction by up to 200ka.
3. The 'Taung Child' is a famous hominin fossil that was discovered in a South African cave in 1924. It is considered to be the world's first Australopithecine, but has not yet been dated. We have a good unpublished U-Pb age of 1.99 +/- 0.05 Ma from a tufa collected above the hominid, and an imprecise upper age limit of 1.4 +/- 2.7 Ma on a calcrete deposit below it. Applying the new algorithms to the latter date will greatly improve its precision. This will be further improved with additional measurements, in time for the 100th anniversary of the Taung Child's discovery.
4. Depth profiling of the U-Pb ages in rutile and apatite provides an exciting new way to constrain the thermal evolution of lower crustal rocks. However, the laser ablation data used for this research are prone to strong error correlations that are not accounted for by current data reduction protocols. These protocols will be revised using the new software, permitting better resolution of the inferred t-T paths.
(5) Radiogenic noble gases such as 40Ar (from 40K), 4He (from U, Th and Sm), and 129Xe (from 129I) are lost by volume diffusion at high temperatures. The revised regression algorithms implemented by the research programme will be applied to step-heating 'Arrhenius' experiments. This will improve the calculation of diffusion coefficients for these gas species, resulting in further improvement of (noble gas) thermochronology.

Academic Beneficiaries

Describe who will benefit from the research [up to 4000 chars].

Entering the word 'geochronology' in the Web of Science search box (at http://webofknowledge.com) currently yields some 1700 academic publications per year, reflecting the importance of geochronology in the (Earth) Sciences.

1. Geochronologists have long relied on a powerful Excel add-in called 'Isoplot' for data processing and presentation. Unfortunately Isoplot is no longer maintained and does not work properly in recent versions of Excel. This is causing real problems for geochronologists, to the point where some laboratories keep an old Windows XP computer with Excel 2003 around just for the purpose of running Isoplot. The proposed work centres around an open and future proof replacement for Isoplot called 'IsoplotR'. The latter program will be extended to accommodate inter-sample correlations that are ignored by Isoplot, and to facilitate the combination and intercalibration of multiple chronometers. These developments are essential if geochronologists are to take full advantage of the improvements in mass spectrometry that have been made in recent years.
2. Meteoriticists will enjoy much improved resolution into the early history of the Solar System thanks to the improved (isochron) regression algorithms provided by the proposed research.
3. Palaeobiologists will benefit from improved age estimates for volcanic eruptions and meteorite impacts that have been linked to mass extinction events, and from better constraints on the recovery rate of ecosystems from these crises.
4. Anthropologists will be able to date a wider range of (carbonate) lithologies thanks to the improved precision offered by the new data processing tools.
5. Thermochronologists, geomorphologists and metamorphic petrologists will benefit from better thermochronology using established noble gas methods and novel LA-ICP-MS depth profiling approaches.
6. Noble gas geochemists will have access to better estimates of the 'time zero' intercept of mass spectrometer signals under static vacuum. The new software will be particularly useful for low intensity ion beams for which conventional (linear, polynomial or exponential) regression may yield physically impossible negative intercepts. The new approach produces values that are guaranteed to be positive and are ideally suited for subsequent processing using logratio statistics.
7. Eventually the International Union of Pure and Applied Chemistry (IUPAC) will need to update its table of isotopic

abundances to account for the significant uncertainty correlations that are bound to exist between the experimentally determined isotope abundances of any element.
8. Further down the line, (historic) geologists will benefit from an improved Geologic Time Scale. The GTS is regularly revised by the International Commission on Stratigraphy (ICS), which operates under the umbrella of the International Union of Geological Sciences (IUGS). Over the decades, various statistical approaches have been used to calibrate the GTS, including the chronogram, spline interpolation and, most recently, Bayesian methods. The software ecosystem under proposal will allow these approaches to take into account inter-sample correlations that have been all but ignored thus far. Such correlations have a strong effect on the precision and accuracy of the GTS.
9. Statisticians and data scientists of any discipline (from Biology to Finance) will benefit from the development of a lightweight alternative to the popular 'shiny' interface between R and Javascript. In its current form, shiny implements its own version of the HTML markup language, and discourages the incorporation of native Javascript and HTML in interactive websites using R. The proposed 'shinylight' package will remove this limitation and facilitate the integration of spreadsheets, canvasses and other dynamic widgets that are not part of shiny, but are available through free and open Javascript libraries.

Impact Summary

Impact Summary (please refer to the help for guidance on what to consider when completing this section) [up to 4000 chars]

1. Community uptake of the proposed software will be promoted by:
a. The incorporation of existing data reduction packages into the new software ecosystem. This will ensure a seamless transition to rigorous inter-sample error correlation for existing users of those packages.
b. The addition of a series of video tutorials to the online IsoplotR data reduction platform (http://isoplotr.london-geochron.com). These tutorials will not only document IsoplotR, but will also serve as a general introduction to geochronological data processing, similar to the PI's 'virtual petrographic microscope' at https://www.ucl.ac.uk/~ucfbpve/intro and the free lecture notes that he has released at https://eartharxiv.org/sj4ft . They will turn IsoplotR into a unique teaching tool.
c. The organisation of a summer school, at UCL, for 50 junior scientists during the final year of the project. This event will cover all aspects of geochronology including sample collection, mineral separation, mass spectrometry and, of course, data processing. It will be taught by the PI and guest lecturers, including some of the Project Partners.

2. The existence of creation myths in many world religions points at a deep and fundamental fascination of all people with the origin of the world. Geochronology represents the scientific answer to this question. It is important that the underlying principles of this discipline are communicated to the general public. The proposal includes a significant budget for science communication that will be used to:
a. Produce a 15-20 min video about geochronology and the geologic time scale, presented by renowned science communicator Prof. Iain Stewart and similar in scope to his 'Anatomy of an Earthquake' video on https://youtu.be/8QNigxTN384 ;
b. Develop a 'geochron@home' app that will allow citizen scientists to participate in an 'online dating' experiment using the fission track method (http://geochron-at-home.london-geochron.com);

Summary of Resources Required for Project

Financial resources

Summary fund heading	Fund heading	Full economic Cost	NERC contribution	% NERC contribution
Directly Incurred	Staff	179739.00	143791.20	80
	Travel & Subsistence	20950.00	16760.00	80
	Equipment	0.00	0.00	100
	Other Costs	136810.00	109448.00	80
	Sub-total	**337499.00**	**269999.20**	
Directly Allocated	Investigators	77824.80	62259.84	80
	Estates Costs	84614.00	67691.20	80
	Other Directly Allocated	4887.00	3909.60	80
	Sub-total	**167325.80**	**133860.64**	
Indirect Costs	Indirect Costs	189634.00	151707.20	80
	Total	**694458.80**	**555567.04**	

Summary of staff effort requested

	Months
Investigator	10.75
Researcher	36
Technician	0
Other	0
Visiting Researcher	0
Student	0
Total	46.75

Research Council Facilities
£ 75810

Other Support

Details of support sought or received from any other source for this or other research in the same field.
Other support is not relevant to this application.

Related Proposals
Proposal is related to a previous proposal to NERC

Reference Number	How related?
NE/S001654/1	Resubmission

Staff

Directly Incurred Posts

			EFFORT ON PROJECT							
Role	**Name /Post Identifier**	**Start Date**	**Period on Project (months)**	**% of Full Time**	**Scale**	**Increment Date**	**Basic Starting Salary**	**London Allowance (£)**	**Super-annuation and NI (£)**	**Total cost on grant (£)**
Researcher	Research Software Engineer	01/01/2020	36	100	Grade 8.37	01/08/2020	40792	3092	14136	179739
									Total	179739

Applicants

Role	Name	Post will outlast project (Y/N)	Contracted working week as a % of full time work	Total number of hours to be **charged** to the grant over the duration of the grant	Average number of hours per week **charged** to the grant	Rate of Salary pool/banding	Cost estimate
Principal Investigator	Dr Pieter Vermeesch	Y	100	1485	11.2	86472	77825
						Total	77825

Travel and Subsistence

Destination and purpose		Total £
Outside UK	AGU x2	4500
Outside UK	Goldschmidt x1	2250
Outside UK	EarthTime meetings x2	4000
Outside UK	Vienna, EGU x2 (2 people)	4000
Within UK	London, academic visit from Noah McLean	3100
Within UK	London, academic visit from Jake Ross	3100
	Total £	20950

Other Directly Incurred Costs

Description	Total £
Permanent server node at the UCL computer cluster	3000
Desktop computer with peripherals for the Research Software Engineer	1500
An introductory video about the geologic time scale presented by project partner Prof. Iain Stewart, plus a series of tutorial videos to be integrated into IsoplotR for training purposes.	30000
Development costs and infrastructure for geochron@home	5000
A summer school for 50 junior scientists, to be organised at UCL during the last year of the project.	20000
Recruitment Cost	1500
Carbonate U-Pb analyses for the Taung Child project, to be carried out by the NERC Isotope Geosciences Laboratory. See the Research Council Facilities section of the Je-S form for further details.	75810
Total £	136810

Other Directly Allocated Costs

Description	Total £
Infrastructure Technicians	4887
Total £	4887

Research Council Facilities

details of any proposed usage of national facilities

Name of Facility	Units	Cost £	Proposed Usage
NERC Isotope Geosciences Laboratory	6	75810	Imaging (SEM and CL), LA-ICP-MS mapping and targeted analyses, U-Th (for residual 234U excess and U-Th as a test of closed system for the past ~0.7 Ma) and ID-TIMS U-Pb for six tufa samples.
	Total £	75810	

Project Partners: details of partners in the project and their contributions to the research. These contributions are in addition to resources identified above.

1	Name of partner organisation		Division or Department	Name of contact	
University of Plymouth			Sch of Geog Earth & Environ Sciences	Professor Iain Stewart	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	presentation of Impact video	5000
secondment of staff			other		
other			Sub-Total		5000

Sub-Total		0		Total Contribution	5000

2	**Name of partner organisation**		**Division or Department**	**Name of contact**	
University of Kansas			Geology	Professor Noah McLean	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Updating ET_Redux, visit to UCL	10000
secondment of staff			other		
other			Sub-Total		10000
Sub-Total		0		Total Contribution	10000

3	**Name of partner organisation**		**Division or Department**	**Name of contact**	
New Mexico Institute of Mining and Techn			New Mexcio Bureau of Geology and Mineral	Dr Jake Ross	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Help integrate Ar-Ar_Redux and timezero into Pychron	20000
secondment of staff			other		
other			Sub-Total		20000
Sub-Total		0		Total Contribution	20000

4	**Name of partner organisation**		**Division or Department**	**Name of contact**	
College of Charleston			UNLISTED	Professor James Bowring	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Assistance with update to ET_Redux	5000
secondment of staff			other		
other			Sub-Total		5000
Sub-Total		0		Total Contribution	5000

5	**Name of partner organisation**	**Division or Department**	**Name of contact**
University of Michigan		Earth and Environmental Sciences	Dr Chris Hall

Direct contribution to project			Indirect contribution to project		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Implement the timezero algorithm	5000
secondment of staff			other		
other			Sub-Total		5000
Sub-Total		0		Total Contribution	5000

6	**Name of partner organisation**	**Division or Department**		**Name of contact**	
Natural History Museum of Denmark		UNLISTED		Dr James Connelly	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Re-evaluation of the age of the Solar System	5000
secondment of staff			other	Sharing Pb-Pb data	50000
other			Sub-Total		55000
Sub-Total		0		Total Contribution	55000

7	**Name of partner organisation**	**Division or Department**		**Name of contact**	
Washington University in St Louis		Physics Department		Professor Alex Meshik	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	Implement the timezero algorithm	5000
secondment of staff			other		
other			Sub-Total		5000
Sub-Total		0		Total Contribution	5000

8	**Name of partner organisation**	**Division or Department**		**Name of contact**	
Birkbeck College		Earth and Planetary Sciences		Dr Philip Hopley	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		

equipment/ materials	Carbonate samples below the Taung Child fossil	10000	staff time	Sample selection, data interpretation, paper writing	5000
secondment of staff			other		
other			Sub-Total		5000
Sub-Total		10000		Total Contribution	15000

9	**Name of partner organisation**		**Division or Department**	**Name of contact**	
Pennsylvania State University			Geosciences	Professor Andrew Smye	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials	Rutile from the Grenville orogen	2000	staff time	Update UPbeat algorithm	5000
secondment of staff			other		
other			Sub-Total		5000
Sub-Total		2000		Total Contribution	7000

10	**Name of partner organisation**		**Division or Department**	**Name of contact**	
NERC British Geological Survey			NERC Isotope Geosciences Laboratory	Dr Daniel Condon	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment		
equipment/ materials			staff time	30 days of staff time for the Taung Child project	30000
secondment of staff			other		
other			Sub-Total		30000
Sub-Total		0		Total Contribution	30000

11	**Name of partner organisation**		**Division or Department**	**Name of contact**	
Free (VU) University of Amsterdam			Earth Sciences	Professor Klaudia Kuiper	
Direct contribution to project			**Indirect contribution to project**		
	Description	**Value £**		**Description**	**Value £**
cash			use of facilities/ equipment	40Ar/39Ar dating of K-Pg materials	20000
equipment/ materials			staff time	Analysis of old and new 40Ar/39Ar data	20000
secondment of staff			other		
other			Sub-Total		40000
Sub-Total		0		Total Contribution	40000

Total Contribution from all Project partners	£197000

Classification of Proposal

(a) Scientific Area (mandatory)

Assign % relevance (in multiples of 5) to one or more areas, totalling 100%.

Scientific Area	%
Atmospheric	5
Earth	75
Freshwater	0
Marine	0
Terrestrial	20
	Total = 100%

(b) Secondary Classification

Assign % relevance (in multiples of 5) to any areas that are relevant. Otherwise, leave blank.

Scientific Area	%
Co-funded	
Cross-Research Council	
Earth Observation	
Polar North	
Polar South	
Science Based Archaeology	20

(c) ENRI (mandatory)

Assign % relevance (in multiples of 5) to one or more ENRIs, totalling 100%.

Scientific Area	%
Biodiversity	25
Environmental Risks and Hazards	25
Global Change	25
Natural Resource Management	25
Pollution and Waste	0
	Total = 100%

(d) Beneficiary Countries

Will the research focus address the challenges faced by developing countries or territories? If so, select those that apply.

OTHER INFORMATION

Nominated Reviewers

1	Name	Organisation	Division or Department	Email Address
Professor Simon Kelley		University of Edinburgh	Sch of Geosciences	simon.kelley@ed.ac.uk

Nominated Reviewers

2	Name	Organisation	Division or Department	Email Address
Dr Clare Warren		Open University	Faculty of Sci, Tech, Eng & Maths (STEM)	clare.warren@open.ac.uk

Nominated Reviewers

3	Name	Organisation	Division or Department	Email Address
Dr David Richards		University of Bristol	Geographical Sciences	david.richards@bristol.ac.uk

Nominated Reviewers

4	Name	Organisation	Division or Department	Email Address
Professor Blair Schoene		Princeton University	Geosciences	bschoene@princeton.edu

Proposal Classifications

Research Area:

NERC's 'primary' Research Areas (second level) are listed here (Research Areas), but other Research Areas can be selected which may relate to other Research Councils. Up to five of these Research Areas may be chosen, and a percentage should be attributed to each such that the total is 100. To add or remove Research Areas use the links below.

Subject	Topic	Indicator %	Keyword
Chemical measurement	Analytical Science	80	
Chemical measurement	Analytical Science	0	Mass Spectrometry
Geosciences	Palaeoenvironments	0	Dating - isotopic
Geosciences	Palaeoenvironments	20	

Qualifier:

Qualifiers are terms that further describe the area of research. Please ensure you complete this section if relevant. To add or remove Qualifiers use the links below.

Type	Name
Project Engagement by Sector	Academic Users
Project Engagement by Sector	General Public
Project Engagement by Sector	Student Teachers & Undergrads

Free-text Keywords:

Free-text keywords may be used to describe the science within your application in more detail. These will facilitate reviewer-matching and may form the basis of a more detailed classification in the future.
Add freetext keywords below (50 character max per keyword):

Free-text Keywords
geochronology
mass spectrometry
software
statistics

Previous Track Record

The **London Geochronology Centre** (LGC) is a joint facility between University College London (UCL) and Birkbeck, University of London. Building on the pioneering work by William Ramsay, Lord Rayleigh, Arthur Holmes and Tony Hurford, the LGC continues to lead the way in geochronological methods development and applications. Its laboratory facilities provide access to a nearly comprehensive suite of radiometric dating techniques including U-Pb, K-Ar, U-Th-He, fission tracks and cosmogenic nuclides. These methods are used to understand how continents deform and how surface topography develops over different spatial and temporal scales. This work is carried out with many UK and international collaborators. The LGC currently employs three full time member of staff (Prof. Andrew Carter, Dr. Pieter Vermeesch and Dr. Matthew Fox). Funding sources include the ERC, NERC and the Leverhulme Trust, supplemented by commercial contracts.

Dr. Pieter Vermeesch (BSc. Ghent 1999, MSc. MIT 2000, PhD. Stanford 2005) is a Reader in geochronology at UCL and the PI of this proposal. His research covers a wide range of topics, from thermochronology to aeolian geomorphology, and has been funded by NERC (Standard Grants NE/K003232/1 and NE/I009248/2), the ERC (Starting Grant #259504), and the Leverhulme Trust (grants RPG-2014-410 and RPG-2015-020). During his PhD. studies at Stanford University, Vermeesch completed six statistics and four computer science modules. This advanced training forms the foundation of his methodological research into the statistical aspects of geology and geochronology. His first and most cited publication calculated the sample size requirements for sedimentary provenance studies by detrital geochronology (Vermeesch 2004). Two more statistical papers published during his PhD. developed new approaches to the tectonic discrimination of oceanic basalts (Vermeesch 2006a,b). The first of these papers introduced the principles of compositional data analysis into this field of research. These principles form the core of the proposal under consideration.

Following his PhD, Vermeesch completed a Marie Curie postdoctoral research fellowship in terrestrial cosmogenic noble gas geochronology at ETH Zürich under the CRONUS-EU Research and Training Network. During this fellowship, he developed the `CosmoCalc` Excel add-in for cosmogenic nuclide calculations (Vermeesch 2007). In a side project, the U-Th-He age equation was the first to be recast in a logratio context by Vermeesch (2008). This work was further developed by Vermeesch (2010), who introduced logratio covariance matrices as a basis for data reduction and error propagation. These ideas form the nucleus of data exchange format presented in Section 5.1 of the DOW. Shortly after transferring to London, Vermeesch (2009) developed `RadialPlotter` for his colleague Andy Carter. This software produces radial plots, which are an extremely useful graphical device for the visualisation of heteroscedatic fission track data that is generalised to all geochronometers by the `IsoplotR` software discussed in the proposal. `RadialPlotter` was written in `Java` to avoid the compatibility issues that plague `CosmoCalc` after every update of Microsoft Office, and which have made Ken Ludwig's `Isoplot` add-in unusable. In a short but influencial paper (170 citations per year), Vermeesch (2012) introduced Kernel Density Estimates (KDEs) as a means of visualising detrital age distributions. `RadialPlotter` was forked to form a separate program called `DensityPlotter` whose code is shared on `GitHub`.

Prompted by the flood of data generated under NERC Standard Grant #NE/I009248/1, Vermeesch developed novel methods and software for 'Big Data' analysis in detrital geochronology (Vermeesch 2013; Vermeesch & Garzanti 2015; Vermeesch et al. 2016). All these contributions were quickly adopted by the provenace community. Vermeesch (2015) completely revised the data processing chain and error propagation routines used for ^{40}Ar/^{39}Ar geochronology. These methods were implemented in a prototype software package called `Ar-Ar_Redux` that is discussed in Section 5.4 of the DOW and forms the backbone of the present proposal.

The UCL **Research Software Development** Group, part of UCL Research IT Services and led by Jonathan Cooper, is a nationally leading scientific programming group, currently consisting of ten experienced research software engineers. Founded in 2012, the group was the first of its kind in the UK, and the UCL model is now being replicated by at least seven leading research-intensive universities in the UK. RSD collaborates with researchers to build and maintain readable, reliable and efficient scientific software, focusing on compute- and data- intensive software engineering.

REFERENCES:•**Vermeesch**, P. 2004, EPSL, 224, 441.•**Vermeesch**, P. 2006a, G-Cubed, 7.•**Vermeesch**, P. 2006b, GCA, 70, 1839.•**Vermeesch**, P. 2007, G-Cubed, 8, 8003.•**Vermeesch**, P. 2008, Chemical Geology, 249, 339.•**Vermeesch**, P. 2009, Radiation Measurements, 44, 409.•**Vermeesch**, P. 2010, Chemical Geology, 271, 108 .•**Vermeesch**, P. 2012, Chemical Geology, 312-313, 190.•**Vermeesch**, P. 2013, Chemical Geology, 341, 140.•**Vermeesch**, P. 2015, GCA, 171, 325.•**Vermeesch** et al. 2015, Chemical Geology, 409, 20.•**Vermeesch** et al. 2016, Sedimentary Geology, 336, 14-25.

Case for Support

Description of Work

1 Preface

This proposal aims to create a 'software revolution' in geochronology. It will build an internally consistent ecosystem of computer programs to account for **inter-sample error correlations** and **systematic uncertainties**. This is a **resubmission** and complete rewrite of a previous proposal[1] that was unsuccessful but received an exceptionally detailed and encouraging decision letter from the Moderating Panel.

In its letter, the Panel agreed that "there is a huge amount of blind faith placed in the business-as-usual model for [geochronology]". It thought that the proposed work "could potentially have very high impact throughout the geochron community and by extension all of the geological sciences." Therefore, the "Panel were content that this work is needed and should be done."

However, the first submission was viewed as not suitable for funding by the NERC Discovery Science scheme because it did not include any specific applications. The Panel wrote that "Technology-led proposals still need to justify the impact and significance they will have on the science discipline". It requested "that the proposal needed to include a key case study to demonstrate the technological development and enhance the engagement of the wider community and thus the ultimate outcomes and impact of the work."

This resubmission follows the Panel's advice by applying the proposed software ecosystem to no fewer than **five detailed case studies** involving **ten Project Partners**. They will (1) refine the age of the Solar System; (2) re-evaluate the timing of the K-Pg extinction; (3) date the famous Taung Child hominin fossil; (4) test competing models for the formation of cratonic lithosphere by rutile U-Pb thermochronology; and (5) reassess linear fits to Arrhenius relationships in noble gas diffusion experiments. These applications demonstrate the far-reaching implications of the proposed software revolution, which may open up entirely new geochronological applications as well.

2 Introduction: linear regression revisited

The proposed research will create a breakthrough in the statistical treatment of inter-sample error correlations. These have a first order effect on the precision and accuracy of geochronology but are largely ignored by current geochronological data processing protocols. The huge implications of this problem can be illustrated using one basic statistical operation that geochronologists perform on a daily basis, namely linear regression.

York (1966) developed a weighted least squares algorithm to fit a straight line through bivariate data with variable uncertainties in both the x- and the y-variable. He soon realised that correlated uncertainties have a first order effect on the quality of the fit and modified his algorithm accordingly (York 1969, further refined by York et al. (2004)). These correlated uncertainties are usually shown as rotated error ellipses, as illustrated with a synthetic example in Figure 1i.

The York algorithm has become a mainstay of geochronology, and is implemented in virtually all geochronological software. However, this proposal argues that further improvements to linear regression are possible and, indeed, absolutely necessary for many applications. The problem with York regression is that it only accounts for error correlations between variables, but not **between samples**. The PI has developed an algorithm that fixes this problem[1]. Figure 1ii shows that this modification has just as big an effect on the goodness of fit as York's solution did compared to ordinary least squares (OLS). Importantly, it can be shown that the algorithm of York (1969) is a special case of the new algorithm, just like York (1966) is a special case of York (1969), and OLS regression is a special case of York (1966). Therefore, the revised regression algorithm is **universally applicable**.

3 Correlated uncertainties are pervasive throughout geochronology

The regression example of Section 2 has far reaching implications for geochronology. Linear regression is a fundamental tool for the calculation of isochron and discordia ages. It is used to correct U-Pb data for common Pb, and U-series data for detrital Th. It is also used in lower level data processing steps, such as the extrapolation of mass spectrometer signals to 'time zero' (see Section 5.5).

But regression is just the tip of the iceberg. Other basic statistical operations in geochronology are equally affected by correlated errors. For example, the calculation of a weighted mean is effectively a special case of linear regression with a zero slope. Section 4.2 shows that inter-sample error correlations could potentially shift the age estimates of important chronostratigraphic marker beds **beyond the currently assumed uncertainties**. Similar effects are expected for the calculation of concordia ages, the interpolation of dates across stratigraphic boundaries, etc.

All these examples demonstrate that inter-sample error correlations can have a major effect on the accuracy

[1] The previous version of this proposal can be viewed at `http://doubleblind.dynu.net` along with further details about the regression algorithm and the code to reproduce Figure 1i-ii

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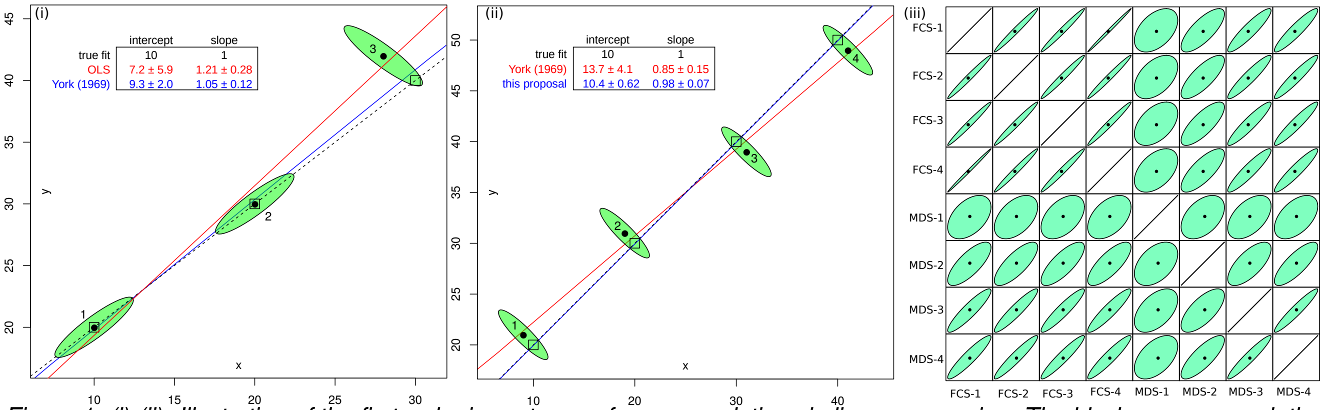

Figure 1: (i)-(ii). Illustration of the first order importance of error correlations in linear regression. The black squares mark the true (x,y)-coordinates of samples drawn from a (dashed) line with intercept $\boldsymbol{a}=10$ *and slope* $\boldsymbol{b}=1$*. The black dots mark random realisations of these samples, given Gaussian uncertainties shown as 95% confidence ellipses. (i) three samples with correlated uncertainties in both the x- and y-variable. Ignoring the error correlations yields the red fit (*$a=7.2, b=1.21$*). Accounting for the error correlations using the algorithm of York (1969) produces the blue fit (*$a=9.3, b=1.05$*). (ii) four samples whose analytical uncertainties are not only correlated within each sample, but also* ***between*** *samples (1 & 2 and 3 & 4, respectively). Ignoring these inter-sample correlations produces the red fit (*$a=13.7, b=0.85$*). Taking into account the inter-sample correlations using the proposed algorithm produces the blue fit (*$a=10.4, b=0.98$*); (iii) Correlation matrix of a* $^{40}Ar/^{39}Ar$ *dataset comprising four Fish Canyon Sanidine (FCS) and four Mount Dromedary Sandine (MDS) analyses, calculated by Vermeesch (2015). Error correlations between samples are as high as 0.9, resulting in highly elliptical confidence regions. Ignoring those correlations has a detrimental effect on the precision and accuracy of weighted means, isochrons, and spline interpolations.*

and precision of geochronology. And unfortunately, such correlations are ubiquitous in geochronology. Vermeesch (2015) showed that inter-sample error correlations commonly exceed $r^2>0.8$ in the context of $^{40}Ar/^{39}Ar$ dating (Figure 1iii). McLean et al. (2016) came to similar conclusions for U-Pb dating by LA-ICP-MS.

By solving the inter-sample error correlation problem, the proposed research will also address the important issue of **systematic uncertainty** in geochronology. Systematic errors, such as decay constant uncertainties, simultaneously affect multiple samples. They are characterised by perfect inter-sample error correlations. In contrast **random uncertainties**, such as detector noise, exhibit zero inter-sample error correlations. The proposed software ecosystem will process both sources of uncertainty together, in contrast with current *hierarchical* error propagation routines (Renne et al. 1998; Min et al. 2000), which process them separately.

Section 4 of this proposal presents five geological problems that will benefit from the ability to handle inter-sample error correlations. These case studies will be used to demonstrate the immediate scientific impact of the proposed software. The five geological problems require a new class of data reduction software, and this is the main deliverable of the proposed research. Section 5 introduces a constellation of computer codes that will keep track of all sources of correlated uncertainty in a self-consistent manner. The proposed toolbox aims to modify existing data reduction programs when possible and supplement these with new computer codes when necessary. By partnering with the developers of existing data reduction platforms, the proposed research will speed up development and accelerate the adoption of the new tools by the user community.

4 Five geological problems that are affected by inter-sample error correlations

This section presents a selection of 'low hanging fruits' for the new data reduction software. It includes two high precision and three low precision examples.

4.1 Age of the Solar System

The age of the Solar System represents the most coveted prize in geochronology. First estimated at $\sim$3000 Ma by Holmes (1946) using Pb-Pb dating of terrestrial lead-ores, it has been regularly refined over the past seven decades (e.g., Holmes 1947; Patterson 1956; Amelin et al. 2002). The earliest solids preserved from the protoplanetary disk occur as inclusions in chondritic meteorites. A weighted mean of these has been dated to 4567.30$\pm$0.16 Ma, which includes a single chondrule age of 4567.32$\pm$0.42 Ma (Connelly et al. 2012).

These isochron data are **underdispersed** with respect to the formal analytical uncertainties (MSWD=0.15, Connelly et al. 2012). One likely cause for this underdispersion is the inability of the York (1969) algorithm to account for inter-sample error correlations. This is similar to the synthetic example of Section 2, which is characterised by a similarly low MSWD of 0.42 using York (1969) regression. Reanalysing the synthetic data with the revised regression algorithm fixes this underdispersion whilst dramatically improving the precision and accuracy of the fit (Figure 1ii). A similar improvement is expected for the meteorite data.

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An evaluation of the effect of inter-sample error correlations will made for Connelly et al. (2012)'s Pb-Pb data using the new data reduction scheme. This work will be carried out in close collaboration with Project Partners **James Connelly** and **Noah McLean**. Applying the new data reduction paradigm to other classes of meteorites will allow further refinement of early Solar System history (Connelly et al. 2017). The proposed re-evaluation may reveal previously undetected geological **dispersion**. Statistical approaches to dealing with such dispersion were introduced by Ludwig (2003a); Vermeesch (2010, 2018) and others. These approaches can be reformulated to accommodate inter-sample error correlations, as shown in the draft manuscript linked under the first footnote of this Description of Work.

4.2 The K-Pg boundary

Tektites from the famous Chicxulub impact event have been dated by the ^{40}Ar/^{39}Ar method to 66.04 $\pm$ 0.05 Ma, i.e. a precision of <1‰ (Figure 2i). These data establish that a bolide impact happened within 32,000 years from the Cretaceous-Palaeogene (K-Pg) impact that wiped out the dinosaurs (Renne et al. 2013). Ultra-precise data like this put important constraints on the timescales required for ecosystems to recover after mass extinctions. However, Vermeesch (2015) showed that strong inter-sample error correlations are commonplace in ^{40}Ar/^{39}Ar geochronology. These correlations affect the precision and accuracy of the results, and may shift the age of the K-Pg events by up to 200,000 years (Figure 2i).

The proposed research will re-evaluate the age of the K-Pg boundary in two parallel ways. First, it will reprocess the raw data from the original studies by Kuiper et al. (2008) and Renne et al. (2013). Second, Project Partner **Klaudia Kuiper**, who was involved in both of these studies, will analyse duplicate samples from them with modern mass spectrometer equipment. Processing these new analyses with the same software will further refine the age of this important stratigraphic boundary and the biogeological processes associated with it.

4.3 U-Pb dating of carbonates and the Taung Child

Zircon is the workhorse mineral of U-Pb geochronology, because (1) it tends to incorporate relatively high concentrations (of up to 1‰) of U and low concentrations of Pb in its crystal lattice during crystallisation; (2) it is resistant to secondary overprinting during weathering, diagenesis and metamorphism; and (3) it is commonly found in many lithologies including (felsic) igneous, metamorphic and siliciclastic rocks.

However, zircon also has serious limitations such as (1) its tendency to be recycled, which makes it difficult to 'see' the difference between new and inherited geological signals; and (2) its absence from common lithologies such as mafic igneous rocks and carbonates.

To overcome these limitations, there is much interest in applying U-Pb dating to other mineral phases with less favourable initial U/Pb-ratios. The ability to routinely date **'low-μ' phases** such as calcite, apatite, rutile and titanite holds the potential to revolutionise several scientific fields including tectonics (Smye et al. 2018), structural geology (Hansman et al. 2018) and archaeology (Hellstrom & Pickering 2015).

Unfortunately, U-Pb dating of low-μ phases is technically challenging because it requires a substantial common-Pb correction. Figure 2ii shows a typical example of a carbonate sample that lacks sufficient spread to permit a reliable extrapolation to purely radiogenic lead. Like the Pb-Pb isochrons of Connelly et al. (2012), also this discordia line exhibits underdispersion, which is a telltale sign of hidden error correlations[2].

We will use the new discordia regression algorithm to determine the age of one of the world's most famous hominin fossils. The 'Taung Child' was discovered in 1924 by quarrymen working at the Buxton Limeworks, Taung, who passed it on to Raymond Dart at the University of the Witwatersrand. Dart described it as a new genus and species, *Australopithecus africanus* (Dart 1925), and it became the first evidence to support Darwin's assertion that humans evolved in Africa. The Taung Child remains an iconic fossil with immense historical importance and is still the subject of new scientific investigations. However, the age of the Taung Child remains uknown to this date.

Since its discovery it has been assigned ages ranging from 3 Ma to 1 Ma, and the most commonly cited estimate of its age is approximately 3.0 Ma to 2.5 Ma, based on the recognition of fossil primate and ungulate species from the Taung site. Early attempts to date associated tufa deposits using bulk uranium-thorium methods led the perception that the deposits were undatable (Tobias et al. 1993). However, recent advances in uranium-lead dating of young carbonates has lead to the successful dating of flowstones associated with other early hominins from South Africa (e.g., Walker et al. 2006; Pickering et al. 2011).

Using National Geographic funding awarded to Project Partner **Philip Hopley** in 2010, the sedimentology and stratigraphy of the site were studied and samples collected (Hopley et al. 2013). After screening a number of samples for U-Pb using LA-MC-ICP-MS, samples of the hominin-bearing layer were deemed undatable. However,

[2] The absence of underdispersion does, of course, *not* prove the absence of inter-sample error correlations!

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a sample of tufa from the top of the outcropping sequence produced a robust date of 1.95$\pm$0.05 Ma. This fits well with new magnetostratigraphic data that show a reversal to normal polarity by this sample (i.e. the base of the Olduvai Chron). The normal polarity of the hominin-bearing strata can be tentatively attributed to the Gauss Chron, but this is a long magnetochron ranging from 3.59 Ma to 2.59 Ma. In 2012, two cores (depths of 13 and 51 m) were recovered from the site.

Preliminary results from a small pilot study of these cores yielded an upper age estimate of 1.4$\pm$2.7 Ma. With the new algorithms and software, we will be able to significantly reduce the uncertainty of this date. We will augment it with additional measurements from five new cores that were collected in March 2018. This proposal seeks funding to screen and date six tufa samples from these cores for U-Pb dating using LA-ICP-MS and isotope dilution methods, including high precision U activity ratio measurements. The new dataset will be combined with the re-processed 1.4 Ma result and the unpublished 1.99$\pm$0.05 Ma lower age limit to form a robust bracketing range for this important hominin fossil, in time for the centenary of its discovery.

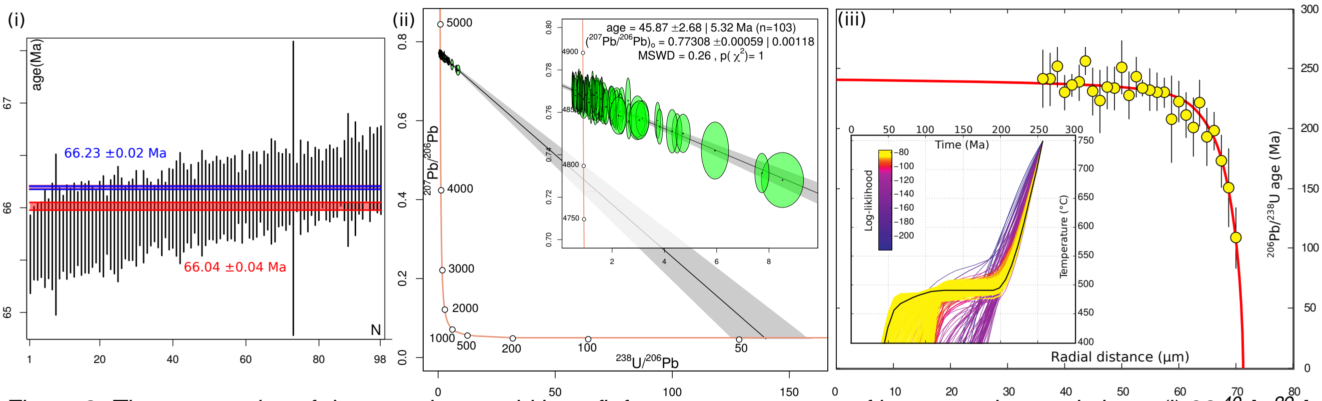

Figure 2: Three examples of datasets that would benefit from an assessment of inter-sample correlations. (i) 98 ^{40}Ar/^{39}Ar dates from an Ir-rich bentonite 80-120cm above the Cretaceous-Palaeogene boundary (Renne et al. 2013). Error bars show 2σ confidence limits. The red lines and rectangle represent the 2σ interval for the weighted mean age, assuming that all age estimates are statistically independent. The blue interval represents a 'worst case scenario' in which the analytical uncertainties for the different aliquots are perfectly (and positively) correlated with each other. This would shift the Cretaceous-Palaeogene boundary by 200,000 years. (ii) 103 U-Pb measurements in carbonate define a linear mixing array between radiogenic and common Pb on a Tera-Wasserburg diagram (data from Nick Roberts). Unfortunately data spread is insufficient to extract a precise age from these data. Taking into account inter-sample error correlations will greatly improve this situation and increase the low MSWD as well. (iii) A U-Pb depth profile in lower crustal rutile from the Grenville orogen (Smye et al. 2018). The inset shows the best fitting thermal history inferred from this profile using `UPbeat`*. This fit ignores the strong error correlations that must exist between the analyses. Taking into account these correlations will tighten the fit whilst improving accuracy as well.*

4.4 U-Pb thermochronology by LA-ICP-MS depth profiling

As explained in Section 4.3, zircon has a tendency to be recycled repeatedly over geologic time. Old zircons may be incorporated into young magmas, acquiring growth layers like tree rings. Whole grain dissolution and TIMS dating of such complex grains yields discordant U-Pb compositions. But even micro-analytical techniques such as LA-ICP-MS may mix reservoirs of different age. As the laser drills into a crystal, it produces a transient signal recording the ages of the growth zones that it passes through. Such 'cycle-by-cycle' geochronology can also be applied to accessory minerals like apatite and rutile. In this case, changes in U-Pb age with depth are not caused by secondary overgrowth but by thermally activated volume diffusion (Cochrane et al. 2014).

In a research collaboration with Project Partner **Andrew Smye**, the PI has developed an inverse modelling code called `UPbeat` to reconstruct continuous time-temperature paths from U-Pb depth profiles (Smye et al. 2018). Here the thermal history information resides in subtle changes in profile curvature, reflecting the competing effects of thermally-activated volume diffusion and radiogenic production that are obscured by analytical uncertainty (Figure 2iii).

`UPbeat`'s existing maximum likelihood algorithm will be modified to accept the full covariance structures produced by the updated `ET_Redux` program (Section 5.7). This will increase the resolution and accuracy of the resulting t-T paths. We will apply the revised algorithm to rutile from the lower crust of the Slave province, NW Canada. Thermal history information will constrain the timing of isostatic equilibration and, in doing so, test competing models for the formation of cratonic lithosphere following continental collision (e.g., McKenzie & Priestley 2016; Lee et al. 2018).

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4.5 Noble gas diffusion experiments and thermochronology

Like Pb in rutile or apatite, radiogenic noble gases can be lost by heating, and diffusion profiles develop in datable minerals during slow cooling. But unlike the diffusion profiles of Pb in rutile or apatite, which can only be reconstructed by (laser) drilling (Section 4.4), noble gas profiles are commonly inferred from step-heating experiments.

An 'Arrhenius diagram' is obtained by plotting the fractional loss of, say, He in apatite against (inverse) temperature (e.g., Shuster et al. 2004). The slope and intercept of a linear array on such a diagram can be used to calculate the diffusivity of the noble gas at any temperature. This diffusivity may then be used to constrain the thermal evolution of the host rock over geologic time.

Similar to the cycle-by-cycle LA-ICP-MS measurements discussed in the previous section, also step-heating experiments are characterised by strong inter-sample error correlations (Vermeesch 2015). The proposed improvements to geochronological data processing will increase the accuracy and precision of diffusion experiments and, hence, of thermochronology.

This aspect of the proposed research also has important applications in *meteoritics*. In collaboration with Project Partner **Alex Meshik**, the revised regression algorithm will be applied to step-heating measurements of xenon isotopes with the aim to improve I-Xe dating of achondritic meteorites (Pravdivtseva et al. 2013). This work will nicely complement the chondritic meteorite study of Section 4.1.

5 New software for accurate and internally consistent geochronology

The geochronological problems introduced in the previous section require a new generation of data reduction software that accounts for inter-sample error correlations. The proposed research will create a modular system of interconnected computer codes that take raw mass spectrometer data as input and produce accurate and precise dates and associated covariance matrices as output. This software ecosystem will modify and extend existing data reduction platforms such as `IsoplotR` and `ET_Redux`, and will augment these with entirely new components such as `timezero` and `shinylight` that will benefit geochronologists and other (Earth) scientists (Figure 3).

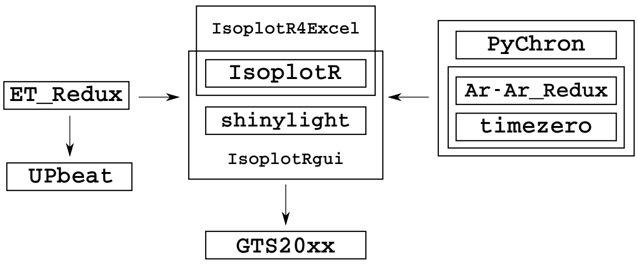

Figure 3: Organigram of the proposed geochronological software. `IsoplotR`, `IsoplotRgui`, `ET_Redux`, `Ar-Ar_Redux`, `PyChron` *and* `UPbeat` *are existing platforms that require modification to accept a common data exchange format.* `IsoplotR4Excel`, `shinylight` *and* `timezero` *are yet to be created. Boxes group components that can be packaged together for separate applications. All software developed under this proposal will be free and open.*

5.1 IsoplotR

Few computer programs have been used as widely in the Earth Sciences as `Isoplot`. This add-in to Microsoft `Excel` takes isotopic data as input and produces publication-ready figures as output, including U-Pb concordia diagrams, isochrons, ^{40}Ar/^{39}Ar-age spectra, etc. (Ludwig 1988, 1999, 2003b, 2012). Unfortunately, after nearly three decades of loyal service, it appears that `Isoplot`'s days are numbered. Recent versions of `Excel` are incompatible with `Isoplot`, whose creator Dr. Kenneth Ludwig (Berkeley Geochronology Center) has retired and no longer maintains the code. These software issues are a major problem for the field of radiometric geochronology, to the point where some laboratories keep an old Windows XP computer with `Excel 2003` around for the sole purpose of running `Isoplot`.

The PI has developed a new computer code to address this pressing issue. Developed over a period of two years without funding, `IsoplotR` aims to provide the geochronological community with a free, open and future-proof alternative for `Isoplot` (Vermeesch 2018). `IsoplotR`'s software architecture uses a modular design with future-proofness and extendability in mind. The software is written in `R` and can be run online (at `http://isoplotr.london-geochron.com.`), offline and from the command-line. The latter option allows `IsoplotR` to be extended and incorporated into automation scripts. Several users are already using this option and have created separate graphical user interfaces for their purposes.

In its present form, `IsoplotR` aims to replicate `Isoplot`'s functionality, whilst expanding it with U-Th-He and fission track functions. `IsoplotR`, (like `Isoplot`) takes into account error correlations between isotopic ratios of the same sample, but assumes that there is no inter-sample error correlation. The proposed research will remove this simplification and implement further improvements to make `IsoplotR` even more user friendly and future proof.

`IsoplotR` currently accepts input data as flat tables with five or nine columns:

$$X, s[X], Y, s[Y], \rho[X,Y]$$

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or $$X, s[X], Y, s[Y], Z, s[Z], \rho[X,Y], \rho[X,Z], \rho[Y,Z]$$

where X, Y and Z are the isotopic (ratio) measurements; $s[X]$, $s[Y]$ and $s[Z]$ are their analytical uncertainties (standard errors); and $\rho[X,Y]$, $\rho[X,Z]$ and $\rho[Y,Z]$ are the error correlations.

Inter-sample correlations such as those shown in Figure 1ii require the addition of a new input format that includes the full covariance structure:

$$\begin{bmatrix}
X_1 & s[X_1]^2 & cov[X_1,X_2] & \ldots & cov[X_1,X_n] & cov[X_1,Y_1] & \ldots & cov[X_1 Y_n] & cov[X_1 Z_1] & \ldots & cov[X_1,Z_n] \\
X_2 & cov[X_2,X_1] & s[X_2]^2 & \ldots & cov[X_2,X_n] & cov[X_2,Y_1] & \ldots & cov[X_2,Y_n] & cov[X_2,Z_1] & \ldots & cov[X_2,Z_n] \\
\vdots & \vdots & \vdots & \ddots & \vdots & & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
X_n & cov[X_n,X_1] & cov[X_n,X_2] & \ldots & s[X_n]^2 & cov[X_n,Y_1] & \ldots & cov[X_n,Y_n] & cov[X_n,Z_1] & \ldots & cov[X_n,Z_n] \\
Y_1 & cov[Y_1,X_1] & cov[Y_1,X_2] & \ldots & cov[Y_1,X_n] & s[Y_1]^2 & \ldots & cov[Y_1,Y_n] & cov[Y_1,Z_1] & \ldots & cov[Y_1,Z_n] \\
\vdots & \vdots & \vdots & \ddots & \vdots & & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
Z_n & cov[Z_n,X_1] & cov[Z_n,X_2] & \ldots & cov[Z_n,X_n] & cov[Z_n,Y_1] & \ldots & cov[Z_n,Y_n] & cov[Z_n,Z_1] & \ldots & s[Z_n]^2
\end{bmatrix}$$

where $cov[X_i,Y_j]$ is the covariance between the i^{th} isotopic (ratio) measurements of X, and the j^{th} isotopic (ratio) measurements of Y etc.

This data structure contains all the information required to perform linear regression, calculate multi-sample averages and, eventually, calibrate the Geologic Time Scale (GTS). Casting it in a `.json` or `.xml` database format will allow data to be passed from lower-level data acquisition codes such as `Ar-Ar_Redux`, `PyChron` or `ET_Redux` to `IsoplotR`, as discussed below.

5.2 shinylight

The code base for `IsoplotR`'s GUI and its core data processing algorithms are surgically separated from each other. The command-line functionality is grouped in a lightweight package called `IsoplotR`, which has minimal dependencies and works on a basic `R` installation. It only uses commands that have been part of the `R` programming language for many decades and are unlikely to change in the future. In contrast, the GUI is written in `html` and `Javascript` and interacts with `IsoplotR` via an interface library. This interface is currently provided by the `shiny` package (Chang et al. 2017).

`shiny` is free, open, and popular amongst `R` developers but has three limitations: (1) it was created and is owned by a private company, which reduces the software's future proofness; (2) `shiny` is a rather 'bloated' piece of code that does much more than is needed for `IsoplotRgui`. Third, the free version of `shiny` does not accommodate simultaneous requests from multiple users.

To avoid all these issues, we will implement a light-weight alternative to `shiny` called `shinylight` that will allow websites to call `R` functions in a similar fashion to the way in which `node.js` allows websites to use `Javascript` as a server language. `shinylight` will be created by 'forking' `shiny` from the popular code sharing platform `GitHub`. It is anticipated that `shinylight` will find uses in many other fields of science besides geochronology.

5.3 IsoplotR4Excel

Arguably the most important reason for `Isoplot`'s remarkable success over the past three decades has been its integration within `Excel`'s familiar spreadsheet environment. Although `IsoplotR`'s existing web-interface aims to replicate the look and feel of `Isoplot`, some users might prefer to have the full power of `Excel` at their disposal during data processing.

Fortunately, `R` is able to interact with `Excel` via different interface packages such as `RExcel` (Heiberger & Neuwirth 2009). The research team will develop a menu-based user interface called `IsoplotR4Excel` that will offer the same user experience as `Isoplot` but without the limitations of the original `VBA` add-in.

5.4 Ar-Ar_Redux

Isotopic data are **compositional data**, which are defined as *vectors representing parts of a whole that only carry relative information* (Pawlowsky-Glahn & Buccianti 2011). For example, in the context of U-Th-He geochronology, the age does not depend so much on the absolute abundances of U, Th and He, but on their relative abundances. In other words, U, Th and He form a ternary system and the U-Th-He age equation can be visualised on a ternary diagram (Vermeesch 2008, 2010).

Similarly, ^{36,39,40}Ar data form a ternary system as well. This can easily be generalised to four or more components. Thus, the full ^{36,37,38,39,40}Ar system fits within the constraints of a four-dimensional pentahedroid. The compositional nature of isotopic data impose a covariant structure on their analytical uncertainties. A random error in the ^{36}Ar measurement, say, will simultaneously affect the ^{37}Ar/^{36}Ar, ^{38}Ar/^{36}Ar and ^{39}Ar/^{36}Ar ratio estimates. Thus, **correlated uncertainties are embedded in the very DNA of isotope geochemistry**

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and, hence, geochronology.

The statistical analysis of compositional data is fraught with problems and common statistical operations such as averaging and regression may produce counterintuitive results when applied to such data (Chayes 1949, 1960). Based on the work of Aitchison (1982, 1986), Vermeesch (2008, 2010) showed that all these problems can be avoided using a **logratio transformation**. This same approach also facilitates the calculation of the covariance matrices that are central to the proposal at hand.

The $^{40}Ar/^{39}Ar$ method was the first geochronometer that was re-evaluated entirely in a logratio context by Vermeesch (2015). The resulting algorithms were implemented in an `R`-package called `Ar-Ar_Redux` to demonstrate the extent of the error correlation problem discussed in Section 2. Figure 1iii shows a real dataset of Fish Canyon and Mount Dromedary sanidine ages that exhibit error correlations of 0.9 and more.

`Ar-Ar_Redux` is proof-of-concept code that is currently limited in a number of ways: (1) in its current version, the program is command-line based. This provides too steep a learning curve for many users; (2) the software currently only reads Argus-VI data; (3) it uses a rather simplified way to extract isotopic ratios from the raw mass spectrometer signals.

The proposed research will fix these issues by (1) developing a user-friendly GUI similar to the one that already exists for `IsoplotR`; (2) integrating `Ar-Ar_Redux` within an existing data acquisition platform called `PyChron` (Section 5.6); and (3) introducing a radically new way to regress noble gas mass spectrometer signals to 'time zero' (Section 5.5).

5.5 timezero

$^{40}Ar/^{39}Ar$ ratios are obtained by *regression* of transient electronic signals in a noble gas mass spectrometer. All subsequent calculations are then based on the signal intercepts at 'time zero'. For low intensity ion beams, this procedure may yield physically impossible negative values. The proposed research will develop a novel way to avoid this problem. The new approach is based on two separate innovations by Project Partners Alex Meshik and **Chris Hall**.

Project Partner Meshik proposed an elegant new definition of 'time zero', as the moment when the high voltage supply is switched on some time after the sample gas is let into the mass spectrometer (Meshik et al. 2012). This innovative procedure removes the gettering effects that are often observed during the initial stages of a noble gas measurement. It thus creates optimal conditions for a physics-based regression algorithm based on an idea from Project Partner Hall, which was adopted for logratio statistics by the PI.

Dr. Hall's algorithm determines the time-zero intercept using a mathematical description of the physical process that takes place during a noble gas measurement. If $c[i]$ is the time-resolved mass spectrometer signal (count rate or current) of the i^{th} isotope, then

$$\frac{dc[i]}{dt} = -\Lambda c[i] + k[i] \tag{1}$$

where Λ controls the rate at which the noble gas of interest is consumed by the mass spectrometer, and $k[i]$ represents the rate at which the i^{th} isotope accumulates into the mass spectrometer under static vacuum.

This differential equation can be solved for $c[i](t)$, the mass spectrometer signal expected t seconds after 'time zero':

$$c[i](t) = e^{0[i]-\Lambda t} + \frac{k[i]}{\Lambda}\left(1 - e^{-\Lambda t}\right) + \epsilon[i](t) \tag{2}$$

where $\epsilon[i](t)$ is the *residual*, which can follow a Poisson or Normal distribution if isotope i was measured on an electron multiplier or Faraday collector, respectively.

The (strictly positive) time-zero intercept is then given by $e^{0[i]}$, where $0[i]$ (along with Λ and $k[i]$) is obtained from Equation 2 by the method of Maximum Likelihood. The parameter Λ can be safely assumed to be identical for all isotopes of a single element such as argon. This constraint reduces the number of fitting parameters, resulting in more precise estimates of $0[i]$ and $k[i]$. Of course, using a single value of Λ for multiple isotopes naturally introduces covariance between their time-zero intercepts.

The new algorithm will be implemented in `R` and `Python` under the name `timezero`. This code will be incorporated into $^{40}Ar/^{39}Ar$ data reduction packages such as `Ar-Ar_Redux` and `PyChron`, but will also be released as a standalone program for other applications in noble gas geochemistry.

5.6 Pychron

`Pychron` is an NSF-funded suite of software to collect and process noble gas mass spectrometer data. Created by Project Partner **Jake Ross**, `Pychron` aims to provide a free, open and future proof alternative for the widely used `MassSpec` software of Dr. Alan Deino (who, like Kenneth Ludwig, is also employed by the Berkeley Geochronology Center). The program includes low level commands to automate gas handling (`PyValve`), heat

Case for Support

samples (`PyLaser` and `furPi`), control the mass analyser and set up analysis batches (`PyExperiment`) etc.

`Pychron` also implements functions that visualise and process the data to calculate ^{40}Ar/^{39}Ar dates (`PyView`). However, these operations use conventional (non-compositional) statistics that suffer from the issues described in Section 5.4. The proposed research will incorporate `Ar-Ar_Redux` and `timezero` into `Pychron`.

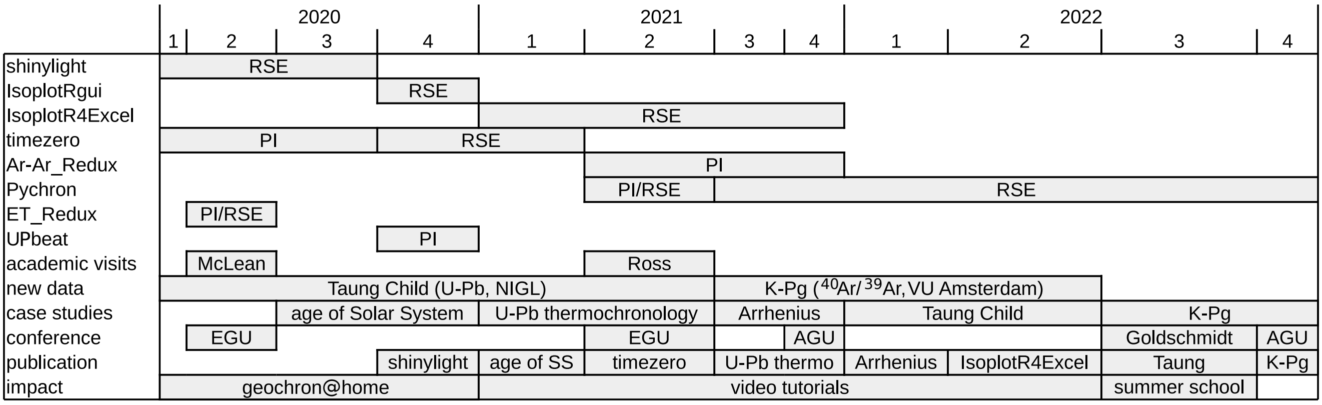
5.7 ET_Redux

One of the key achievements of the international EARTHTIME initiative was the development of a `Java` program called `U-Pb_Redux` for high precision U-Pb geochronology by Thermal Ionisation Mass Spectrometery (TIMS, Bowring et al. 2011). `U-Pb_Redux` propagated analytical uncertainties in a matrix format (McLean et al. 2011) but did not yet take into account the compositional nature of the isotopic data. The program was retrofitted with logratio statistics, modified to accommodate LAICPMS data, and rebranded as `ET_Redux` (McLean et al. 2016).

Like `Ar-Ar_Redux` and `Pychron`, `ET_Redux` is free and open software whose code is shared via `GitHub`. The proposed research will add an export function to `ET_Redux` that will allow the program to pass its output on to `IsoplotR` for further manipulation and combination with other chronometric datasets. See supporting letters by Project Partners **Jim Bowring** and Noah McLean.

6 Gantt chart

The proposed work will carried out by close collaboration between the PI and a Research Software Engineers (RSE) recruited by UCL's Research Software Development team. Further details of this are provided in the *Justification for Resources* section of this proposal. The source code for all software will be released through `GitHub` under the GPL-3 license, which permits re-use and modification provided that any derived code is released under the same conditions (Free Software Foundation 2007).



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Case for Support

Justification for Resources

Research Staff

The proposed work can be divided into two parts:

1. The development or modification of ten different computer programs, written in `R` (`IsoplotR`/`IsoplotRgui`, `timezero`, `Ar-Ar_Redux`), `Javascript/html` (`IsoplotRgui`, `shinylight`), `Python` (`Pychron`, `timezero`), `Java` (`ET_Redux`), `Matlab` (`UPbeat`), and `C/C++` (`shinylight`); and the creation of a cyber-infrastructure to accommodate the online components of this software constellation.

2. The application of this software to five different case studies. These involve the reprocessing of existing mass spectrometer data (e.g., the age of the Solar System; Section 4.1), supplemented by new measurements (e.g., the Taung Child study; Section 4.3).

This ambitious work plan will be carried out by PI Vermeesch (*directly allocated*) and a Research Software Engineer (RSE, *directly incurred*). The PI will spend 30% of his time on the project. Although this is more than usual for a NERC Standard Grant, it is a conservative estimate that is based on the two-year development period for the first version of `IsoplotR`. This –unfunded– program, which forms the heart of the proposed software ecosystem, was developed during evenings and weekends. The requested funds will allow the PI to carry out the proposed work plan during normal working hours. Even with the help of a designated RSE, the PI will need to invest far more time than was required for `IsoplotR 1.0`. He will modify `IsoplotR` to accommodate inter-sample correlations, work out the details of time zero regression and the revised isochron equation, write pilot (`R`) code for `timezero` and include it in `Ar-Ar_Redux`, collaborate with the Project Partners on the case studies, write papers and supervise the RSE.

The ideal candidate for the RSE position would be a postdoctoral research associate (PDRA) with a background in the Earth Sciences and strong credentials in programming and statistics. Although such people do exist (Project Partners Ross and McLean are two excellent examples), they are not easy to find. If the search for such a multi-talented geologists does not yield any suitable candidates, then a computer scientist will fill the position instead. This person will be recruited by UCL's Research Software Development (RSD) team. (S)he will be physically located at the Department of Earth Sciences during the project, but will join the RSD team after completion of the project.

The five case studies represent a significant amount of work. A case could be made to recruit a second PDRA, but this would nearly double the requested budget. The revised proposal manages to avoid such an inflation of costs with the help of ten Project Partners, all of whom have agreed to contribute data and time to the project. Additionally, Project Partner Kuiper has agreed to provide new ^{40}Ar/^{39}Ar data at no additional cost to NERC. However, a financial contribution is requested for the involvement of the NERC Isotope Geoscience Facility (NIGL) in the Taung Child study.

The Taung Child project will be carried out by NIGL using samples collected by Project Partner Hopley. In 2012, field and drilling work by Hopley recovered two cores (depths of 13 and 51 m) from the site. We have identified a number of detritus-free tufa and calcrete samples that look well-suited for uranium-lead dating methods, and which when dated will provide a bracketing maximum age for the 'Taung Child'. Six samples will be analysed by the following methods: imaging (SEM and CL), LA-ICP-MS mapping and targeted analyses, U-Th (for residual ^{234}U excess and U-Th as a test of closed system for the past $\sim$0.7 Ma) and ID-TIMS U-Pb. This work will be carried out by NIGL staff member Nick Roberts, who will also reprocess the old data with the revised version of `ET_Redux`, as explained in the Case for Support.

Other directly incurred

Computer infrastructure As explained in Section 5.1 of the Case for Support, `IsoplotR` can be accessed online, offline and from the command line. The online version of the program is currently hosted on a 7-year old desktop computer in the PI's office at UCL. This machine is struggling to handle the levels of traffic that the app is already generating (currently 100 individual users per day and growing). Funds are requested to acquire a state-of-the-art computer server to host this crucial piece of software. Eventually the contents of this server will be mirrored by computers abroad to further improve speed and robustness. We also request funds for one desktop computer for the RSE during his/her residence in the Earth Science Department.

Conference attendance The software deliverables will be officially launched at international conferences, including EGU, AGU and Goldschmidt. Additionally, funds are requested to attend EARTHTIME meetings, which

Justification for Resources

are often organised before the GSA annual convention.

Academic visits The proposed research builds on existing software such as `IsoplotR`, `Pychron`, `ET_Redux`, `Ar-Ar_Redux` and `shiny`. This is a key aspect of the proposal and a departure from previous geochronological software development efforts. We will actively collaborate with the creators of `Pychron` and `ET_Redux` and seek funds to support two three-week visits from Dr. Jake Ross (New Mexico Tech) and Prof. Noah McLean (University of Kansas) to facilitate this collaboration.

Impact

Educational videos The cost estimate for the educational video is based on Prof. Iain Stewart's 'Anatomy of an Earthquake' that is mentioned in the Pathways to Impact. The video –and the `IsoplotR` tutorials– will require a significant CGI component. This will be supplied by an independent creative media outfit, many of which exist in London.

Summer School During the final year of the project, we will organise a one week summer school at UCL for 50 junior scientists (PhD students and postdocs). The purpose of this event is to promote statistical awareness among the next generation of geochronologists, and to promote the use of the free software tools that will be developed under the proposed research programme. Funds are requested to subsidise housing and catering for the attendees, and to cover the expenses of guest lecturers such as Project Partners McLean and Ross who will contribute content to the school. After project completion, the curriculum of the summer school will be incorporated into the workshops that NIGL already runs on a bi-annual basis.

geochron@home Funds are requested to develop a `geochron@home` app for online fission track dating, and for its installation on the same server that will also host the online version of `IsoplotR`. A rudimentary version of this app was developed by King's College physicist and freelance programmer Jiangping He. The requested funds will cover Dr. He's time to finish the code and transfer control to the RSE at UCL.

Justification for Resources

Pieter Vermeesch

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EDUCATION

- ◇ Stanford University, Stanford, CA, United States.
  Ph.D. in Geology, June 2005.
  Thesis title: *Contributions to detrital thermochronology.*
- ◇ Massachusetts Institute of Technology, Cambridge, MA, United States.
  M.Sc. in Geosystems, July 2000.
  Thesis title: *Thermal evolution of a compositionally stratified Earth, including plates.*
- ◇ Universiteit Gent, Gent, Belgium.
  B.Sc. in Geology, July 1999.
  Thesis title: *Studie van de recente evolutie van het Issyk Kul Bekken (Tien Shan, Kirghistan) met behulp van warmtefluxmetingen, hoge-resolutie reflectie-seismische profielen en veldwaarnemingen.*

WORK EXPERIENCE

- ◇ Reader, University College London (2014 – present)
  Teaching: Isotope geology, (geo)statistics and data analysis, Dorset field trip
- ◇ Senior Lecturer, University College London (2012 – 2014)
- ◇ RCUK Academic Fellow, Birkbeck College (2007 – 2012)
  Teaching: Introduction to Geology, Assessed field techniques I
- ◇ Marie-Curie postdoctoral researcher, ETH-Zürich (2005 – 2007)
- ◇ Research Assistant, Stanford University (2001 – 2004)
  Assisted students and faculty in the School of Earth Sciences GIS lab.
- ◇ Field Engineer, Schlumberger Wireline, Ras Shukeir, Egypt (2000 – 2001)
  Performed borehole measurements on- and off-shore.

RESEARCH INTERESTS

(detrital) geochronology and thermochronology, terrestrial cosmogenic nuclides, statistical analysis of geochemical data, remote sensing, aeolian geomorphology.

HONOURS AND AWARDS

- ◇ 2017 GSA Bulletin Exceptional Reviewer
- ◇ 2011 Birkbeck Excellence in Teaching Award (BETA)
- ◇ 2010 Birkbeck College's Ronald Tress Prize for excellence in research
- ◇ 2009 Geology Exceptional Reviewer
- ◇ Most cited paper award 2004-2007 for the EPSL article "How many grains are needed for a provenance study?"
- ◇ Best oral presentation at the 2005 Stanford School of Earth Sciences research review
- ◇ Francqui Fellow of the Belgian American Educational Foundation
- ◇ 1999 Valère Billet Award for best geology student of Ghent University

COMMUNITY SERVICE

- ◇ Reviewer for Aeolian Research; American Chemical Society; Austrian Science Foundation; Anais da Academia Brasileira de Ciências; Basin Research; Chemical Geology; Computers & Geosciences; Earth and Planetary Science Letters; Earth Surface Processes and Landforms; Estuarine, Coastal and Shelf Science; Geochemistry, Geophysics, Geosystems; Geochimica et Cosmochimica Acta; Geology; Geological Journal; Geological Magazine; Geological Society of London Special Publications; Geomorphology; Geophysical Journal International; Geophysical Research Letters; Geosciences; Geoscience Frontiers; Geosphere; Geostandards and Geoanalytical Research; Global and Planetary Change; Gondwana Research; GSA Bulletin; Icarus; International Journal of Earth Sciences; International Journal of Applied Earth Observation & Geoinformation; Journal of Asian Earth Sciences; Journal of Analytical Atomic Spectrometry; Journal of Geology; Journal of the Geological Society; Journal of Geophysical Research (JGR) Earth Surface; JGR Solid Earth; Journal of Mountain Science; Journal of Quaternary Science; Journal of Sedimentary Research; Lithosphere; Marine Geology; Mathematical Geosciences; National Science Foundation; Nature; Nature Communications; PLoS ONE; Quaternary Geochronology; Quaternary Science Reviews; Radiation Measurements; Radiocarbon; Remote Sensing; Remote Sensing of Environment; Science; Scientific Reports; Swiss Science Foundation; Tectonics; Terra Nova; Water.

- ◇ Member of the NERC Peer Review College (2012 - present)
- ◇ Steering Committee member of NERC's Cosmogenic Isotope Analysis Facility (CIAF, 2018-present).

Research Grants

- ◇ 2018: Thesiger-Oman Scholarship from the Royal Geographical Society (£8,000)
- ◇ 2015-2018: Leverhulme grant RPG-2015-020: "Assessing the potential of lunar geology as a window into galactic history" (Co-I with Prof. Ian Crawford, £174,468)
- ◇ 2015-2017: Leverhulme grant RPG-2014-410: "Determining erosion rates to revive the LOREX neutrino experiment (Macedonia)" (PI, £119,337)
- ◇ 2013-2015: NERC standard grant NE/K003232/1: "^{4}He/^{3}He laser microprobe analysis: a disruptive new technology for in-situ U-Th-He thermochronology" (PI, £295,452)
- ◇ 2011-1014: NERC Standard Grant NE/I009248/2 for "Dust storms and Chinese loess over the last 22 million years." (Co-PI with Dr. Thomas Stevens, £360,996)
- ◇ 2011-2016: ERC Starting Grant 259504 for "K-Ar and Ar-Ar geochronology by stepwise dissolution." (PI, €580,992)
- ◇ 2011: NERC-CIAF award for "Sediment storage and recycling in the Namib Sand Sea and its Miocene ancestor" (PI, £13,200)
- ◇ 2009: NERC-CIAF award for "Measuring the residence time of sand in Namib dunes with cosmogenic nuclides."(Pi, £8,565)

Admin

- ◇ 2015-present – Undergraduate admissions tutor
- ◇ 2009 - 2011 – MRes Earth Science programme director

Papers

- ◇ 75 publications of which 35 as first author and 20 as single author.
- ◇ 3286 citations of which 439 in 2016, 589 in 2017 and 867 in 2018; h-index = 27.
- ◇ Full list of publications available at `https://tinyurl.com/pvbib`

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Saturday, December 29, 2018

Dr. Pieter Vermeesch
Department of Earth Sciences
University College London

Dear Pieter,

I am delighted that you asked me to be a part of the team that you are assembling for your project to update and maintain a new set of standard statistical tools for geochronologists. As you point out in your NERC proposal, many of us old timers are getting "long in the tooth" and some of the standard bits of software are no longer maintained. Additionally, you have introduced some new concepts that could be very important for fundamental issues that the community must wrestle with (e.g. the age of the Earth). Derek York was my PhD supervisor and ever since my first days as a graduate student, I have been keenly aware of the importance of correlated errors!

As you mentioned in your e-mail, my approach to extrapolating noble gas data back to the time of sample inlet could be a useful contribution to the "timezero" section of your project. It has the charm of being based on simple physical parameters and it achieves performance similar to parabolic fits with one fewer fitted parameter. It also has the ability to stably handle low signal sizes, particularly in cases where the signal decay rate is comparable to the rate of rise due to memory effects.

I would also be interested in helping out with sections dealing with constrained least squares minimization problems as I have implemented some of the algorithms of Mifflin and Menke in fitting distributions, where the sum of all items must equal one and no member's contribution can go negative. This could be useful for things like isotopic abundance calculations.

I wish you good luck with your proposal and let me know how I can contribute further.

Yours truly,

Chris Hall

Assoc. Research Scientist

Dr Philip Hopley
Lecturer in Palaeoclimatology
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Tel: +44 207 6798029
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7th January 2018

Dear Sir / Madam,

Letter of Support for NERC Standard Grant by Dr Pieter Vermeesch

I would like to take this opportunity to offer my support for Dr Vermeesch (P.I.) and his application for NERC funding to work on the above project, specifically his Case Study on the U-Pb dating of carbonates in relation to human evolution.

I have been working on the geological context of Plio-Pleistocene hominin fossils from South Africa for a number of years now (Hopley et al., 2007; 2018; Maxwell et al., 2018). Early hominin fossils have been collected from the "Cradle of Humankind" in South Africa since the first australopithecine fossil, the Taung Child, was discovered by Raymond Dart in 1924 (Dart, 1925). None of these globally important fossils could be radiometrically dated until the pioneering U-Pb study of Walker et al. (2006). Since then, most of the South Afridan early hominins have been associated with one or more U-Pb ages (e.g. Pickering et al., 2018). However, the age uncertainty on most of these dates is large (100,000s of years), and the current methods used to correct for initial ^{234}U-^{238}U disequilibrium add a large amount of additional uncertainty to the corrected ages. In addition, some hominin specimens remain undated, such as the iconic Taung Child.

In collaboration with Project Partner Nick Roberts, and with support from National Geographic and NERC Isotope Facilities (IP-1489-1114), I have been working on U-Pb dating the Taung Child (e.g. Hopley et al., 2013). We have successfully produced an unpublished minimum age of 1.99 ± 0.05 Ma for the fossil, but have been unable to produce a meaningful age for the underlying cored sediments, preventing us from producing a bracketed age for the hominin. The Taung core material is generally low in U, making age determination difficult. Using conventional statistical treatments we have produced a poorly constrained maximum age of 1.4 ± 2.7 Ma. It is highly likely that the PI's proposed improvements to the age calculations of carbonate U-Pb ages will improve the precision and accuracy of this U-Pb dataset, resulting in a meaningful age. In addition to this reanalysis of existing data, we propose to improve the dating of the Taung sedimentary sequence through the collection of additional U-Pb data.

I would be very happy to offer support for this Project, through the sharing of unpublished U-Pb datasets and through the provision of carbonate material from Taung. I also have carbonate material from additional South African hominin localities, should it be considered necessary to produce additional ^{234}U-^{238}U measurements to improve published U-Pb age calculations.

The proposed geochronological research will clearly be of huge importance to many different scientific fields. For my particular field of interest, palaeoanthropology, the opportunity to improve both the accuracy and precision of carbonate U-Pb ages is potentially transformative. Many more “young” carbonates will yield meaningful ages, with substantial gains in the understanding of patterns diversity, speciation and extinction in hominin evolution (e.g. Maxwell et al., 2018). The proposed improvements to carbonate geochronology will also have major implications for speleothem climate reconstructions in the Neogene; see Hopley et al. (2018) for an example of a speleothem climate record that would benefit from the proposed improvements to U-Pb dating. There are many more Plio-Pleistocene carbonates from South African caves, most associated with hominins or other fossil mammals, that if datable, will transform our understanding of both the climatic and evolutionary history of southern Africa.

I have known Dr Vermeesch as a colleague at UCL and Birkbeck for a number of years now. I have always been impressed by his analytical abilities and his vision for geochronology. I have no doubt that, if funded, he will be able to make a success of this project and to deliver the proposed scientific goals. I hope you view his proposal favourably.

Yours Sincerely,

Dr Philip Hopley

References:
Dart, R. A. (1925). *Australopithecus africanus*: The Man-Ape of South Africa. *Nature* **115**: 195-199.
Hopley, P. J., et al. (2007). High- and low-latitude orbital forcing of early hominin habitats in South Africa. *Earth and Planetary Science Letters* **256**: 419-432.
Hopley, P. J., et al. (2013). Beyond the South Africa cave paradigm - *Australopithecus africanus* from Plio-Pleistocene paleosol deposits at Taung. *American Journal of Physical Anthropology* **151**: 316-324.
Hopley, P. J., et al. (2018). Orbital precession modulates interannual rainfall variability, as recorded in an Early Pleistocene speleothem. *Geology* **46**(8): 731-734.
Maxwell, S. J., Hopley, P. J., Upchurch, P., Soligo, C. (2018). Sporadic sampling, not climatic forcing, drives observed early hominin diversity. *Proceedings of the National Academy of Sciences* **115**(19): 4891-4896.
Pickering, R., et al. (2018). U–Pb-dated flowstones restrict South African early hominin record to dry climate phases. *Nature*.
Walker, J., et al. (2006). U-Pb Isotopic Age of the StW 573 Hominid from Sterkfontein, South Africa. *Science* **314**(5805): 1592-1594.

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January 7th 2019

Dear Dr. Pieter Vermeesch,

Project Partner Letter for Grant Application

This letter is in addition to the NERC Facilities technical assessment letter provided and outlines additional contributions to the proposed project, in addition to the dating itself. Your proposal outlines the development of data reduction algorithms and software that will allow the compositional nature of radio-isotopic data to be better accounted for, considering covariance within and between samples. This work builds upon the partial implementation of log ratios and capturing covariance terms in both the Ar-Ar_Redux and the ET_Redux system developed by PP Noah McLean and others. Importantly, this will all be connected to your IsoplotR software, which is rapidly being adopted by the community.

Having discussed with you in detail the project objectives, we are able to offer support as a project partner in the following areas:

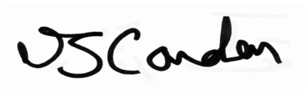
- *Access to a wide range of U-Pb, Th-Pb and U-Th data and metadata.* We have a wide array of example data sets that will cover the wide range of data types and arrays; these data can be used to test functionality of your algorithm and software. We also have significant knowledge of limiting uncertainties (e.g., disequlibrium corrections for young carbonates, $^{238}U/^{235}U$ in chondrules) to support your role in the overall improvement of geochronological data and methods.
- *Continue to beta-test software.* We will contribute to the project by working with you to beta-test the software and inter-operability with IsoplotR, the output from the 'community standard' data reduction software we use. We are also Project Partners on the NSF funded project '*EarthCube Integration: Geochronology Frontier at the Laboratory-Cyberinformatics Interface*' and will be able to test links between the various units of the emerging geochronology data infrastructure being developed.
- *Uptake in the wider community.* Getting the community to use new data tools is a challenge. We work with a wide range of end-users, both in the UK and internationally, and once developed, we will work with you to help build greater awareness of the utility of these tools as part of broader efforts to make geochronological data findable, accessible, interoperable, and reusable (i.e., FAIR). We teach early stage researchers through short courses (50+ students taught/year) and

include sections on data reduction and tools, and we would welcome your contribution to such courses.

These are areas of current activity within our facility. We are involved with a number of efforts as part of the newly commissioned National Environment Isotope Facility (NEIF) where developing systems for FAIR data is a work package. Internationally, as part of the international EARTHTIME Initiative (which includes both the high-precision and high-spatial resolution U-Pb communities) we are involved in a number of calibration experiments where new data reduction algorithms are key. As such, we're able to make an additional contribution to your project in addition to the analytical programme requested via the NERC Facility (see separate Technical Assessment letter).

Having discussed the project at length with you, we are happy to offer the assistance outlined above. We will be available to your project and will commit about thirty days of time to the project with a notional in-kind value of £30k.

Yours sincerely,



Dr. Dan Condon, on behalf of the NIGL Geochronology group:
Dr Matt Horstwood
Dr Ian Millar
Dr Steve Noble
Dr Nick Roberts
Dr Diana Sahy
Dr Simon Tapster

GEOGRAPHY, EARTH AND ENVIRONMENTAL SCIENCE WITH PLYMOUTH UNIVERSITY

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Dr Pieter Vermeesch
Department of Earth Sciences
University College London

08 January 2019

Dear Pieter,

I am delighted to write in support of the 'Beyond Isoplot' project, and in particular to confirm my interest in being involved in the educational impact component of the work.

Here at the University of Plymouth we have considerable experience in the communication of geoscience to public audiences. In addition to mainstream broadcast media, I have been actively involved in creating bespoke digital media products, much of that in relation to NERC-funded geoscience. As well as receiving funding for video-based media output associated with a current standard NERC grant on 'earthquakes in the lower crust' (PI: L. Menegon), I initiated and coordinated the production of the popular NERC-sponsored 'Anatomy of an Earthquake' video. The aim was to showcase world-class science with high-end, sophisticated graphic animation of Earth science information, working with leading media professionals to create a digital product that is globally disseminated and widely used in the school science curriculum.

That same goal will be an objective of your "Beyond Isoplot" project. Excellent science ought to generate excellent impact in the wider public, and in today's busy and fragmented media landscape that means producing a high-quality product that competes in quality with conventional gaming and broadcast media. An imaginative graphics-led educational film with strong narratives around Earth history would be timely and popular. Moreover, it is a digital format that could be designed to work both as a standard, stand-alone medium-length film (10-15 mins) and as multiple short (~1 min) geo-vignettes on specific methods and applications that might better suit dissemination via social media. Both formats could be hosted as part of NERC's Science Channel on YouTube, and embedded in the online version of your IsoplotR software for training purposes. I offer my help and expertise in implementing this innovative combination research and teaching.

In summary, I would very much welcome the opportunity to explore with you and your project team how we most effectively convey geochronology to a broad new audience.

Sincerely,

Professor Iain Stewart

PennState

Department of Geosciences
The Pennsylvania State University
503 Deike Building
University Park, PA 16802-2714

814-865-6711

NERC Review Panel

January 8th, 2019

Letter of Intent to Collaborate

To Whom It May Concern:

If the proposal submitted by Dr. Pieter Vermeesch is selected for funding by NERC, it is my intent to collaborate and/or commit resources as detailed in the Project Description of the proposal.

Specifically, generation of a new geochronological software suite has the potential to herald a new era for LA-ICPMS U-Pb geochronology, amongst other techniques. Incorporation of error covariance into the U-Pb age profiling inversion code will lead to a state-of-the-art technique, capable of resolving high-resolution thermal history information from single crystals. Such information is paramount in differentiating between competing geodynamical models from continental collision to delamination.

I hope the proposal is selected for funding.

Sincerely,

Dr. Andrew Smye
Slingerland Early Career Assistant Professor
Department of Geosciences
The Pennsylvania State University
814-863-
smye@psu.edu

COLLEGE of CHARLESTON
DEPARTMENT OF COMPUTER SCIENCE

10 January 2019

To whom it may concern,

I am writing in support of Dr. Pieter Vermeesch' application for a NERC Standard Grant to develop a new software ecosystem for geochronology.

I lead as Principal Investigator a computer science undergraduate software engineering initiative at the College of Charleston named CIRDLES.org ('Cyber Infrastructure Research & Development Lab for the Earth Sciences'). We specialize in the collaborative development of free open source software to support science domains. This material is based upon work supported by the National Science Foundation under Grant Numbers 0930223 and 1443037. CIRDLES members are designing and building a novel system for geochronological data processing that links data production to data archiving. The principal software component is ET_Redux and supports uranium-lead geochronology. We are currently extending ET_Redux to include uranium-series geochronology.

ET_Redux keeps track of error correlations by propagating the analytical uncertainties in a matrix format. Following Pieter Vermeesch' lead, it now also includes logratio statistics, which, as explained in the NERC proposal, further improves accuracy in a significant way. The new software ecosystem described in the proposal will generalize these principles to other geochronometers such as 40Ar/39Ar, and will develop an R-package called IsoplotR as a vital tool to combine dates from different chronometers for further processing. Doing this requires a universal data exchange format that accounts for all the relevant error correlations. The proposal introduces such a format, which builds on an existing architecture in ET_Redux. I would be delighted to extend this architecture to support this proposal in collaboration with Pieter and his team of software engineers.

Regards,

James Bowring, Ph.D.
Associate Professor

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Washington University in St. Louis
ARTS & SCIENCES

Department of Physics

January 11, 2019

To whom it may concern,

This letter is to support Pieter Vermeesch NERC proposal to develop new data reduction software for geochronology and cosmochemistry. I met Pieter two years ago at an NSF-sponsored workshop on $^{40}Ar/^{39}Ar$ geochronology in Socorro, New Mexico. At this workshop, he presented the new data reduction workflow that is set out in his 2015 GCA paper entitled "Revised error propagation of $^{40}Ar/^{39}Ar$ data, including covariances" .

In this paper, Pieter gives a detailed account of the prevalence and effect of correlated uncertainties. He solved this problem by casting the noble gas data into a logratio matrix format. This represents an important breakthrough, not only for $^{40}Ar/^{39}Ar$ geochronology but for noble gas geochemistry in general.

For example, the new data reduction method promises to improve the precision and accuracy of the nine-isotope xenon system, for which we have developed a custom-made multi-collector mass spectrometer in my lab at WUSTL. I am keen to collaborate with Pieter to re-analyze some of our I-Xe meteorite data using his new software.

One of the discussion topics of the Socorro meeting was the regression of noble gas signals to 'time zero' (t_0). At WUSTL, we have developed a novel approach to this problem. We introduce the sample gas into the mass spectrometer with the high voltage (HV) supply to the ion source turned off. t_0 is then defined as the moment when the HV is turned back on. Our definition of t_0 is ideally suited for Dr. Chris Hall's regression approach, which Pieter reformulated in terms of logratios.

I look forward to helping Pieter develop his new time zero regression approach, and hereby offer my support and expertise for doing so. We will exchange data and software, and participate in joint EARTHTIME meetings.

Alexander P. Meshik
Prof. of Physics

Washington University in St. Louis, Campus Box 1105, One Brookings Drive, St. Louis, Missouri 63130-4899
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GEOLOGICAL MUSEUM
NATURAL HISTORY MUSEUM
UNIVERSITY OF COPENHAGEN

Dear Panel Members:

I am writing this letter in support of the proposal by Pieter Vermeesch entitled "Beyond IsoplotR". It aims to implement novel data processing algorithms to account for previously undetected inter-sample error correlations in geochronology. The new approach has applications across the entire geological time scale including the chronology of the formative stages of the Solar System, which is my area of expertise. At present, the lack of a standard method of error assessment in this field represents a significant concern given the stated uncertainties on ages as low as ±150,000 years. For example, our 2012 paper in Science (v.338, p.651-655) on the Pb-Pb geochronology of components in chondritic meteorites dates the formation of the Solar System to 4567.30 ± 0.16 Ma and includes an age for a single chondrule of 4564.71 ± 0.30 Ma. The chondrules age is based on an isochron fit using the conventional "York regression" that yields an MSWD of only 0.16, a value that is underdispersed with respect to the analytical uncertainties. As pointed out in Section 4.1 of the proposal, this underdispersion suggests the presence of strong error correlations between the different Pb-Pb measurements in the dataset.

13 JANUARY 2019

James N. Connelly
Geological Museum
Natural History Museum
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GEOCENTER COPENHAGEN

Under the proposed research, I will work in collaboration with Dr. Vermeesch and fellow Project Partner Dr. Noah McLean to investigate the issue of inter-sample error correlation. We will reprocess the raw mass spectrometer data from our 2012 Science paper using an updated version of ET Redux. The output of this software will contain the full covariance structure of the Pb-Pb data set. This output will then be passed on to an updated version of IsoplotR to perform the revised regression analysis. We predict that the results of the proposed re-analysis will no longer be underdispersed. We further predict that the derived age will represent a more accurate and precise estimate of the age of this object. Adapting this method as a standard error assessment method for future work in the cosmochronology community will enable us to more confidently compare the results from different laboratories and, thus, construct more a accurate model of Solar System formation.

Given the importance of this issue for the geochronology community specifically and the geological community in general, I am very hopeful your panel will be able to support Dr. Vermeesch's research.

Sincerely,

James N. Connelly

VRIJE UNIVERSITEIT AMSTERDAM

2800-2900

Dr. Pieter Vermeesch
Department of Earth Sciences
University College London

DATE	OUR REFERENCE	YOUR LETTER DATED	YOUR REFERENCE
11.01.2019			
E-MAIL	TELEPHONE	ENCLOSURE(S)	
k.f.kuiper@vu.nl	+31205983559		

Subject: support letter NERC proposal

Dear Pieter,

I have read your proposal to develop "new software for better geochronology" and I am happy to offer my support for the second case study, which aims to re-evaluate the timing of critical events around the Cretaceous-Palaeogene (K-Pg) boundary. These events were constrained by $^{40}Ar/^{39}Ar$ geochronology using the Mass Spec and ArArCalc data reduction programs (Kuiper et al, 2008; Renne et al., 2013). I am keen to find out how your new software will improve the precision and accuracy of these results. Here at the VU Amsterdam, we were already looking into replacing our current data reduction software with for example Jake Ross' open source Pychron software. So I am particularly excited that your algorithms will be implemented in this program.

My contribution to the proposed research consists of two parts. First, I will share my raw mass spectrometer data for the original K-Pg paper by Kuiper et al. (2008). Second, I will reanalyse some leftover sanidine and tektites from the Kuiper et al. (2008) and Renne et al., 2013) studies using new, state-of-the-art mass spectrometers (Argus VI+ and Helix MC) in my lab. Together these data will showcase the effect of inter-sample error correlations whilst refining the timing of the most notorious mass extinction in Earth history.

I wish you success with securing NERC funding for this project and I am looking forward to a fruitful collaboration.

Best regards,

Prof. Dr. Klaudia Kuiper

FACULTY OF SCIENCE

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January 11, 2019

Dear Pieter,

I have read your NERC proposal entitled "Beyond IsoplotR: new software for better geochronology" and am excited to be involved in this important work. More than eight years have passed since we first met at an NSF-sponsored pre-AGU workshop in San Francisco, and had our first discussions about overdispersion and logratio statistics. Since then, we have implemented these concepts in several programs (HelioPlot, ET_Redux, Ar-Ar_Redux), whilst continuing to discuss the far-reaching implications of compositional data analysis for geochronology. More specifically, we came to realize that that compositional data problems and unresolved error correlations affect every aspect of geochronology, from the earliest stages of data acquisition to the calibration of the geologic time scale. Properly keeping track of these correlations requires a new generation of interconnected computer codes. Your proposal sets out a detailed plan for such a software system. The implications of this work can hardly be overstated, as it will enable a recalibration of the geologic time scale and even an improved IUPAC table of isotopic abundances.

The proposed research plan calls both for the modification of existing codes and the creation of entirely new programs. I have been personally involved in the creation of the ET_Redux program for U-Pb data reduction, together with computer scientist Jim Bowring at the College of Charleston. I look forward to working with you and Jim to add an export function to ET_Redux allowing its output to passed on to your IsoplotR program. I also welcome the opportunity to reprocess Jim Connelly's condrite data and thereby revise the age of the Solar System. I wish you all the best with your proposal and look forward to the academic visit at UCL that is discussed in the proposal.

Sincerely,

Noah M. McLean

New Mexico Tech

To whom it may concern,

I hereby confirm my support for Dr. Pieter Vermeesch' NERC proposal to develop new software for better geochronology, particularly where it relates to Pychron. Pychron is an NSF-funded suite of software that I am developing as a free and open source replacement for the widely used 'Mass Spec' software for 40Ar/39Ar data acquisition and processing. Pychron consists of a constellation of plugins that are used to control hardware (valves, lasers, mass spectrometers); record, format and archive data; calculate ages and generate (isochron, spectra or density) plots. Written in Python and shared on Github, Pychron is designed as a collaborative project, although I am its principal developer at this moment. I am excited to get Pieter and his software engineers on board. Back in June of 2017, Pieter was invited to a 40Ar/39Ar workshop at New Mexico Tech. In his presentation, he made a convincing case for a complete revision of 40Ar/39Ar data reduction and error propagation, using log-ratio statistics and matrix algebra. During the same workshop, we also had a lively debate about the thorny issue of 'time zero' regression. It soon became clear that nearly everyone in the 40Ar/39Ar community uses a different definition of time zero and employs different strategies to fit their data. These methodological differences may go a long way to explaining the difficulties that the 40Ar/39Ar community sometimes has in reproducing each other's results within the stated analytical uncertainties. One of the attendees of the workshop, Prof. Alex Meshik (Washington University of St. Louis) uses a novel solution to the time zero problem in which the high voltage supply of the mass spectrometer is used as a trigger to start the isotopic measurements. Combining this approach with the regression algorithm introduced in Section 5.5 of Pieter's proposal promises to provide a logical and internally consistent solution to this long-standing problem in noble gas geochemistry. Thanks to Pychron's modular design, it is possible to implement this and other innovations in the code. I look forward to visiting UCL and work together with Pieter and his team to make these important changes.

Signed,

Jake Ross

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January 7th 2019

Dear Sir/Madam,

Technical Assessment for Grant Application including access to the NERC-funded NIGL Geochronology and Tracers Facility

The analytical program outlined in the proposal entitled "Beyond IsoplotR: new software for better geochronology" is technically tractable, and I can confirm that the Geochronology and Tracers Facility, NERC Isotope Geoscience Laboratory has the technical expertise, and capacity, to deliver the suite of analyses requested.

Based upon discussion with the PI, we plan a three phase approach: (1) screening of slabbed carbonate samples via laser ablation ICP-MS, SEM and CL imaging; (2) targeted U-Pb LA-ICP-MS in primary domains that have sufficient U concentrations to generate U-Pb 'isochrons', and (3) subsequent high-accuracy U-Pb and ^{234}U-^{230}Th determinations by isotope dilution TIMS/ICP-MS on carbonate micro-sampled aliquots guided by the LA-ICP-MS data. This staged approach will provide the best chances of obtaining the robust absolute age constraints for the materials provided, and the complete data required for the covariance analyses. The U-Th analyses will provide the required constraints on ^{234}U disequilibrium correction and serve as a check for closed system behaviour for the past ~700 ka. We estimate that the programme of combined high-spatial resolution and isotope dilution U-Pb and U-Th analyses has an estimated cost of £75,810 which we request to be costed into the facilities section in the JeS submission.

In summary, I can confirm that the NIGL chronology facility has the capacity, analytical capability and in-house expertise to supply the analytical and scientific support to facilitate this proposed study.

Yours sincerely,

DJCondon

Dr. Daniel J. Condon,
NERC Isotope Geosciences Laboratory
British Geological Survey.

Dr. Pieter Vermeesch
University College London
+44 (0)20 3108 6369
p.vermeesch@ucl.ac.uk

UCL

12 January 2019

To whom it may concern,

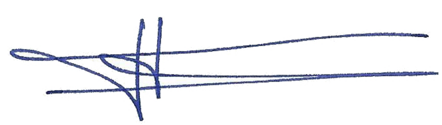
The proposal entitled "Beyond `IsoplotR`: new software for better geochronology" is a re-submission of a proposal that was rejected in the January 2018 Standard Grant round. In its decision letter, the Moderating Panel requested that a revision would "need to include a key case study to demonstrate the technological development and enhance the engagement of the wider community and thus the ultimate outcomes and impact of the work." I took the Panel's advice on board and have established contacts with six new Project Partners to develop five new and exciting case studies. These are described in Section 4 of the revised proposal and demonstrate the wide ranging impact of the proposed software.

Choosing the five case studies among a myriad of possible applications was not an easy task. A previous iteration of the proposal included a large $^{40}Ar/^{39}Ar$ investigation of the Permo-Triassic (P-T) boundary, involving SUERC Professor **Darren Mark** as a Co-Investigator. However I was worried that the £150k cost of this case study combined with the lack of space to properly describe this complex project, would elicit criticism from the reviewers. So I replaced the P-T work with a lower risk re-analysis of the Cretaceous-Palaeogene (K-Pg) boundary. Prof. Mark was understandably disappointed with this change of plans and decided to leave the project. Given this prior history, I would request that Prof. Mark not be appointed as a reviewer of this proposal.

The four nominated reviewers are well respected geochronologists with whom I have never collaborated, and two of whom (Richards and Schoene) I have never even met before. This avoids any possible conflict of interest. I obviously did not discuss any aspect of this proposal with any of the nominated reviewers.

Sincerely yours,

Dr. Pieter Vermeesch
Department of Earth Sciences
University College London



Cover Letter

Pathways to Impact

1 Summer School

Community uptake of the proposed algorithms will be accelerated by (a) their incorporation into existing data reduction software, and (b) their adoption by the Project Partners, who are among the world's leading geochronologists. To increase awareness of inter-sample error correlations and other statistical concepts of geochronology, the research team will organise a summer school at UCL during the third year of the project. This one week event will introduce 50 junior scientists (PhD students and postdocs) to geochronological data processing using the new software ecosystem. The summer school will be taught by the PI and guest lecturers including Project Partners Ross and McLean. The teaching materials will be shared on EarthArXiv, to complement the PI's "Introduction to Geochronology" lecture notes, which are already available there (`https://eartharxiv.org/sj4ft`). After the project's completion, the contents of the summer school will be transferred to the Project Partners at NIGL for incorporation into their existing biannual training courses.

2 Video tutorials

`IsoplotR`'s GUI runs within a web browser. One of the advantages of this design is the ability to embed video tutorials into the software. This will turn `IsoplotR` into a unique teaching environment. The video tutorials will be hosted on the PI's YouTube channel, which already has more than 125,000 views thanks to a popular series of optical petrography videos that are embedded in his 'Introduction to Geology' website (`https://ucl.ac.uk/~ucfbpve/intro`). `IsoplotR`'s video tutorials will not only document the software, but will also introduce the theoretical principles behind all the geochronometers implemented in it. The videos will be produced with the help of the UK's leading Earth science communicator, **Prof. Iain Stewart** (Univ. Plymouth, see Letter of Support), who will also oversee the outreach activities, which are discussed next.

3 Outreach

Geologic time is a powerful concept that captures the imagination of the general public. It is therefore surprising that, apart from a 2003 Radio 4 presentation by Melvyn Bragg, the BBC has never presented any programme on the subject. To fill this void, we will create a 15-20 minute video about geochronology and the Geologic Time Scale (GTS). The video will be similar in format and scope to Prof. Stewart's NERC-funded film 'Anatomy of an Earthquake' (`https://youtu.be/8QNigxTN384`). With over 60,000 views, this is the most watched video on NERC's YouTube channel, combining a presenter-led narrative and high-end virtual reality animation to convey the bare essentials of seismic hazard to intermediate- and advanced-level secondary school children taking science and geography around the world. The new film will show Prof. Stewart walking along a virtual geological time line, highlighting key geological events and introducing the isotopic methods that are used to date them.

Specific examples will include (a) a review of nucleosynthesis prior to the formation of the Solar System, which resulted in the formation of radioactive elements. This will be illustrated with examples of extinct nuclides such as ^{129}I, which are used to constrain the timescales over which the meteorites and planets were accreted (case study 5 of the DOW); (b) the oldest rocks and minerals on Earth, the Moon, and in space (meteorites), as dated using the U-Pb and Pb-Pb methods (case study 1); (c) the extinction of the dinosaurs, as dated by the K-Ar and ^{40}Ar/^{39}Ar-methods (case study 2); (d) cooling rates and vertical motions in the crust constrained by U-Pb, U-Th-He and fission tracks (case studies 4 and 5 of the DOW and the `geochron@home` software discussed below); and (e) human evolution (case study 3).

4 geochron@home

All the geochronological methods described in the proposal require expensive and complex mass spectrometers that are inaccessible to non-specialists. The fission track method is the only exception to this rule, which makes it ideally suited for outreach activities. Spontaneous fission of ^{238}U produces trails of damage in the crystal lattice of actinide-bearing accessory minerals such as apatite and zircon. These fission tracks can be etched out with acids and counted under an ordinary microscope, thus allowing geochronologists to determine the age of the mineral and hence the rock from which it was separated. Since its development in the 1970s and 80s, the fission track method has been widely adopted by geologists interested in reconstructing the tectonic and thermal evolution of ancient mountain belts and sedimentary basins (Malusà & Fitzgerald 2018).

Despite significant technical and methodological advances over the past three decades, the actual counting of the tracks is still very much a manual process. `geochron@home` is a *crowd-sourcing* platform for fission track counting of digital image stacks by citizen scientists. Besides serving as a visually accessible introduction to geochronological data acquisition, the tool will also improve the accuracy of fission track data. Interlaboratory

Pathways to Impact

comparison studies have shown that (a) the accuracy of fission track data is not correlated with the level of expertise of the analyst; and (b) the average estimate of many analysts is more accurate than the estimate of any one individual (Miller et al. 1985). `geochron@home` will allow each sample to be counted by dozens of analysts, beating down the noise caused by observational bias.

A basic version of `geochron@home` was developed by the PI and Dr. Jiangping He (King's College London) and is accessible from `http://geochron-at-home.london-geochron.com`. The tool has been successfully used for teaching purposes at UCL. A small budget is requested to complete the software development by (a) creating a fully fledged tutorial; (b) porting the browser-based code to native iOS and Android apps; (c) saving the image database and resuls on a standalone server (these currently reside on a virtual server on an ordinary desktop computer at KCL); (d) releasing the source code through `GitHub`; and (e) integrating the output of `geochron@home` within `IsoplotR`.

REFERENCES:•**Malusà** et al., 2018, Fission-Track Thermochronology and its Application to Geology, Springer.•**Miller** et al. 1985, Nuclear Tracks and Radiation Measurements, 10, 383.

Pathways to Impact

Outline Data Management Plan

Project Title	Beyond Isoplot: new software for better geochronology.
Principal Investigator(s)/Grant Holder	Dr. Pieter Vermeesch, University College London
Will the grant produce data Y/N?	Y
Nominated Data Centre(s)	National Geoscience Data Centre

The proposed research will produce six U-Pb datasets for the Taung Child hominin fossil, including SEM and CL images, LA-ICP-MS maps and targeted analyses, U-Th measurements (for residual 234U excess and U-Th as a test of closed system for the past ~0.7 Ma) and ID-TIMS U-Pb data.

The K-Pg case study will reanalyse previously dated samples of bentonite and tektites using the 40Ar/39Ar method. These data will be processed using Ar-Ar_Redux in both its R and Python/Pychron implementation. The raw isotopic data of this study will be stored along with an R script detailing the entire data processing chain that was used to produce the figures of the results paper. This cradle-to-grave approach is increasingly adopted by other fields of science. See, for example, the LIGO gravitational wave experiment at https://losc.ligo.org.

Making geochronological data processing more transparent and reproducible is one of the main goals of the proposed software ecosystem. The data exchange format introduced in Section 5.1 plays a central role in this. The software itself will be free, open, and shared on the popular GitHub version control service. The project team strongly believes that such openness is key to future progress in the (geo)sciences.

Data Management Plan