**Meeting Report - Workshop on Detrital Zircon U-Pb Geochronology**
*13th-14th August 2011, Prague Congress Centre, room "Club D"*

**Convenors:** Jan Kosler, Matt Horstwood, George Gehrels
**Sponsors:**
Centre for GeoBiology University of Bergen,
International Association of Geoanalysts (IAG),
Nu Instruments,
Australian Scientific Instruments (ASI),
ESI/New Wave Research,
Photon Machines

50 people attended the workshop over the two days (see attendance list at the end of the report).

Jan Kosler opened the meeting and introduced the programme. Matt Horstwood then thanked the sponsors and provided a brief recap of the outcomes of previous workshops. This included highlighting the community-derived recommended tables for the reporting of data and data acquisition information and uncertainty propagation protocol for LA-ICP-MS U-Pb dating, available on http://cirdles.org/LA-ICP_MS_Data_Handling

Jan Kosler presented the results of the detrital zircon inter-laboratory comparison exercise which had been undertaken by 9 laboratories (7 ICP-MS, 2 SIMS) in preparation for this workshop. The conclusions from this study were broadly:

- LA-ICP-MS U-Pb data are currently limited at the +\- 2% (2SD) level
- LA data were no more precise nor accurate than SIMS data
- There appeared to be a general shift in LA results to younger ages compared to TIMS data
- This shift to younger ages was likely a result of minor Pb-loss effects c.f. chemical abrasion (CA-)TIMS values and that the Seiland reference zircon likely demonstrated greater Pb-loss characteristics.
- Probability Density Plots (PDP's) of the results don't show the details of differences illustrated in accuracy (meas/true) plots
- most labs identified a 5% population within 36 analyses, and a 3% population after 67 analyses
- there was a natural tendency towards sampling bigger grains

**Action – Interlaboratory comparison study to be published, Jan Kosler to lead**

Jan Kosler presented a study addressing questions of sampling bias. Particular questions in this area posed prior to the workshop were:

- What are the potential biases involved in separating accessory minerals from rock?
- What are the best procedures for making unbiased selections of zircon grains for analysis?
- Should the grains be selected/mounted randomly or should we use another strategy to ensure that all age populations are mounted and analyzed?
- Should all the grains be imaged prior to the LA-ICPMS/SIMS dating to reveal their internal structures?
- For grains with multiple age zones, which zones should be analyzed – Cores? Rims? Both?

The results of the study and discussions highlighted that strong biases resulted from mineral separation procedures (hydraulic separation, magnetic separation, handpicking) but that natural bias in samples (due to deposition and winnowing mechanisms, relative erosion rates, etc) were much stronger and fundamentally limited data interpretation. It was determined that every separation procedure was likely to bias the sample but that all procedures were OK for identifying age peaks but not their relative abundance. Best option to limit biasing was seen to be not to separate where possible and use a sampling protocol using thin sections but that this still left natural bias as fundamentally limiting. Imaging (e.g. CL/BSEI for zircon, electron probe mapping for monazite) prior to analysis was considered to be essential for informed interpretation of the data. It was considered that where apparent, both core and rim phases should be targeted for analysis to obtain all the information available from the sample but it was recognised that this would bias interpretation of a PDP. However, if not interpreting relative abundance, only presence or absence of age peaks, this is not problematic.

The ability to use relative abundance as an accurate quantifier of similarity between samples was seriously questioned and appeared flawed. It was noted that the published statistical studies indicating the required number of analyses (N) from a sample were generally conservative and should be followed. It was noted that separation procedures typically used should best be changed when addressing detrital problems to better limit separation bias and that a more considered approach to separation methods was generally required for all studies rather than a 'one-size fits all' assumption.

***Recommendation*** *- relative abundance within and between samples in detrital studies is not to be used for interpretation unless significant proof demonstrates that the abundances have not been skewed by separation procedures. Separation procedures typically used can only allow identification of the presence of peaks not relative abundances. Natural bias likely prevents interpretation of relative abundances. Targeted analyses form the other end of the spectrum where relative abundance is obviously not representative. It should be noted that absence of age components does not mean that they were not present in the source, just that they have not been sampled by the depositional process or have been lost in transit/deposition.*

**- Action – manuscript is being prepared on the highlighted study by Jan Kosler and co-workers**

Alexander Nemchin gave a presentation highlighting data filtering. Particular questions in this area posed prior to the workshop were:

- What discordance cut off should be recommended, for the plotting of PDP's, 5%?
- Is it better to use the Nemchin & Cawood (2005) idea of Concordia ages for each data point with their importance in the PDP weighted according to their discordance? Can we develop a software tool to calculate this?
- Should different ratios be used to represent age in PDP's when they are more precise (i.e. switch between $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ ages at c. 1 Ga?)

It was suggested that the level of discordance used as a discriminator in deciding which points to plot in a PDP, made little difference to the overall age profile. However, variations do occur at small scale and interpretations of PDP's should therefore be made carefully and/or on a broad scale. Using a concordia age result for each data point as a representation of its age provides a more robust age assessment but is heavily biased to the Pb/Pb age which for strongly discordant data will still represent a significantly younger age than the true age. However, using a data point concordia age double weighted for concordancy and uncertainty is likely the best representation method available and avoids the need to make subjective decisions on discordance discrimination level and which ratio (Pb/Pb or Pb/U) to represent in a PDP. It was noted that a software tool available to all which allowed this assessment would be useful. The presentation also displayed the viewing of data and defining of populations using 3D probability plots. The coding for these plots is available in MatLab.

**Action: Alexander Nemchin willing to modify coding and make available**

Keith Sircombe gave a presentation discussing statistics and uncertainties. Particular questions posed prior to the workshop were:

- How do you identify (significance?) a population peak and quantify its age and uncertainty?
- How are the uncertainties on the defined population to be expressed (are they asymmetric)?
- Should we accept a 1-2% limit on the level of uncertainty on a defined population age until such time as we can prove we can do better? Since 2% (2s) is the likely ILC limit why are ages interpreted at better than this resolution anyway??
- Should we be using Gaussian or non-Gaussian distribution statistics for these data?
- N – how many concordant and/or total analyses do we need?

Mathematicians have already been engaged by the SIMS community (led by K. Sircombe) to answer many of these questions. Pritchard et al 'Provenance of sedimentary rocks' www.maths-in-industry.org/miis/277 summarises the thoughts and outcomes of this engagement. Key conclusions from this previous exercise included:
- there are no silver statistical bullets
- understanding the exact nature of our data and how data are acquired is critical to knowing how data can be used and managed, and that
- these data are heteroscedastic

This ‘Maths in Industry Study Group’ meeting recognised that detrital data likely dont fit an assumption of a Gaussian distribution but that there is little else to use - populations probably have an asymmetric distribution but for all practical purposes they must be assumed to be normal at this time. It is likely that astronomers, biologists and fission track practitioners can probably give valuable insight into this and better tools are required.

New tools are required by the detrital zircon community for identifying populations and defining their uncertainties but it was noted that these are essentially present and in use by other communities and could be adapted. In light of current capabilities, reference materials and the ILC results reported above, there was general agreement that a 2% (2SD) uncertainty should be considered limiting when quantifying and interpreting detrital zircon data. The current publications suggesting the number of grains to be analysed in a detrital zircon study should be followed, noting that with increased degree of discordance there will be a low probability that all of the age peaks in the sample have been successfully identified.

**Action – Pieter Vermeesch agreed to do some software modifications to a programme for the identification and quantification of peaks with an assigned uncertainty for these peaks.**

**Action – Colleagues (Sircombe/Paton/Nemchin/Dunkl) with mathematician/astronomer co-workers to instigate discussions on the nature of detrital zircon data and peak identification (e.g. subtracting major peak contributions to look at validity of small peaks).**

George Gehrels gave a presentation discussing interpretation limits in LA U-Pb detrital zircon data. Particular questions posed prior to the workshop were:

- When is a population geologically meaningful (n=1)? Answers may vary depending on whether data are used to determine provenance, correlation, or maximum depositional age.
- N – Does the required number vary depending on the question to be solved?
- What is the best method of describing the age and uncertainty of the youngest age component and the maximum depositional age? How should these data be interpreted? What limits are there?
- clustering versus concordancy as a measure of ‘robustness’ of age identification
- How does the discordant nature of data affect/limit the level of interpretation?
- What is the best method for comparing the age distributions of several samples?

- Is presence/absence or proportion of ages more important? In light of sampling bias issues, should we be interpreting abundance?
- Should core and rim determinations giving the same age from the same grain be included in a PDP?

It was demonstrated that data need to be assessed for analytical robustness using plots of age vs U, U/Th, 206/204, Hg and LIEF corrected 206/238 for example. It was clear that the number of data points required to represent a population (n) as meaningful, varied with the total number of data points (N). Probabilities for the data set should be quoted to illustrate this. The required number of total data points (N) does vary depending on the question being addressed. In trying to determine a maximum depositional age the current practice of relying on the youngest data point is not reliable. Very low confidence can be assigned to a single data point result. Multiple analyses of a single grain are required to establish concordance. Even then, whole grain Pb-loss could be present. In this case, taking populations with n=3+ where n represents the number of different grains, is a more reliable estimator of maximum depositional age. It should also be remembered that other minerals might define this parameter better (e.g. rutile) or even another method (e.g. Ar-Ar white mica). It should not be forgotten during interpretation that the true depositional age of a sediment could be considerably younger than the youngest components constituting the sediment, depending on the age of materials sampled by the sedimentary process. Also, since sedimentary rocks are predominantly heterogeneous (they have beds!), it is better to analyse multiple samples than perform thousands of analyses on one sample. It was proposed that since populations are essentially clusters, clusters are a better arbiter of a robust result than concordance. A concordant cluster is better still. Since populations constitute collections of grains which may have different origins, the 'peak age' may not have geological meaning. Weighted means should not therefore be used to define population ages and their uncertainties. Some members of the community argued for including all data from a sample during interpretation, no matter how discordant, using different statistical mechanisms to reduce the impact of highly discordant data, whilst others believed that only near concordant data should be interpreted and better samples found to replace those that have suffered extensive Pb-loss. Clearly there is some debate still to be had here. It is clear that the community lacks software tools by which comparisons of similarity can be made between samples. Over the course of the workshop George Gehrels, Keith Sircombe and Pieter Vermeesch showed examples of possible new tools and were encouraged to work these up to be useable for the community. From discussions in the workshop so far it is clear that presence/absence of an age component is a more important characteristic in a sample than proportion and if abundance is not being interpreted core and rim ages from the same grain, even if the same, can be included in the same PDP.

*Recommendation*

- *single data point results should not be used to define maximum depositional age. Use populations with data points (n=3+) with overlapping uncertainties or multiple analyses of a single grain to define confidence in this interpretation. Preferably use other information/minerals (e.g. rutile) and isotope systems (e.g. Ar-Ar white mica) to get better assessment of maximum depositional age*
- *weighted means and uncertainties should not be used to define detrital populations*

**Action - Vermeesch, Sircombe, Gehrels, to derive better tools for quantification of populations and uncertainties and similarity between populations.**

Istvan Dunkl presented on data reporting and alternative tools for the expression and interpretation of detrital zircon U-Pb data. Particular questions posed prior to the workshop were:

- How should U-Pb detrital zircon data be presented to best convey the age information and quality of the data?
- Are there better methods for the expression of detrital age data rather than the PDP?
  - Residual error analysis of age-provenance data

- Are there software programs used by heavy mineral researchers (or other scientific disciplines) that we may adopt or modify for our purposes?
- Can better software tools be developed for representing detrital age spectra?

It was concluded that there is a need for more information to be shown in published diagrams (e.g. discordance, age of sedimentation where known) than is currently displayed. New tools are required and some have already been offered in this workshop (see previous actions). This presentation also confirmed that the youngest single data point age in a data set had very little meaning, it is not an age component. It was suggested that a PDP is not a good diagram for the community, it is a 'broken tool' and something better is now needed. Kernel distribution functions are a better tool statistically than PDP's but they ignore data point uncertainties. They could be used in combination with PDP's. A 'discordance corrected (Dc)PDP' (Dunkl) and a 'dendrogram & 'DNA plot' (Sircombe) were offered as better tools for visualisation of comparison between samples. New tools should also include the capacity to visualise or recover quality information (e.g. uncertainty, concordance). At this stage in new tool development, users and developers should look to design sophisticated solutions possibly including interactive software with multiple visualisations (DcPDP, DNA, concordia, 3D).

**Action – Dunkl/Sircombe/Nemchin/Vermeesch/Gehrels encouraged to work up new visualisation tools for release/publication**

An evening poster session (see list of posters below) allowed further discussion of the days events.

On day 2, George Gehrels discussed archiving of new U-Pb data and the re-use of legacy data. Particular questions posed prior to the workshop were:

- Why do we need to archive data?
- How do we do this?
- How should detrital zircon U-Pb data be archived/tagged such that specifically targeted data are not over-represented in data populations? E.g the presence of young rims in a detrital sediment.
- How should database queries of detrital zircon U-Pb data be performed, e.g. should samples with less than the ideal number (80-100?) of analyses be omitted from a database query for regional studies to prevent apparent absence of components within small datasets biasing the query?

It is clear that archiving of data is rapidly becoming a prerequisite of the funding organizations in order to maximize the value of their investment. Tens of thousands of analyses are published each year but little agreement is present on the appropriate format under which detrital zircon analyses should be archived. The structure and content of a new database ('Geochron' http://www.geochronportal.org/) was detailed. Community input into the design and construction of the database for legacy data was encouraged. Correlation of the inputs and outputs for the database with previously recommended data and information reporting tables would be beneficial. Discussion regarding some specifics, particularly quality assurance, validation and the inclusion of data not corrected for common-Pb, ensued. It was suggested that the Working Group should compile a proposal detailing requirements for legacy data in a database.

**Action – Working Group to propose a standard for entry of legacy laser ablation U-Pb data into databases.**

During the workshop it also became clear that the terminology used in detrital analytical science needed defining and standardising. Some terms needed to be used with care, in particular the use of 'age' which suggests 'a definitive igneous event recorded in the rocks'.

Discussion of ‘ages’ should be avoided unless supported by strong geological evidence or robust statistical analysis. In light of the breadth of the detrital science community any recommendation on terminology would need to be made in consultation with colleagues in other disciplines.

**Action – Proposal on detrital zircon science terminology standardisation to be compiled.**

Attendees requested that presentations were made available. Presenters have agreed and their presentations will be posted on the cirdles website. **- Action**

**Summary**

***Actions***

1) Meeting report to be compiled and made available
2) Interlaboratory comparison study to be published, Jan Kosler to lead
3) Manuscript on sampling bias is being prepared on the highlighted study by Jan Kosler and co-workers
4) Alexander Nemchin to modify coding for 3D probability plots and make available
5) Pieter Vermeesch to do some software modifications to a programme for the identification and quantification of peaks with an assigned uncertainty for these peaks.
6) Colleagues (Sircombe/Paton/Nemchin/Dunkl) with mathematician/astronomer co-workers to instigate discussions on the nature of detrital zircon data and peak identification (e.g. subtracting major peak contributions to look at validity of small peaks).
7) Vermeesch, Sircombe, Gehrels, to derive better tools for quantification of populations and uncertainties and similarity between populations.
8) Dunkl/Sircombe/Nemchin/Vermeesch/Gehrels encouraged to work up new visualisation tools for release/publication
9) Working Group to compile a standard for entry of legacy laser ablation U-Pb data into databases.
10) Proposal on detrital zircon science terminology standardisation to be compiled.
11) Presentations to be made available on the web

***Recommendations***

1) Relative abundance within and between samples in detrital studies is not to be used for interpretation unless significant proof demonstrates that the abundances have not been skewed by separation procedures. Separation procedures typically used can only allow identification of the presence of peaks not relative abundances. Natural bias likely prevents interpretation of relative abundances. Targeted analyses form the other end of the spectrum where relative abundance is obviously not representative. It should be noted that absence of age components does not mean that they were not present in the source, just that they have not been sampled by the depositional process or have been lost in transit/deposition.

2) Single data point results should not be used to define maximum depositional age. Use populations with data points (n=3+) with overlapping uncertainties or multiple analyses of a single grain to define confidence in this interpretation. Preferably use other information/minerals (e.g. rutile) and isotope systems (e.g. Ar-Ar white mica) to get better assessment of maximum depositional age

3) Weighted means and uncertainties should not be used to define detrital populations

**Evening Poster Session**

1) *Matrix effects on down-hole U/Pb fractionation among well-recognized zircon standards* (Charlotte M. Allen)
2) *A considered approach to detrital zircon U-Pb geochronology and microtextural relationships* (Laura Bracciali, Randy Parrish and Matt Horstwood)
3) *UranOS: a quick data reduction system for processing laser ablation ICP-MS data* (István Dunkl, Tamás Mikes, Dirk Frei, Axel Gerdes and Hilmar von Eynatten)
4) *Less zircons from more samples* (Sebastien Meffre)
5) *Zircons in metasedimentary rocks: using trace elements to distinguish youngest detrital ages, metamorphic overgrowths and Pb loss* (J. Michael Palin and James M. Scott)
6) *An introduction to Iolite's data reduction module for U-Pb zircon geochronology* (Chad Paton)
7) *Zircon provenance studies in Precambrian Metassedimentary sequences from Central and Southern Brazil: implications to the evolution of West Gondwana amalgamation* (Carla Porcher and Márcio Pimentel)
8) *U-Pb dating by SHRIMP IIe of Brazil in super homogeneous detrital zircon (quartzite) from Santa Catarina - South American Platform* (Kei Sato)
9) *Detrital zircon perspective on provenance of the Permian-Triassic sandstones in the Banda Arc, SE Asia* (Inga Sevastjanova and Robert Hall)
10) *Factors affecting detrital zircon age distribution - natural samples and experimental approach* (Jiri Slama and Jan Kosler)
11) *U-Pb Detrital zircon ages from the Beiras Group – implications for the neoproterozoic evolution of the SW Iberia* (Rita Sola)
12) *Principle component analysis applied to 3.0-4.35 Ga detrital zircon populations within ca. 3.0 Ga metasediments of the Yilgarn Craton* (Eric Thern)
13) *The (ab)use of statistics in detrital studies* (Pieter Vermeesch)

**Prague Laser ablation U-Pb detrital zircon workshop - Attendees**

1. István Dunkl University of Göttingen
2. Tonny B. Thomsen Stockholm University
3. Tamás Mikes University Frankfurt Germany
4. Luigi Solari UNAM,
5. Paul Sylvester Memorial University
6. Laura Bracciali NERC Isotope Geosciences Laboratory (British Geological Survey) and Lancaster University
7. J. Michael Palin University of Otago
8. Delia Rösel University of Mainz
9. Leonid Danyushevsky University of Tasmania
10. Jeffrey Oalmann University of Kansas
11. Dirk Frei Stellenbosch University
12. Sebastien Meffre University of Tasmania
13. Kate Souders Memorial University
14. Miguel A S Basei University of São Paulo Brazil
15. Charlotte M Allen Australian National University
16. Matt Horstwood NERC Isotope Geosciences Laboratory, British Geological Survey
17. Brad Hacker UCSB, USA
18. Andrew Kylander-Clark UCSB, USA
19. Zuzana Tasáryová Charles University
20. Kei Sato Sao Paulo University
21. Altug Hasozbek New Brunswick Lab, U.S Department of Energy
22. Martin Whitehouse Swedish Museum of Natural History
23. Diane Seward University of Wellington
24. Siv Hjorth Dundas University of Bergen Norway
25. Eric Thern Curtin University of Technology, Perth, Australia
26. Kenshi Maki Kyoto University
27. Inga Sevastjanova Royal Holloway University of London,
28. Nick M W Roberts NERC Isotope Geosciences Laboratory, UK
29. Chad Paton University of Copenhagen
30. Axel Gerdes Goethe University Frankfurt
31. Pieter Vermeesch Birkbeck, University of London
32. Yaron Be'eri-Shlevin Hebrew University of Jerusalem
33. Steffen Allner ETH Zurich
34. Fabian Kohlmann University of Bergen
35. Andreas Moeller University of Kansas
36. Carla Porcher Universidade Federal do Rio Grande do Sul Porto Alegre - RS - Brazil
37. Jan Kosler University of Bergen Norway
38. Charles Magee Australian Scientific Instruments
39. Rita Sola Laboratório Nacional de Energia e Geologia, Amadora, Portugal
40. Norman Pearson Macquarie University, Sydney, Australia
41. Thanusha Naidoo University of Stavanger, Norway
42. Jeff Vervoort Washington State University, United States
43. Jon Woodhead University of Melbourne, Australia
44. Janet Hergt University of Melbourne, Australia
45. George Gehrels University of Arizona, United States
46. Keith Sircombe Geoscience Australia
47. Sasha Nemchin Curtin University of Technology, Perth, Australia
48. Steve Shuttleworth Photon Machines
49. Kerstin Drost University of Bergen
50. Jiri Konopasek University of Bergen