DATA PROCESSING PACKAGES FOR LA-ICP-MS U-PB AGE DATING

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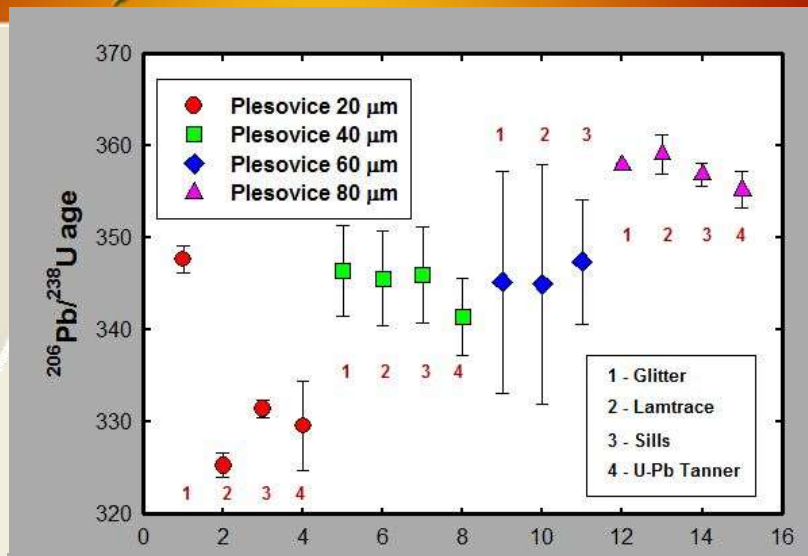
The Initiative

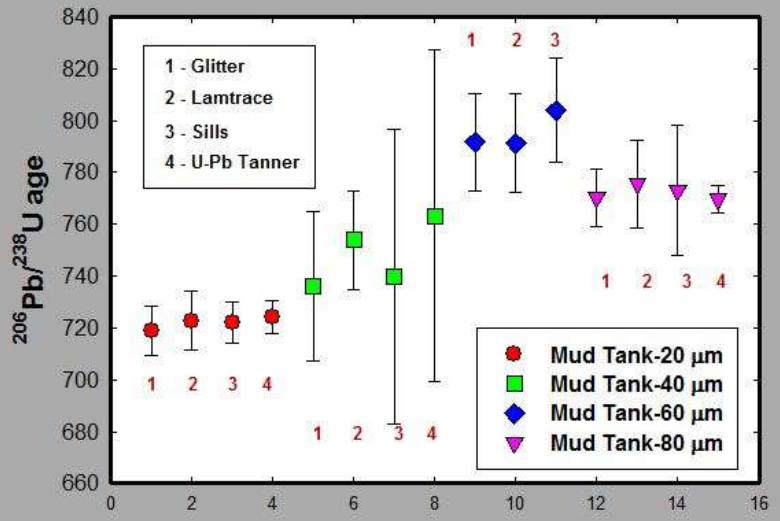
- To determine best practices in LA-ICP-MS U-Pb data processing
- Provide a set of (reasonably) standardized procedures
- Publish these as a paper in a thematic issue

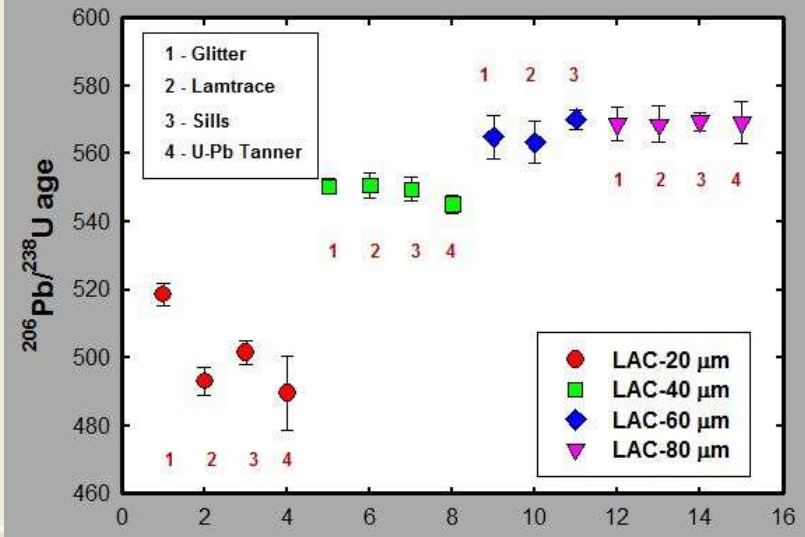
Software Round Robin

- Software comparison proposed at San Francisco Workshop, Dec. 2009.
- Develop and distribute “synthetic data sets” to a group of users
  - Create synthetic data to be reduced by all packages
  - Have ten (10) users, with a range of expertise, reduce data with each package to evaluate operator bias.
  - Use the revised data reduction systems to evaluate new ILC data and then compare results.
- Aims to to evaluate & improve existing data-reduction packages
  - Create versions of existing packages that follow the recommended flow

Issues?


Plesovice 20 µm
Plesovice 40 µm
Plesovice 60 µm
Plesovice 80 µm
1 - Glitter
2 - Lamtrace
3 - Sills
4 - U-Pb Tanner
$^{206}Pb/^{238}U$ age


1 - Glitter
2 - Lamtrace
3 - Sills
4 - U-Pb Tanner
Mud Tank-20 µm
Mud Tank-40 µm
Mud Tank-60 µm
Mud Tank-80 µm
$^{206}Pb/^{238}U$ age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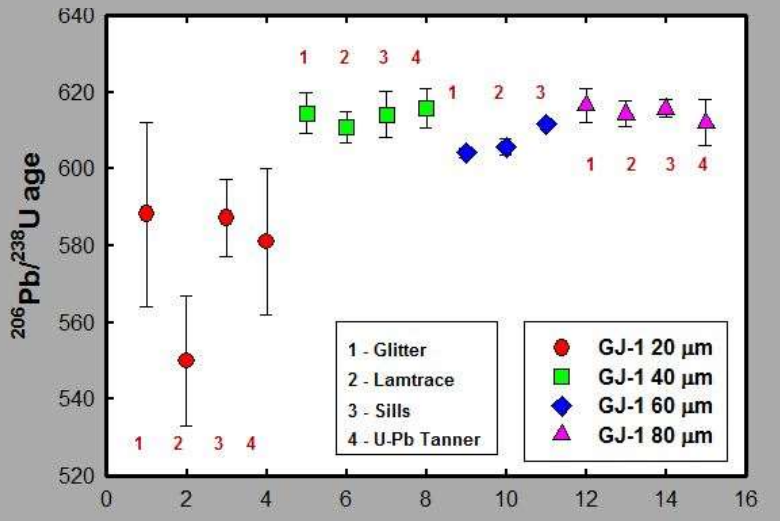
2 - Lamtrace
3 - Sills
4 - U-Pb Tanner
LAC-20 µm
LAC-40 µm
LAC-60 µm
LAC-80 µm
$^{206}Pb/^{238}U$ age


1 - Glitter
2 - Lamtrace
3 - Sills
4 - U-Pb Tanner
GJ-1 20 µm
GJ-1 40 µm
GJ-1 60 µm
GJ-1 80 µm
$^{206}Pb/^{238}U$ age

Software Round Robin

Issues at the time:

- Comparison of 4 key packages just presented (Von Quadt et al., Goldschmidt 2009) – problems identified
- Biases and universal underestimation of uncertainties being identified (Hanchar round robin, Klotzli et al., 2009)
- Premature to conduct a further comparison (GLITTER and PepiAge only now being upgraded)
- ……

Free Or Commercially Available Software

Software	Platform	Contact
AgeCalc	MS Excel	George Gehrels
GLITTER	IDL	Norman Pearson et al. - http://www.glitter-gemoc.com/
ICPMSDataCal		
Iolite	Igor Pro	Chad Paton et al. - http://www.earthsci.unimelb.edu.au/isotope/iolite/index.html
LaDating@Zrn	MS Excel	Zhenhui Hou http://staff.ustc.edu.cn/~zhenhui/icpms/icpms.html
LAMBern	MS Excel	Tonny Thomsen and Thomas Pettke
LamDate	MS Excel	Jan Kosler
LAMTRACE	Lotus 1-2-3	Simon Jackson
PEPI-AGE	Standalone Win/Mac/Linux	Istvan Dunkl - http://www.sediment.uni-goettingen.de/staff/dunkl/software/pepi-age.html
UPb.age	R	Martin Tanner et al.

Logistics of a Software Round Robin

Logistics:

- Still so many different data acquisition and processing approaches, data formats, etc.
- Many data processing packages are protocol specific (e.g., aspirated Tl/U/Np normalisation, Si/Zr normalisation, common Pb correction (Hg and ^{204}Pb)
- Require different inputs and data formats (constantly changing)
- Processing using multiple programs by multiple (10) persons requires very large investment in time and $
- Sending data sets to single users, or even multiple users, of different packages risks user biases

Aims of a Software Round Robin

Aims: What are we evaluating?

- *"Pre-defined and well-specified targets have to be set"*
- *Proficiency testing* - does software meet certain specifications? If not, then what?
- *Comparison* – which software provides the most accurate ages and most realistic uncertainty estimates?
- But, how do we evaluate? One software may have the best Pb/U fractionation algorithm but perform worst due to limited drift correction options.
- Options and ease of use? e.g., method of integration interval selection, common Pb corrections, fitting options?

Processes and Corrections

1. Read in data from multiple ICP-MS platforms
2. Detector dead time and cross calibration
3. Spectral skew – single collector instruments
4. Correction of signal intensities
   - background
   - common Pb
     - if so, ^{204}Pb? – if so, correct for ^{204}Hg? Criteria required
     - ^{207}Pb or ^{208}Pb methods?
5. Outlier elimination
   - if so, what algorithm? All isotopes?
6. Integration selection
   - matching sample and standard integration intervals
   - manual- or auto-optimize for lowest uncertainty or best concordance?

Processes/Corrections

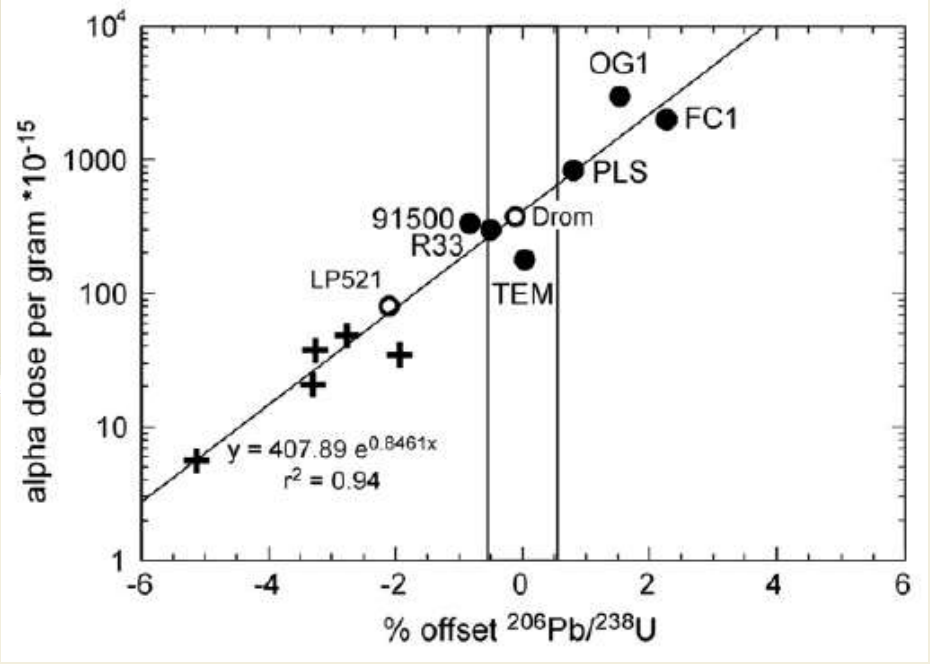
7. U-Pb fractionation
   - matched standard and integration intervals (GLITTER)
   - linear regression to time zero (or other) intercept (LAMDATE)
   - model Pb/U fractionation with exponential or more complex function (Iolite)
   - Si/Zr normalization (LAMTRACE)
8. Ratio calculation (Fisher et al., 2010)
   - ratio of mean signals
   - mean of individual ratios
   - zero (or other) intercept of linear regression
9. Standardization (instrumental mass bias and drift)
   - on-line aspirated tracers and/or
   - external standard
     - frequency of standards (Fisher et al., 2010)
     - options for interpolation between standards

Uncertainties

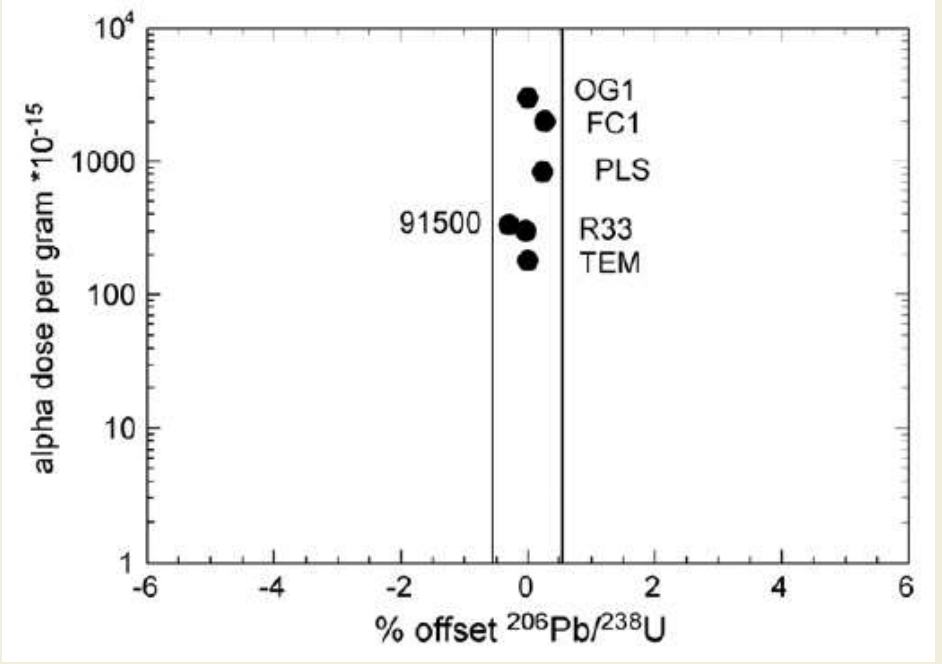
1. Analytical uncertainty of ratios of interest, both sample and standard
   - counting statistics (noise in LA-ICP-MS not counting statistics limited)
   - or, standard error of ratios
2. Uncertainty in drift correction of standardization factor
   - LIEF, Mass bias
3. Uncertainty on any corrections and correction ratios used
   - e.g., common Pb, Tl isotope ratio
4. Should corrections be applied on a time slice by time slice basis or be applied to integrated data and uncertainties propagated statistically?
5. Uncertainty on the reference ratios of standardisation materials
6. Uncertainties on decay constants
7. Long term reproducibility vs. single session (1 secondary standard?)
   - Still not sufficient to account for systematic matrix-induced biases
   - Alpha dose, REE variations

The game changer?
Sub 1% accuracy at last?

No annealing

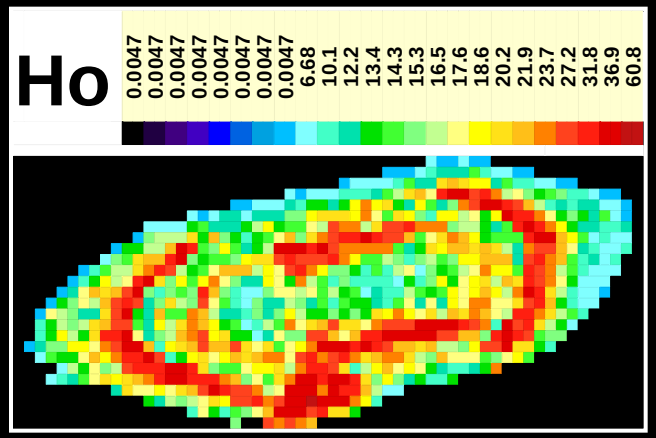


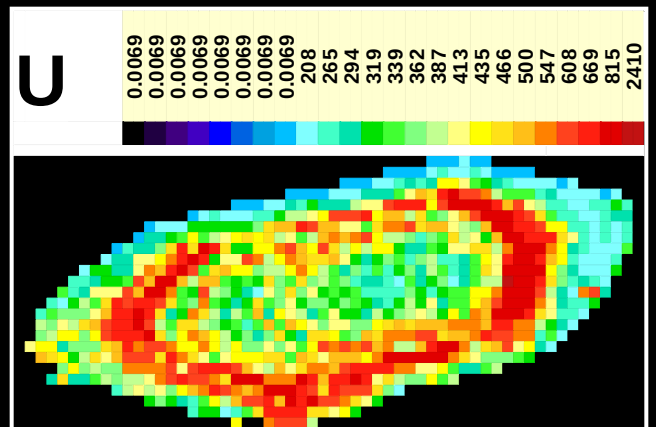
Annealed

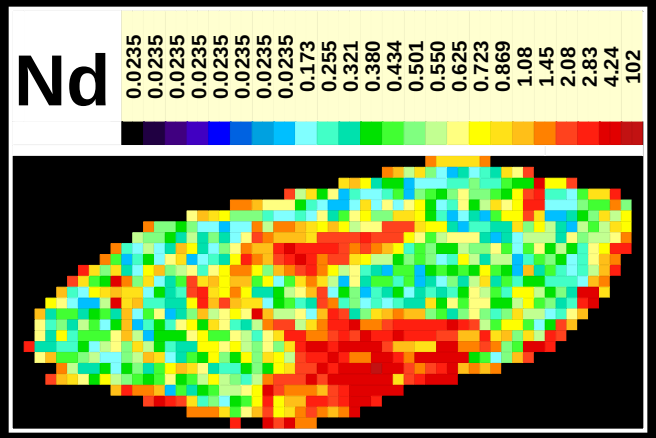


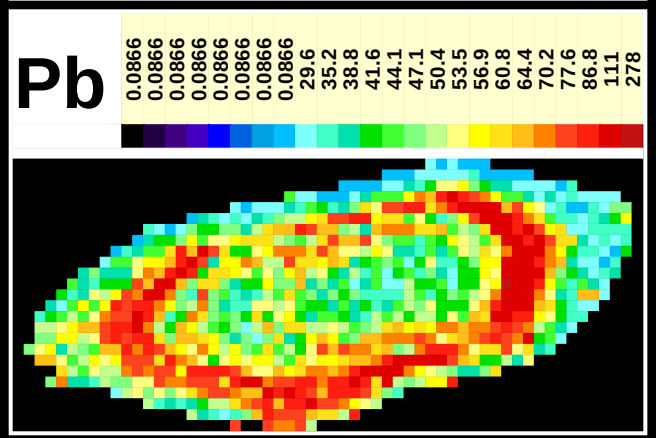
C.M. Allen, I.H. Campbell (2012),
Chemical Geology, v. 332–333, p 157–165

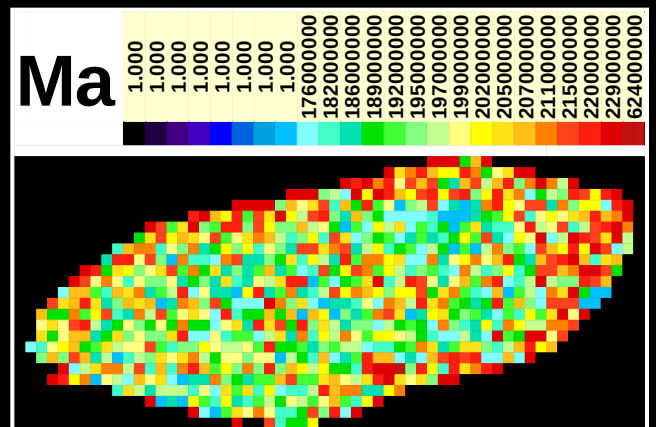
Element and age mapping











Conclusions

- Still large variations in analytical protocols and data processing software
- Need to work towards consensus on best analytical protocols and data processing strategies
  - Common Pb corrections
  - Handling Pb-U fractionation
  - “Matrix effects”
  - Uncertainty estimates
- Would a data processing software round-robin help determine best-practice in data processing?
- If so, what do we want to get out of it?
- How should it be run?