Automating U-Pb IDTIMS Data Reduction and Reporting: Cyberinfrastructure Meets Geochronology James F. Bowring¹, Noah M. McLean², J.D. Walker³, Jason M. Ash³. (1) Col of Charleston, Charleston SC 29424, (2) MIT, Cambridge, MA 02139, (3) Univ of Kansas, Lawrence, KS



Tripoli imports raw data files generated by the Sector 54, Isoprobe, and Triton mass spectrometers. Tripoli facilitates interactive visualization of temporal trends and scatter during measurement, statistical filtering of data, point-bypoint corrections for isobaric interferences, spike stripping, fractionation corrections and calculation of statistical parameters.

Tripoli is an interactive tool (Win OS) that allows the analyst to correct, save and export processed raw isotopic data. Tripoli supports live workflow from a mass spectrometer to aid in monitoring data flows. Tripoli provides several types of ratio-by-ratio corrections:

- uranium oxide corrections
- fractionation (U & Pb double spike)
- barium phosphate isobaric interferences - thallium isobaric interferences

For each correction, the analyst can specify parameters, such as a tracer (see below) or a model of the U sample components. *Tripoli* also supports the tracking of long-term trends in standard measurements and faraday gains.

Active Hotel	
Tracer	ET2535 Version 2
Tracer Type	mixed 202-205-233-235
Lab	EARTHTIME digits, NOT in scientific notation.
Date Certified	2008-04-27 1-sigma PCT
Ratios r206_204t	3.36668548197461000000 0.100000000000
r207_206t	0.80521716304278700000 0.030000000000
r206_208t	0.50519171725315400000 0.030000000000
r206_205t	0.00029893852895987800 0.03000000000
r207_205t	0.00024071043421325700 0.03000000000
r208_205t	0.00059173283874343000 0.30000000000
r202_205t	0.9998900000000000000000000000000000000
r238_235t	0.00308700000000000000000000000000000000
r233_235t	0.99464000000000000000000000000000000000
r233_236t	0.0000000000000000000000000000000000000
-	
r235_205t	100.18000000000000000000000000000000000
Isotope Concentrations	in moles/gram
concPb205t	0.000000000993073600 0.030000000000
concU235t	0.0000000099525836175 0.030000000000
	ОК

Tripoli provides interactive graphs of each ratio, allowing the analyst to discard outliers, blocks of data, or to utilize built-in filters such as 2-sigma or Chauvenet's criterion. The new statistics are displayed live (see below).

Tripoli - Selected Graphs from: ET2535 LB4, Ph tri

S	Tripoli: ET2535_LB4_Pb.trip		
T	Fripoli File DataFile DataFolder Settings Corrections Annotate Control Pa	nel l	Resource
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	1 + alphaPb		Synch
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	204/205 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	206/205		Synch
	206/205 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	207/205		Synch
	207/205 [BaP02IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	208/205		Synch
	208/205 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	206/204 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	207/204 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	208/204 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	206/207 [BaPO2IC: EARTHTIME v:1; TIIC: EARTHTIME v:1; FC: ET2535 v:2]		Synch
	206/208 [BaPO2IC: EARTHTIME v:1: THIC: EARTHTIME v:1: FC: ET2535 v:2]		Synch
	Select All Select None Select User Func Select Ratios	Sh	ow Sele

Tripoli exports the processed isotopic data to reduction software, carrying all applied corrections. *Tripoli* supports PbMac-Dat, but is designed to communicate in realtime with *U-Pb_Redux* using a publishsubscribe protocol that automates data transmission using extensible markup language (XML) schema and documents.

Live Workflow Automation *Tripoli*'s novel Live Workflow mode automatically detects new mass spectrometer data and refreshes its display. *Tripoli* lets affected by baselines, choose outliers, and calculate statistics in realtime. A button click transmits this data to U-Pb_Redux, which provides a variety of analytical tools to monitor data quality (next panel).

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Graph PrintAll Layout Clipboard Help													
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U-Pb_Redux is an open-source Java application for full U-Pb data reduction and uncertainty propagation for any U-bearing phase. U-Pb_Redux provides sophisticated graphical and statistical tools for data analysis and compilation, and produces publication-ready data tables, concordia, and weighted-mean plots. U-Pb_Redux outputs standardized analysis results—as an aliquot XML file—for export to the Geochron database. It can also import one or several aliquots from Geochron for compilation, visualization, and detailed analysis.

[New Fraction	🗹 zrc	ET2535 v.2	\$ 0.01	0.0000	0.10000	137.8800	137.8800	0.00200	example Pb Bl 🛟	Stacey-Kramers 🛟	0.0000	1.0000	0.5000	0.90000	2.8000	1.1000	0.00010	0.01000	0.01000	0.01000	0.00002	0.30000	0.50000	0.10000
(ADD	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL	FILL
Е	EDIT Fraction	ZRC?	Tracer	Tracer Mas	s Fraction mas	s U Blank mass	238/235smpl	238/235blnk	180/160Uox	Pb Blank	Initial Pb Model	Est Date	SK % Unct	SK Rhos	Pb Blank mas	s rTh_Umagma	ar231_235s	lo-ABS tracer mass	lo-ABS U blank mass	1σ-ABS 238/235 smpl	10-ABS 238/235 blnk	10-ABS 180/160 WOR	lo-ABS Pb Blank mass	lσ-ABS rTh_Unagma	1c-ABS ar231_235s
	z1	🗹 zrc	ET2535 v.2	\$ 0.01000	g 0.00000 g	0.10000 pg	137.8800	137.8800	0.002050	example Pb Bl 🛟	Stacey-Kramers 🜲	0.0	1.0000	0.5000	0.90000 P	2.80000	1.10000	0.00010	0.01000	0.01000	0.01000	0.000020	0.30000	0.50000	0.10000
	z2	🗹 zrc	ET2535 v.2	\$ 0.01000	g 0.00000 g	0.10000 pg	137.8800	137.8800	0.002050	example Pb Bl 🛟	Stacey-Kramers 🜲	0.0	1.0000	0.5000	0.90000 P	2.80000	1.10000	0.00010	0.01000	0.01000	0.01000	0.000020	0.30000	0.50000	0.10000
	z3	🗹 zrc	ET2535 v.2	\$ 0.01000	g 0.00000 g	0.10000 pg	137.8800	137.8800	0.002050	example Pb Bl 💲	Stacey-Kramers 🔹	0.0	1.0000	0.5000	0.90000 P	2.80000	1.10000	0.00010	0.01000	0.01000	0.01000	0.000020	0.30000	0.50000	0.10000
	z4	🗹 zrc	ET2535 v.2	\$ 0.01000	g 0.00000 g	0.10000 pg	137.8800	137.8800	0.002050	example Pb Bl 🗘	Stacey-Kramers 🛓	0.0	la 1.0000	0.5000	0.90000 p	g 2.80000	1.10000	0.00010	0.01000	0.01000	0.01000	0.000020	0.30000	0.50000	0.10000
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U-Pb_Redux supports the analyst with aliquot-based fast entry of fraction-specific parameters featuring "fill" buttons and keyboard navigation.

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Α	liquot	h	ncl N	lote	Fracti	ion	206/2	204	206/207	206,	/208	206/2	05	207/205	208/205	202/20	05 238/	235 2	33/235	233/236	Tracer
7	ircon		1	N	~ 21		4584.	5970	19.9769	7.	6684	2.7	167	0.1360	0.3543	0.00	2.4	1091	0.9793	0.0000	ET535
							0.	3704	0.0352	٥.	0221	0.0	077	0.0344	0.0206	0.00	000 0.0	0012	0.0013	0.0000	v.2
			v	N	z2		2447.	9602	19.1121	11.	3877	1.1	122	0.0582	0.0977	0.00	00 0.9	9956	0.9895	0.0000	ET535
							0.	4010	0.0558	0.	0405	0.0	143	0.0548	0.0379	0.00	00 0.0	0012	0.0012	0.0000	v.2
			V	N	z3		2763.	2525	19.3002	3.	0102	1.4	197	0.0736	0.4716	0.00	00 1.2	2676	0.9877	0.0000	ET535
							0.	3585	0.0463	0.	0185	0.0	091	0.0464	0.0171	0.00	00 0.0	0011	0.0012	0.0000	v.2
			√	N (z4		4324.	0232	19.9295	3.	4029	2.3	091	0.1159	0.6786	0.00	2.0	0520	0.9819	0.0000	ET535
							0.	3250	0.0360	0.	0176	0.0	079	0.0349	0.0155	0.00	00 0.0	0011	0.0012	0.0000	v.2
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							0.	3498	0.0280	0.	0234	0.0	060	0.0276	0.0229	0.00	000 0.0	0011	0.0011	0.0000	v.2
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	206Pb/	+2σ	207	Ph/	+2σ	207Ph/	+2σ	Corr		Th/	Ph*	Phc	Ph*/	206Pb/	206Pb/		207Ph/		207Pb/		
Fraction	2380-	abs	235	Ū ^a ′	abs	206Pb ^a	abs	coef.	% disc⊾	Ú°	(pg) ^d	(pg)°	Pbc ^f	204Pb9	238U ^h	±2σ %	235U ^h	±2σ %	206Pb ^h	±2σ %	Fraction
zircon																					
z1	70.702	0.035	70	. 70	0.12	70.7	3.6	0.609	0.03	0.39	57.7	0.66	88	5438	0.0110280	0.049	0.07211	0.17	0.04742	5 0.15	z1
z2	70.712	0.040	70	.84	0.19	75.0	6.1	0.536	5.75	0.24	21.4	0.45	47	3072	0.0110296	0.057	0.07225	0.28	0.04751	0.26	z2
z3	70.721	0.036	70	.78	0.17	72.9	5.3	0.532	2.93	1.01	41.3	0.65	64	3372	0.0110310	0.051	0.07220	0.25	0.04747	0.22	z3
z4	70.736	0.034	70	.74	0.12	70.7	3.6	0.569	-0.02	0.90	64.3	0.67	97	5236	0.0110334	0.049	0.07215	0.18	0.04742	5 0.15	z4
z5	70.701	0.033	70	.615	0.099	67.7	2.9	0.603	-4.41	0.26	71.4	0.67	107	6856	0.0110279	0.047	0.07202	0.14	0.04736	5 0.12	z5
z6	70.707	0.034	70	.79	0.11	73.5	3.2	0.649	3.75	0.82	71.7	0.65	110	6102	0.0110287	0.049	0.07220	0.16	0.047480	0.13	z6
z7	70.695	0.035	70	.69	0.15	70.7	4.7	0.451	-0.04	0.35	27.2	0.39	70	4397	0.0110270	0.050	0.07210	0.21	0.04742	5 0.20	z7
z8	70.703	0.035	70	.74	0.12	72.1	3.6	0.541	1.95	0.24	31.7	0.31	103	6657	0.0110282	0.049	0.07216	0.17	0.04745	3 0.15	z8
z9	70.699	0.036	70	.78	0.12	73.6	3.5	0.556	3.96	0.36	36.7	0.33	110	6862	0.0110275	0.051	0.07220	0.17	0.047484	0.15	z9
z10 -11	70.703	0.035	70	.13	0.14	/1./	4.3	0.531	1.45	0.90	47.0	0.58	80 64	4372	0.0110282	0.049	0.07215	0.20	0.04744	0.18	210
712	70.001	0.034	70	.00	0.15	72 1	1 4	0.234	-1.19	0.51	20.9	0.42	04	4072	0.0110248	0.048	0.07207	0.21	0.04740	0.21	712
713	70.720	0.036	70	77	0.14	72.1	3.9	0.516	3.06	0.90	37.8	0.36	109	5975	0.0110318	0.051	0.07218	0.21	0.04743	0.10	713
z14	70.701	0.038	70	.62	0.18	67.9	5.6	0.527	-4.07	0.94	28.2	0.44	64	3445	0.0110278	0.053	0.07203	0.26	0.04737	0.24	z14
z15	70,700	0.035	70	.72	0.12	71.6	3.6	0.576	1.21	0.16	40.3	0.43	93	6164	0.0110276	0.050	0.07214	0.17	0.04744	0.15	z15
		0.000	1.0				5.0	0.0.0		0.10		0.1.5		0101	510220210	0.050				0.13	

U-Pb_Redux produces user-customized data tables. The analyst can choose commonly-used compositional parameters, isotopic ratios (with the option of Th- and Pa-correction), and correlation coefficients, order the columns in any way, and save the data table setup. Uncertainties can be displayed as significant figures or to arbitrary precision, and values may be forced to display the same digits as the uncertainty. The data table automatically adds pertinent footnotes. U-Pb_Redux can export the analyst inspect the data, discard blocks || this table to Excel or to publication-quality SVG and PDF files.



Date interpretation in *U-Pb_Redux* is streamlined and interactive. Each analysis is organized in a hierarchical structure in a panel on the left. On the right, the analyst can visualize data as a full color concordia or weighted mean plot, with customizable display options. Multiple weighted means and York fits to the data may be calculated for any subset of the data, with parameters dynamically calculated as analyses are included or excluded by the user.



U-Pb_Redux makes a major contribution to sample analysis with its in-The cyber infrastructure (above) produced in this collaboration successfully innovative Sensitivity Testing interface, shown above. The left-hand panel tegrates an end-to-end system from sample through analysis and date interdisplays value sliders for every input and its uncertainty. When the anapretation to archiving and retrieval of results. This process standardization lyst moves a slider, the data reduction is re-calculated on-the-fly and the provides a heretofore missing common data reduction protocol, thus promotother display panels react accordingly: ing the interpretation of precise geochronology and enabling inter-laboratory comparison. This emphasis on precision aids in time-scale calibration, in un-A Concordia Panel displays error ellipses for all fractions in the aliquot derstanding processes of crustal evolution and early solar system dynamics.

with the current fraction highlighted. The concordia plot is navigable by panning and zooming with the mouse.

207Pb/206Pb dates with a graphical depiction of the contributions of **II** Chem database. each input's uncertainty to the date's uncertainty. Correlated errors are shown as positive or negative contributions to the variance.

C Dates Graph Panel shows each date with its uncertainty as a red bar representing the data, and a green bar representing the changes caused by the input sliders. The user can select which dates to view and the graph re-scales automatically.



Additional Features

D Uncertainty Selector: the user can choose only analytical uncertainty, or add in either tracer or tracer plus decay-constant contributions.

Auto-Uranium: when only the Pb portion of a fraction is present, the user can use independent constraints on the ²⁰⁶Pb/²³⁸U date to assess discordance and uncertainty budgets. U-Pb_Redux can generate dummy U data to predict ²⁰⁶Pb/²³⁸U and ²⁰⁷Pb/²³⁵U date uncertainties and plot the simulated ellipse on concordia.

AGU 2009 Fall Meeting 14-19 December 2009 San Francisco, California

The screen shot below shows how U-Pb_Redux interacts with SESAR and B Uncertainty Breakdown Panel displays 206 Pb/238 U, 207 Pb/235 U, and I Geochron to publish an XML-schema-compliant sample analysis to the Earth-

				Anquot	# 1 <> 2110011			
liquot Name:	zircon	child IGSN:	XYZ000000	Inst Method:	ID-TIMS	Analyst:	noahmclean	
				Fractionation for	r mono-isotopic Tracer	5		
	Cho	oose AlphaU Model:	example alphaU	* *	Choose Alpha Pb Model:	example alph	aPb 🛟	
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To Publi	sh this ali	quot to the Ge	eochron databa	ase:				
1. Valid	ate your User	name and Password	d for Geochron:	username	••••	Valida	ate Geochron credentials	
2. Valid	ate your User	name and Password	for SESAR:	username	••••	Vali	date SESAR credentials	
3. Valid	ate the Parent	t SESAR IGSN for thi	is Child Aliquot:	NONE		Valio	late parent SESAR IGSN	
4. Requ	est a child IG	SN from SESAR for t	this Aliquot:			Reque	st child IGSN from SESAR	
5. SAVE	and preview /	Aliquot:				Save and	Preview Aliquot in browser	\supset
6. SAVE	and UPLOAD	this aliquot to Geo	ochron:			Save and	Upload aliquot to Geochron	
7. Test	by downloadi	ng this aliquot from	n Geochron and savi	ng it as a local XM	ML file.	Test if al	iquot successfully uploaded	
		Fract	ion Fast Details	Fraction Notes	Measured Ratio Check	and Meta-Data	Publish	
Save & Cl	ose	Save Close	e Revert	to Saved	Save and Export 4	liquot as local)	(ML file	

🚳 research supported by NSF through EarthChem, a project of Columbia University's Lamont-Doherty Earth Observatory and the University of Kansas