CustomMassRanging 3.0

Ranging, Composition, and Multi-Hit Analysis Extension for IVAS

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Overview

The **"CustomMassRanging" extension** provides an automated re-ranging scheme for existing IVAS™ (Integrated Visualization & Anaysis Software) ranges that provides composition determination based on background correction, as well as multi-hit analysis features for .APT format datasets with the necessary data sections. The motivation for this extension is to provide users with the tools necessary to replicate the analysis reported in a previous publication (Prosa and Oltman, "Study of LEAP® 5000 Deadtime and Precision via Silicon Pre-Sharpened-Microtip™ Standard Specimens", Microsc. Microanal. 2022).

Standard IVAS features for range and background determination are limited. This extension takes as input a mass spectrum and an initial list of ranges made by a user. Based on a set of user-selected parameters, 1) additional peaks are discovered, 2) range definitions are optimized based on an algorithm that maximizes the net counts for each peak (based on a selected background ranging scheme), and 3) computes ionic and decomposed compositions after background subtraction with 4) assessment of statistical significance. Should the user choose, the optimized definitions for the original user-identified ranges (or all ranges, user and discovered) are returned to the main IVAS session. Once applied-remembered, using the standard IVAS feature "Save Analysis Tree" will save the parameter setting used by the extension and these will be re-loaded when a new IVAS session starts from that saved analysis tree.

In addition, multi-hit analysis features are also available for suitable datasets. A variety of multi-hit tables are computed to allow users to see how various ion events are correlated in space and time. Separation plots, which plot multi-event types as a function of separation distance (as measured in the reconstruction or detector coordinates) are also made available. Normalization of these curves can allow for estimates of ion events missing due to detector deadtime. See the paper for a more complete discussion.

Primary Requirements and Enabled Function

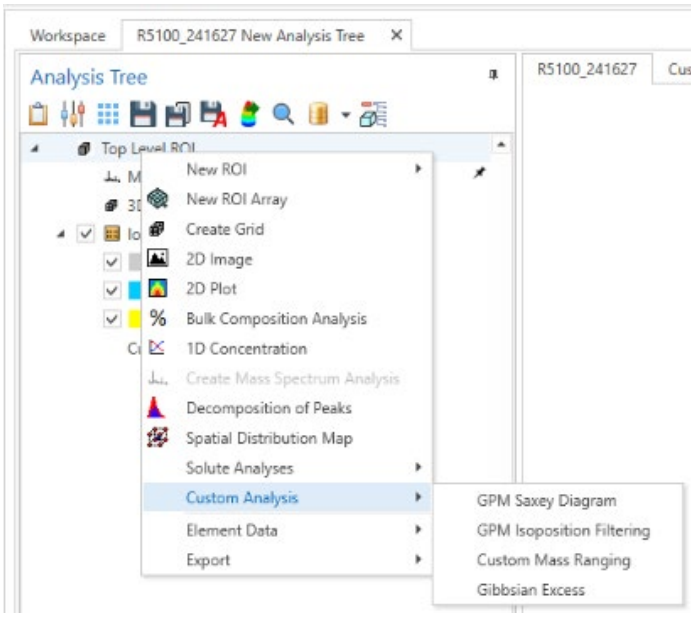
- IVAS session with mass spectrum – allows for re-ranging and composition analysis
- ROIs (regions of interest) with created mass spectrum – same
- .APT format dataset that includes EPOS, pulse, and pulseDelta sections – multi-hit processing features (see IVAS documentation for more information)

Extension Installation

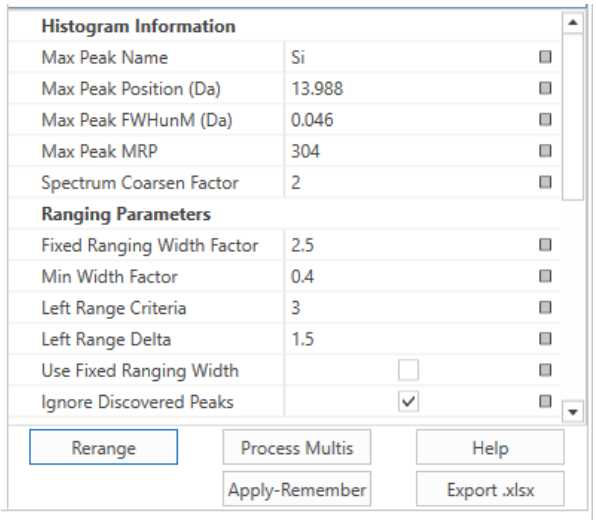
Go to the Cameca GitHub site: https://github.com/CamecaAPT.

Find the CustomMassAnalysis extension and install (see the AP Suite User Guide, available within a running IVAS session, section 2.8.3 Detailed Instructions for Installing, Updating, or Uninstalling and Extension to AP Suite Using the Extension Ecosystem).

QuickStart



1. Start an IVAS analysis session.
2. Right click hold on any exiting ROI.
3. Select “Custom Mass Ranging”.
4. A blank “Custom Mass Ranging” tab will appear with an “Update” button. Click on the “Update” button.
5. The mass spectrum and existing range definitions are loaded and Histogram Information is extracted. Users can modify the default parameters that affect the ranging process in the Parameters section: Ranging, Tail, and Peak Discovery Parameters.
6. Click the “Rerange” button.
7. At this stage, all peaks have been discovered, initial ranging schemes have been determined by the extension, range definitions have been optimized, and compositions have been determined. The user can change parameters and re-range as many times as desired until an acceptable result has been achieved.
8. At any time, the user can save all information (all tabs, ranges, and parameters) to a multi-tab Excel file via the “Export .xlsx” button.



9. At any time, should the proper data sections exist in the dataset, multi-hit tabs “Multi-hit Information” and “Separation Plots” can be populated via the “Process

Multis" button. Again, parameters can be changed and "Process Multis" repeated as desired.

10. Finally, selecting the "Apply-Remember" button will update the ranging information used in the main IVAS session for this ROI, update the Properties section pertaining to this extension, which makes it savable via the "Saved Analysis Tree" function.
11. Note: Tool tips are available for most variables. Just hover the mouse over an item and a helpful description should appear.

Re-Range

Automated Range Definition Determination:

The **"CustomMassRanging" extension** provides an automated re-ranging scheme for existing IVAS ranges. Adding or deleting ion ranges must be done in IVAS, before passing them on to this extension. A peak discovery feature displays found peaks and allows the user to add all these ranges (which can be passed back to IVAS for identification and then returned to the extension for computation).

Histogram Information:

Max Peak Name: Ion range of found max counts position
Max Peak Position (Da): Bin position with maximum counts
Max Peak FWHunM (Da): Full width of max peak at hundredth max
Max Peak MRP: Mass resolving power of max peak (1/FWHunM)
Spectrum Coarsen Factor: Binning of the extension mass spectrum (integer number x IVAS binning). Since IVAS default binning is 0.001 Da, coarsening factor = 2 would result in a 0.002 Da binning.

Range boundaries are determined by maximizing the net counts for a given peak (ranged events minus background estimate). Four ranging schemes exist and are initially populated by the algorithm on a peak-by-peak basis, but subsequent re-ranging allows the user to override the background scheme for any peak. The schemes include: Left, Half, Quarter, and LeftTail.

The LeftTail option attempts to fit the tail of the peak with a decaying exponential fit to unranged regions in the tail. Ionic and decomposed ion bulk compositions use the tail estimate and full statistical consideration is made for detection threshold and resulting compositional uncertainty. When using the LeftTail option, the user specifies an estimated uncertainty in the tail estimate and that error is propagated to the bulk compositions.

Ranging Parameters:

Ranging Width Factor: Number x FWHunM for left-ranging scheme width (or the fixed ranging width)
Min Width Factor: Number x FWHunM for min range width (all ranges must be at least this wide)
Left Range Criteria: Required pre-peak region (Da) empty of other discovered ranges for left-ranging

Left Range Delta: Position left of peak (Da) to center left-background range
Use Fixed Ranging Width: Use fixed ranging width (range width determined by Ranging Width Factor)
Ignore Discovered Peaks: Ignore discovered peaks when determining ranges (and compositions)

Schemes

Left (and LeftTail): Designed for peaks with no pre-peaks (flat background with no peak tails overlapping peak region). Uses a fixed range-width, positioned to provide maximum counts. Peak width is set to RangingWidthFactor x FWHunM.

Half: First a range of minimum width (even number of bins) is centered about the maximum peak position. Immediately adjacent ranges of ½ width are used to approximate the background. The range width is increased two bins at a time (and each adjacent background range by one bin) with the position moved right or left, depending on which gives the maximum net counts. The range width continues to grow and move two bins at a time until the net counts begin to decrease.

Quarter: Used when peaks are too close together to allow for ½-range background ranges. The difference is that the immediately adjacent background ranges are ¼ width and the range width is increased by four bins at a time.

Note: The background estimates are plotted as straight lines in the Mass Histogram plot as this is the equivalent interpretation for the adjacent ranging method.

LeftTail

There are occasions where one or two dominant peaks both interfere with adjacent peaks and also represent significant numbers of ion events such that any compositional analysis that ignores these will systematically underrepresent these species and provide inaccurate results. The LeftTail feature first determines ranging for such a peak using the Left method described above. The tail region (or region immediately to the right of the peak) is then fit with an exponential curve (straight line in a log plot). Any bins where a range from another peak is defined are ignored. The counts in the fit, extending down to where the tail meets the background, are tallied and used in composition analysis. Any unrealistic tail fits are ignored (e.g., tail extends beyond Tail Range Maximum).

Tail Parameters

Considered Tail Range (Da): Range beyond right-range-edge to fit exponential tail
Tail Estimate Uncertainty: Estimated fractional uncertainty of tail counts for error propagation
Tail Range Maximum: Fit tail intersection with background maximum width (or error)

Peak Discovery

Any missing peak are “Discovered”, and the user can optionally add all these ranges or ignore them (default). Added ranges become part of the ionic composition but are

excluded from the atomic composition calculations (unless the user identifies the ion types in IVAS and then returns the ranges to the extension).

Discovery is down via a kernel with a width defied by RangingWidthFactor x FWHunM. This kernel width is adjusted relative to the Max Peak in time-of-flight (ToF). That means that for the region near the Max Peak, the kernel has this width, but the kernel will be more narrow for low mass-to-charge (equivalent ToF width) and wider for higher mass-to-charge (equivalent ToF width), and at least some minimum bin width as defined in the parameters. The constant ToF kernel moves across the mass spectrum using ½-width background ranging to decide if a statistically significant net signal exists for the kernel. If this exceeds a 99% confidence level that a signal is above background (and minimum counts parameter is satisfied), then a peak has been discovered and the range extent defined.

Peak Discovery Parameters

Sensitivity: Number times FWHunM for left-ranging or fixed ranging kernel width
Min Bin Pairs: Minimum bin width for peak evaluation in coarsened bin pairs
Min Counts for Peak Max Bin: Discovered peaks must have a bin with at least this many counts
*Note: Minimum and Fixed Width Scaling: Generally, minimum and fixed peak widths scale in ToF (or $\sqrt{(m/z)}$) relative to the Max Peak, so only the Max Peak will have the specific values as set forth in the parameter table. Ranges to the left will be slightly more narrow, and those to the right more broad. Depending on parameter definitions, very low m/z peaks might require near zero-width minimums, so the "Min Bin Pairs" parameter prevents this.

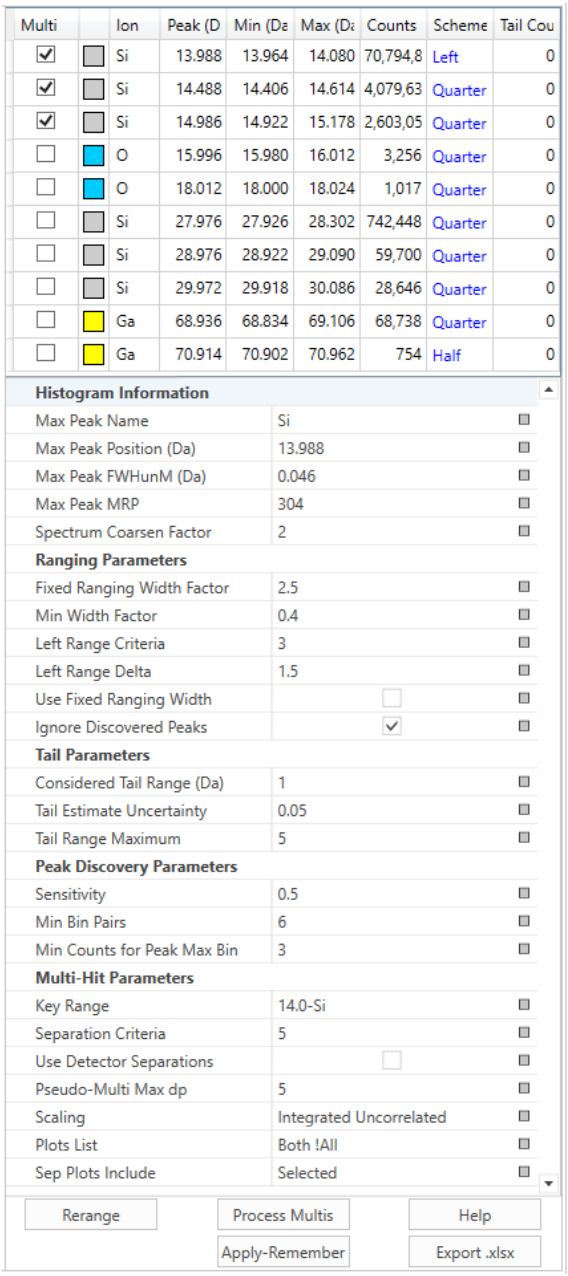
Ranging & Composition Details:

The initial ion list and range definitions are the RRNG-type data passed from IVAS, and the range list items cannot be added to or deleted within the extension (the user needs to do that in IVAS and then pass that list to the extension). The ranging procedure is consistent with the analysis described in Prosa and Oltman, 2022 (attached at end):

Overlapping initial range definitions are not allowed (although IVAS does allow). An exception will be generated and the user notified when input ranges have overlaps.

1) The most intense histogram bin in the mass spectrum is discovered and processed for peak m/z position and full-width-hundredth max (FWHunM, note in the publication, the FW0.001M was used, but that metric may is not sufficiently robust for general mass spectra).
2) FWHunM is used to determine the histogram m/z resolution. Typically, the input mass histogram has a resolution of 0.001 Da. The algorithm coarsens the resolution so that 15-30 bins encompass the FWHunM of the main peak (typically, somewhere between 0.002 Da to 0.01 Da).

3) The peaks are processed from left to right along the mass spectrum to determine the appropriate ranging scheme. Ideally, a background range of the same width as the ranged peak is used to estimate the background for a given peak. The scheme is determined as follows: If there are no peaks defined within a certain distance to the left of a given peak (as defined by "Left Range Criteria"), then the Left ranging scheme will be used. That is, a range defined at some specified distance to the left (as defined by "Left Range Delta") of the given peak and the same width. If the left-ranging criteria fail, then an evaluation is made for nearest peaks on either side of the given peak. Nearest peak >0.9 Da away is the criteria for a Half-width ranging scheme. Immediately adjacent to the left and right of a prospective peak range, background ranges of half the prospective peak range width are defined and used to estimate the background. The Half scheme is equivalent to estimating a linear background correction for that peak. Otherwise, the Quarter-width ranging scheme is used. Same as the Half scheme, except background counts need to be doubled to account for the range width and provide a linear background correction (and consequently the background uncertainty will be doubled as well).



Multi		Ion	Peak (D	Min (Da	Max (Da	Counts	Scheme	Tail Cou
☑		Si	13.988	13.964	14.080	70,794,8	Left	0
☑		Si	14.488	14.406	14.614	4,079,63	Quarter	0
☑		Si	14.986	14.922	15.178	2,603,05	Quarter	0
☐		O	15.996	15.980	16.012	3,256	Quarter	0
☐		O	18.012	18.000	18.024	1,017	Quarter	0
☐		Si	27.976	27.926	28.302	742,448	Quarter	0
☐		Si	28.976	28.922	29.090	59,700	Quarter	0
☐		Si	29.972	29.918	30.086	28,646	Quarter	0
☐		Ga	68.936	68.834	69.106	68,738	Quarter	0
☐		Ga	70.914	70.902	70.962	754	Half	0

Histogram Information	
Max Peak Name	Si
Max Peak Position (Da)	13.988
Max Peak FWHunM (Da)	0.046
Max Peak MRP	304
Spectrum Coarsen Factor	2
Ranging Parameters	
Fixed Ranging Width Factor	2.5
Min Width Factor	0.4
Left Range Criteria	3
Left Range Delta	1.5
Use Fixed Ranging Width	☐
Ignore Discovered Peaks	☑
Tail Parameters	
Considered Tail Range (Da)	1
Tail Estimate Uncertainty	0.05
Tail Range Maximum	5
Peak Discovery Parameters	
Sensitivity	0.5
Min Bin Pairs	6
Min Counts for Peak Max Bin	3
Multi-Hit Parameters	
Key Range	14.0-Si
Separation Criteria	5
Use Detector Separations	☐
Pseudo-Multi Max dp	5
Scaling	Integrated Uncorrelated
Plots List	Both !All
Sep Plots Include	Selected

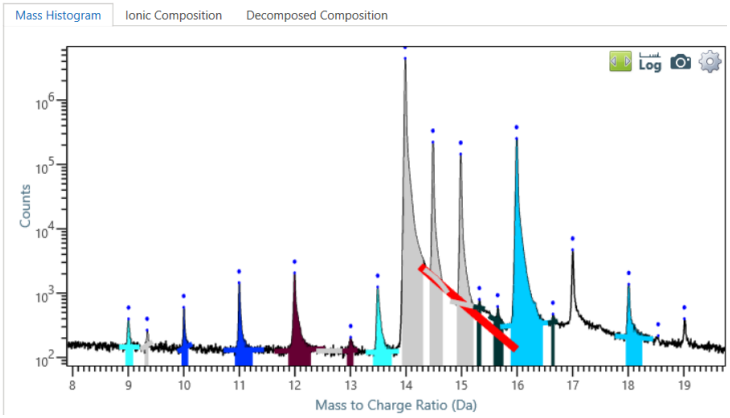
Rerange | Process Multis | Help | Apply-Remember | Export .xlsx

4) Optimum ranges are determined given the initial ion range definitions and auto-determined schemes as follows:
    a. A minimum range-width is defined based on the FWHunM.
    b. The local maximum is determined for each initial ion range.
    c. Left-scheme peaks use a fixed range width as specified in Parameters. The position of the fixed-width range is adjusted to yield the maximum number of total/net counts, and a same-width range is defined to the left of this peak (as specified in Parameters) as a background estimate.

d. For half-width and quarter-width schemes, the minimum range-width is positioned so that the net counts (total counts in ion range, minus the immediately adjacent background estimate) is maximum. Then the prospective range width is expanded 2 bins (or 4 bins for quarter-width ranging) at a time and re-evaluated. The process stops when the net counts begin to decrease.

e. Background ranging lines are added to the mass spectrum histogram. Note they are lines in linear-scale but curved in log-scale.

f. LeftTail performs an exponential fit to the ToF tail ($\sqrt{m/z}$). Starting at the range maximum point and continuing for "Considered Tail Range", ignoring any values defined by other ranges, these points are fit to an exponential function and those estimated counts are added to the various tables. Should the exponent be non-negative or span more than 5 Da before intersecting with the background, then the tail is rejected. The user specifies "Tail Estimate Uncertainty" as a fraction of the total number of counts. A value between 0.01 and 0.1 might be reasonable (1% and 10%). This uncertainty is estimated and propagated to the final composition results.



Mass Histogram | Ionic Composition | Decomposed Composition

Ion	Composition	Sigma/DT (95% CL)	Counts	Background	Net	Tail
Si	83.187%	0.028%	23,587,420	178,753	23,629,359	217,382
O	5.9438%	0.0044%	1,738,326	50,207	1,688,338	0
SiO2	2.4268%	0.0030%	766,703	77,941	689,343	0
Co	2.2346%	0.0028%	662,016	27,376	634,744	0
SiO	1.9812%	0.0052%	574,335	37,787	562,757	26,206
Ge	1.5898%	0.0025%	510,312	59,169	451,579	0
TiO	1.0701%	0.0022%	379,190	76,041	303,963	0
Ti	0.7554%	0.0021%	294,531	80,496	214,559	0
TiN	0.3105%	0.0011%	100,595	12,418	88,199	0
C	0.08732%	0.00074%	43,452	18,888	24,803	0
SiC	0.07234%	0.00065%	35,881	15,357	20,548	0
Al	0.07061%	0.00075%	38,919	18,969	20,058	0

Mass Histogram | Ionic Composition | Decomposed Composition

Element	Composition	Sigma/DT (9	Counts	Background	Net	Tail
Si	80.881%	0.027%	25,020,914	331,709	24,936,735	243,588
O	12.8237%	0.0070%	4,272,981	347,773	3,953,734	26,206
Co	2.0865%	0.0026%	687,877	44,677	643,304	0
Ti	1.9679%	0.0029%	774,316	168,955	606,721	0
Ge	1.4647%	0.0023%	510,312	59,169	451,579	0
N	0.3978%	0.0013%	159,398	36,851	122,635	0
C	0.1971%	0.0010%	108,640	48,149	60,777	0
Al	0.09551%	0.00081%	58,894	29,608	29,448	0
F	0.05301%	0.00055%	31,095	14,766	16,344	0
B	0.01964%	0.00070%	45,831	39,828	6,054	0
Hf	0.01302%	0.00038%	9,342	5,396	4,014	0
Au	-ND-	0.00069%	2,102	2,063	39	0

5) Once the ranging definitions are finalized, ionic and decomposed ion compositions are calculated. For each range (or ion type) the net counts are evaluated for statistical significance (has a peak been detected with a 95% confidence level).

Note that any Not Detected (-ND-) ranges are removed from composition considerations and the 95% confidence level detection threshold is reported instead of sigma (the amount of that range/element that would be detected 95% of the time).

6) A version of the peak ranging algorithm is used to look for any net counts that statistically might be a peak. The minimum range size is used bin by bin, starting at 0.8 Da. When the net counts are greater than (99%CL-DT/ Sensitivity), this constitutes a discovered peak. The range position is adjusted to yield the maximum net counts for that peak, and then the search process continues starting at the far-right edge of the discovered peak's range extent. Blue dots (limited by plotting options) are displayed on the mass histogram.

Process Multis

Multi-Hit Analysis Tools:

Multi-hit analysis tools have been added to this extension, including various tables, plots, and statistics computed to help the user assess the evaporation behavior within a particular dataset. Note, the **"GPM.SaxeyDiagram" extension** is also available on the GitHub to display 2D correlation histograms.

Input: Multi-hit analysis can only be performed on **.APT files** that have had additional data sections included at the time of reconstruction. The "Mass" and "Position" data is always included in a reconstruction (POS information). The additional sections include some EPOS sections and two additional, specifically:

Required APT Sections:

"Position": EPOS: The reconstructed coordinates (nm)
"Detector Coordinates": EPOS: The detector coordinates (mm)
"Mass": EPOS: Mass-to-charge ratio (Da)
"pulse": Float of pulse number
"pulseDelta": Difference between float and double of pulse
"Voltage": EPOS: Specimen voltage (no pulse)
"Epos ToF": EPOS: Raw Time of Flight minus t0 (ns)

It is noteworthy that EPOS does not include the "pulse" and "pulseDelta" sections, and these would not normally be necessary; however, the assumptions used to decode multi-hit information from an EPOS file (an entire reconstructed dataset) cannot be used when decoding a sub-volume (region of interest or ROI) from the EPOS array of information. Internally, the added sections enable proper decoding of hit relationships for the extracted lines from the EPOS array:

EPOS sections “Multiplicity” and “Delta Pulse” are defined such that the first ion in a multi-ion list indicates the “Multiplicity” or number of multi-hit events detected for a given pulse, with each succeeding ion in the multi-hit list having “Multiplicity” of zero and “Delta Pulse” of zero, indicating no pulses occurred between events.

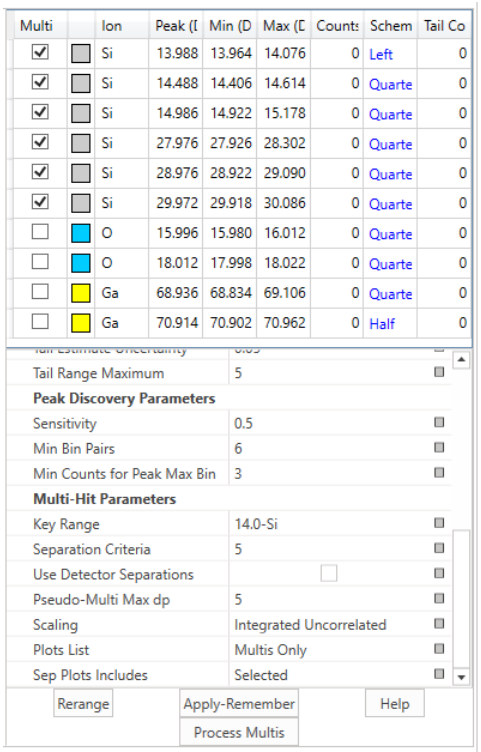
This is not reliable for IVAS ROIs because lines of ion information are stripped from the list, leaving this procedure unreliable.

The true pulse number (realPulse) for all ions is decoded internally by:

```
double realPulse = (double)pulse + (double)pulseDelta;
```

Extension Function: After successful “Rerange” one can depress the “Process Multis” button, and as long as all the required sections above exist, multi-hit statistics and ion separation plots (sep plots) will be compiled and displayed in their output tabs (Multi-hit Information and Separation Plot).

The left-most column in the range table section (top of figure to right) allows the user to select ions (referred to below as “selected” ions) to include for specific multi-hit consideration.



Multi-Hit Parameters:

The Multi-Hit parameters and functions include:

1) Key Range: This isotope-labeled range is used to track average ToF and Voltage for the analyzed data. The user selects by editing the text before processing, or when no match is found, the first range in the list is used and updated in the parameter list.
2) Separation Criteria: The separation distance used to partition the correlated events (those < criteria) and uncorrelated events (those > criteria).
3) Use Detector Separations: Use event separation based on separations in detector coordinates (mm) rather than reconstructed coordinates (nm).
4) Psudo-Multi Max dp: Track pseudo-doubles from dp=1 out to Max dp.
5) Scaling: Rescale non-same-same separation plots according to selection: None, Max Uncorrelated, or Integrated Uncorrelated. Max Uncorrelated integrates the latter half of the sep distribution histograms (consisting only uncorrelated events). The non-same-same histogram is then rescaled so that it has the same area as the same-same sep histogram for that ion species. Integrated Uncorrelated does the

same, but for the range starting with separations defined by the Separation Criteria parameter. Effects of multi-hit deadtime tend to extend beyond the Separation Criteria. The Max Uncorrelated scaling has fewer counting statistics but is less affected by correlated overlaps. Selecting a scaling method allows for estimates of missing counts due to detector deadtime (which are displayed in the legend of the plots).

6) Plots List: The Separation Plot tab includes three sets of plots for combinations from each selected ion in the range table section: same-same or pairs of ions from the same defined range (e.g., 14.0-Si – 14.0-Si pairs of events), non-same-same or pairs of ions from differing ranges, and all or all pairs of events regardless of ion range. Since it is all combinations, three selected ion ranges will result in nine plots. Nine more plots for Pseudo-multis. The Plots List selection allows the user to down-select the plots to display: Multis Only, Pseudos Only, Both, Multis Only !All (the same-same and non-same-same histograms, but not the all ions plots, which is the sum of the same-same and non-same-same histograms), Pseudos Only !All, and Both !All.
7) Sep Plots Include: Selected, Selected & Other Ranged, All. Discussed later is the idea that multi-hit events can be segmented into correlated and uncorrelated. In addition, specific ion correlations are divided into user-selected ions, all other ranged ions, and unranged ions. For purposes of sep plot display and scaling, the user can choose to ignore the non-user selected ions and the unranged ions for these calculations and displays.

Discussion:

As discussed in Prosa and Oltman, 2022, atom probe evaporation events do not occur randomly. They present aspects of both correlated evaporation (one evaporation affecting another evaporation) and uncorrelated evaporation (evaporation events occurring independently and randomly in space and time). As a consequence, multi-hit events are tabulated based on time correlations (dp=0 are same-pulse, commonly referenced multi-hit events, and dp=1, or less than some small dp number, as “pseudo”-multis) and based on spatial correlations (events spaced within a small distance likely being correlated while those farther apart following random correlation statistics). Once tabulated, descriptive tables and plots are presented in the “Multi-hit Information” tab for the user to interpret.

Important Terms:

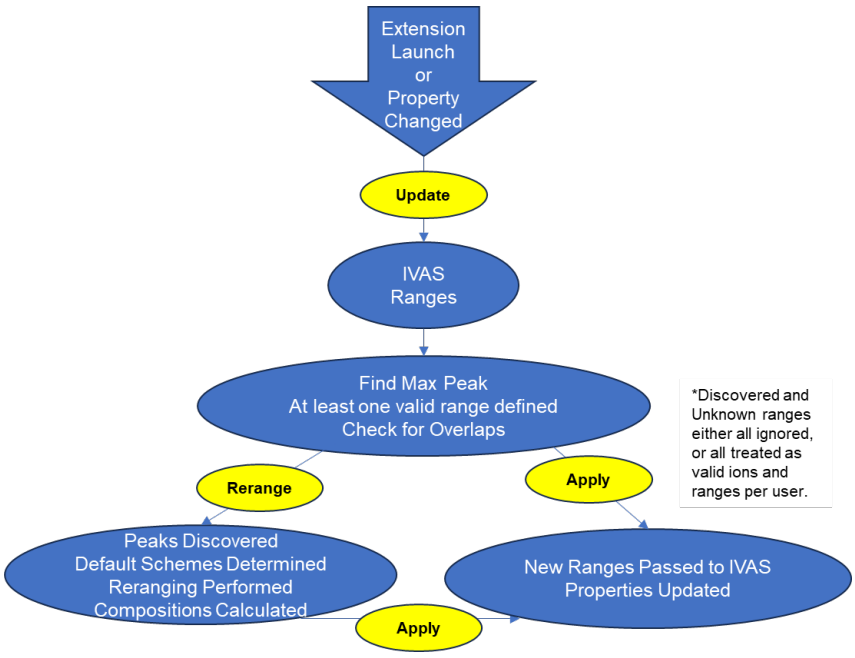
The following are used to help describe the various computed statistics:

- Pulse: Laser or voltage pulse (or both) attempting to cause field evaporation
  Note: Most pulses result in zero detected events

- Event: One or more ions detected during a single pulse
- Multi-hit: Two or more ions detected during a single pulse
- Pseudo-double: Evaporation events separated by a small number of pulses
  Note: Here, critically defined as consecutive single events only
- dp: Pulse difference between detected ions
- Correlated: Events close in both space and time. One event affecting the others.
- Uncorrelated: Events occurring independently. Apparent correlations due to random statistics
- Critical Separation: Spatial separation used to partition correlated and uncorrelated events
- Considered: Ion ranges chosen to be tracked for display
- Other Ranged: Ion ranges defined but not specifically considered
- Unranged: All other ions neither considered nor other
- Same-same: Ions from same ion range. dp=0 events of this type are susceptible to deadtime
- Non-same-same: Ions not from same ion range. Events of this type are not susceptible to deadtime
- hreg: Register used to summary describe numbers of event: single, double, triple, etc.
- PCME: Probability of Multiple Events (PME) defined as Multi-Pulses/All-Pulses, as used by Cojocaru-Mirédin et al. (Advanced Materials, 2024). Here, correlated-multis are used in numerator instead, so PCME
- Overcounting: A double (two ions during an event) represents a single correlation pair, while a triple (three ions) represents three correlation pairs. Multis are represented in tables this way so that the number-of-ions ≠ 2 x any table entry.

Apply-Remember

The user can then choose to pass/apply new ion ranges back to IVAS or change ranging parameters and re-range again. The utilized extension parameters, those from the last apply-remember operation, are moved to the Properties section so that they can be saved as part of any subsequent "Save Analysis Tree" operation. It also requires "Update" to the extension before continuing.



Help

Pressing the "Help" button should launch a view of the most recent .pdf version of this document.

Export .xlsx

Opens a save window enabling the user to choose name and directory for file save. The Excel file includes tabs documenting all displayed data: Parameters, Ranges Table, Mass Histogram, Ionic Composition, Decomposed Composition, Multihit Information, Separation Plots.

Final Notes

1. "Rerange" can be done multiple times (needed when users change Parameters or modify any Schemes).
2. Select/Select-All and Copy/Paste functions should work on all tables (column headers are not captured in this operation). To enable copy/paste in the Multi-hit Information tab, it was made editable. The changes will only temporarily affect the display as any Process Multis operation will restore the display.
3. Double clicking in plot region will unzoom x-axis. A second time is needed to unzoom y-axis. Auto-y-axis scaling is not a current feature.
4. Table columns are also sortable by clicking the column header, but note to control precision display, some numerical columns are of type string, and these will not always sort in numerical order!
5. Quarter-width ranging will have slightly larger uncertainly because the background is scaled by a factor of two (greater background uncertainty).
6. Decomposed compositions error propagation means that any molecular ion with an element that has greater than one atom in the molecular formula (e.g., O in SiO_2) will result in a larger uncertainty because of the scaling of those counts in the decomposition calculation (not historically accounted for in this way in IVAS). This is almost always insignificant, but for materials with a significant fraction of multi-same-atomic molecular species, this could become significant.
7. Tool tips are available for many table column headers, Parameters, and Properties.
8. Any changes in the IVAS ranges associated with an active extension session will force an update of the extension (start from the beginning).
9. Save Analysis Tree saves the current parameters and schemes (those shown in the properties region, which are modified only after apply has been done). Using a Saved Analysis tree will also override auto-scheme (not shown in Properties) with the previously used scheme for any matching ranges (since a Saved Analysis Tree can be applied to a different dataset than the one from which the save was performed, the IVAS ranges/ions list may be different).
10. "Discovered" range names ignored upon load (user needs to assign new range type/name for them so survive initial load).

11. Ignore function: Re-range always starts with the original StartTable (internal for load)—the original Scheme Properties when they exist, or null. When null, then the scheme will be auto determined.
12. Not Ignore: The peaks list of all found peaks is overridden by any StartTable entries. StartTable scheme is applied if found and null otherwise. When null, then the scheme will be auto determined.
13. The discovery process can provide closely spaced peaks, and the auto-ranging can result in overlapping peaks. The code attempts to resolve these overlaps using the following rules: Same named overlapping ranges, the lower net counts range is removed. Overlapping ranges where one is “Discovered”, the discovered is removed. Any other potential outcomes will cause the extension to fail.
14. For versions beyond 3.0, expect modifications to the multi-hit information tab.
15. Send feedback to tjprosa@ua.edu