The GCE Data Toolbox Q/C Framework

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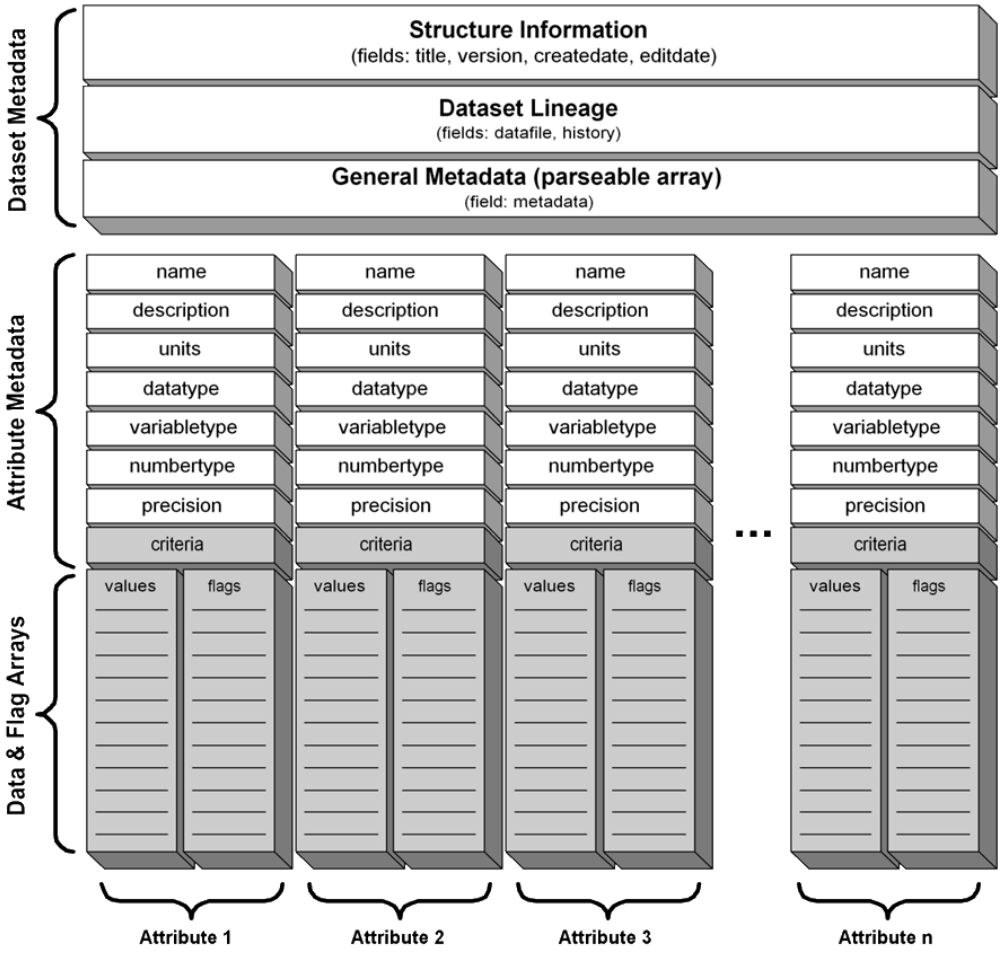
Overview

- Four major facets of Toolbox Q/C framework
  - Data model for storing Q/C rules, qualifiers, Q/C metadata
  - Tools for performing Q/C (assigning qualifier flags)
  - Tools for managing qualifier flag assignments
  - Tools for visualizing and managing qualified values
- Components work together seamlessly
  - Q/C framework integrated with data processing, analysis
  - Supports Q/C throughout the entire data lifecycle
- Q/C strategy important
  - Q/C is an iterative process
  - Operations done in wrong order can nullify flags, waste effort
  - Information can also be lost

Data Model

- GCE Data Structure designed to store data, Q/C info, metadata together
- Dedicated Q/C criteria field
- Paired value/flag arrays
- Q/C fields in doc metadata
  - Data/Codes (flag definitions)
  - Data/Anomalies (Q/C summary)
  - Data/ValueCodes (definitions for instantiated flag columns)
  - Processing history (all Q/C operations)



Data Model – Q/C Principles

- Data and structure validation happens before Q/C analysis
  - No need to add Q/C checks for valid data type, ragged tables, text in numeric fields, ...
- Basic Q/C operations are documented automatically
  - Edits to rules, evaluation of rules, manual/visual Q/C, flagged value removal, ...
- No qualifier vocabularies or semantics are assumed
  - Qualifiers are defined in the data set metadata (or interactively)
  - Just as valid to assign qualifiers for “good” values as “bad” (e.g. “reviewed”)
  - Subtle bias for “bad” interpretation in some tools, but not hard and fast
- Multiple qualifiers can be assigned to a data value
  - Multiple Q/C criteria matched
  - Multiple qualifiers assigned/copied manually
  - Major exception is graphical assignment (1 flag set or all flags cleared)

Assigning Qualifiers

- Qualifiers can be assigned automatically
  - Assigned based on criteria expressions for each column (“rules”)
  - Assigned by specialized flag functions in rules or run in workflows
  - Assigned by tools when values revised, calculated (e.g. gap-filling)
- Qualifiers can be assigned manually/interactively
  - Typed into a data grid or added using workflow functions
  - Graphically assign with the mouse on data plots
- Qualifiers can be copied/imported
  - Copy composite flags from one or more columns to other column(s)
  - Convert text columns to flags to import pre-assigned or 3rd party flags

Automatic Assignment (Rules)

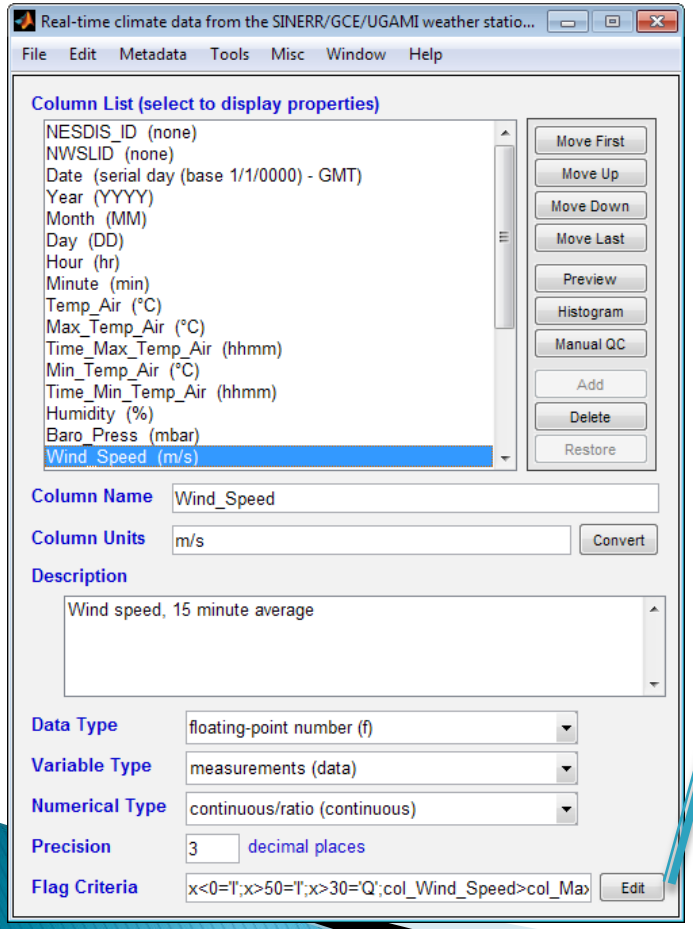
- Basic syntax: [logical expression]='[flag code]'
- Logical Expression =
  - MATLAB expression that evaluates each data value against some criteria and returns true/false (true mean matches criteria)
- Flag Code =
  - Alphanumeric character to assign when expression true (I, q, 9, *)
  - Flag Codes defined in the dataset metadata (I = invalid value, Q = questionable …)
- Examples
  - Conditional statements: x<0='Q'
  - Mathematical/statistical comparisons: x<mean(x)-2*std(x)='Q'
  - Functions for set-based comparisons: flag_notinlist(x,'A,B,C')='I'

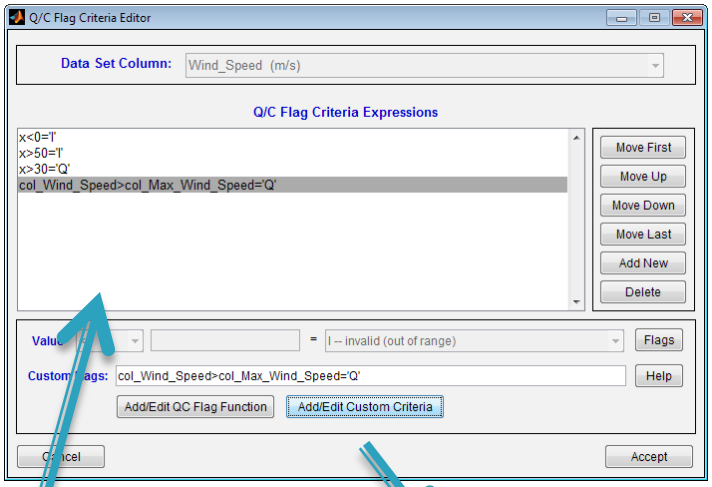
Automatic Assignment (Rules)

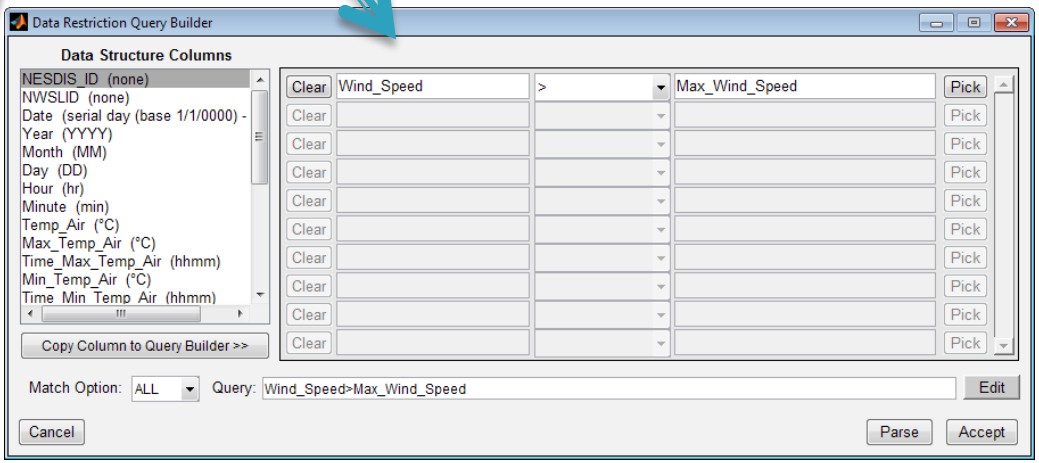
- Rule Characteristics
  - Column values are referenced in rules using “x” or “col_[name]”
  - Rules are evaluated for every value in the column independently
  - Rules can reference corresponding values in other columns
  - Multiple expressions can be combined using Boolean operators (&/|) and include parentheses to create complex criteria
  - Can define any number of rules per column (semi-colon separator)
    - If multiple rules are matched, multiple flags are assigned (e.g. IQQ)
  - Can use mathematical statements, MATLAB (or toolbox) functions to create derived arrays for comparison with column values
    - mean(), max(), std(), sum()
  - Can call functions to retrieve reference data, run algorithms, etc (open-ended)

Automatic Assignment (Rules)

- Rules can be created, edited, deleted, re-ordered using GUI forms

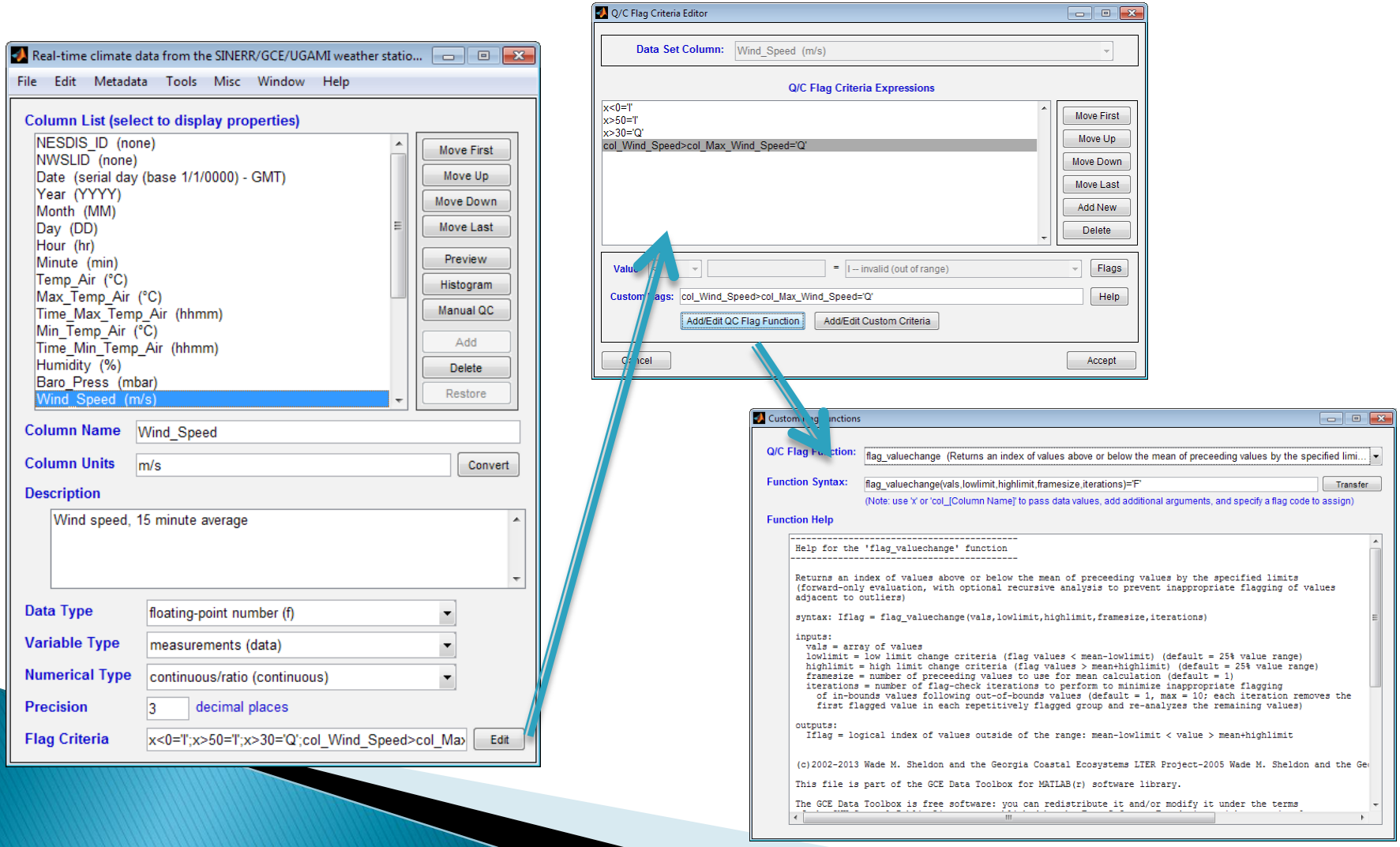






Automatic Assignment (Rules)

- Syntax help displayed for custom flag functions to guide use



Automatic Assignment (Rules)

- Basic Examples (MATLAB conditionals, built-in functions)

Q/C Goal	Rule Type	Example
Limit/range check	simple conditionals	x<0='I';x>37='Q'
		col_Salinity<0='I';col_Salinity>37='Q'
Valid value check	null check function	isnull(x)='M' (numeric or string column)
		isnan(x)='M' (numeric only)
Sanity/consistency check	algebraic equations	col_WetWeight<=col_DryWeight='Q'
		(col_SpartinaPct+col_JuncusPct+col_BorrichiaPct)>100='I'
		(col_NO2+col_NO3)>col_NOX='I'
Outlier detection	statistical tests	x>mean(x)+3*std(x)='Q'
		x>mean(no_nan(x))+3*std(no_nan(x)) ='Q' (NaN-safe)
Condition check	multi-column rules	col_Depth<=0.2='I';col_BatteryVolts<=9='Q' (in Salinity)

Automatic Assignment (Rules)

- More Complex Examples (custom flag functions)

Q/C Goal	Rule Type	Example
Code check	set-based function	flag_notinlist(col_Site,'GCE1,GCE2,GCE3,GCE4')='I'
		flag_notinlist(col_Site, 'plant_list.mat|data|Species')='I'
		flag_notinarray(col_Plot,[1 5 10 15 20])='I'
Pattern check	moving window function	flag_valuechange(col_AirTemp,5,5,3)='Q'
		flag_nsigma(col_Humidity,3,3,10)='Q'
Location check	geographic lookup fnc	flag_locationcoords(x,'Longitude','Latitude',0.5)='Q'
Stuck/fouled sensor	inverse change function	flag_novaluechange(col_Salinity,0.2,0.2,3)='Q'
Derived property	custom function	flag_o2saturation(col_O2Conc,col_WaterTemp,col_Salinity, 100,30,'mg/L')='Q'
Conditional checks	compound rules	flag_valuechange(col_AirTemp,5,5,3)&col_Precip==0='Q'
		col_PAR>0&flag_timeofday(col_Date,{'00:00','06:00', '20:00','23:59:59'})='Q'

Automatic Assignment (Rules)

- Rules are evaluated automatically during processing
  - When data are imported and metadata template is applied
  - When data values are revised or columns added
  - When Q/C criteria edited or new template applied
- When rules are evaluated, any existing flags are overwritten
- Rules with syntax errors will be skipped, warning issued
- Rules can be “locked” & “unlocked” to control automatic assignment
  - Adding the token “manual” to the Q/C criteria locks flags and prevents recalculation
  - Rules are retained, but dataflag() will skip evaluation and never clear flags
  - Removing the token “manual” unlocks flags and triggers recalculation
- Rules are converted to column descriptions when flags are converted to text columns for export

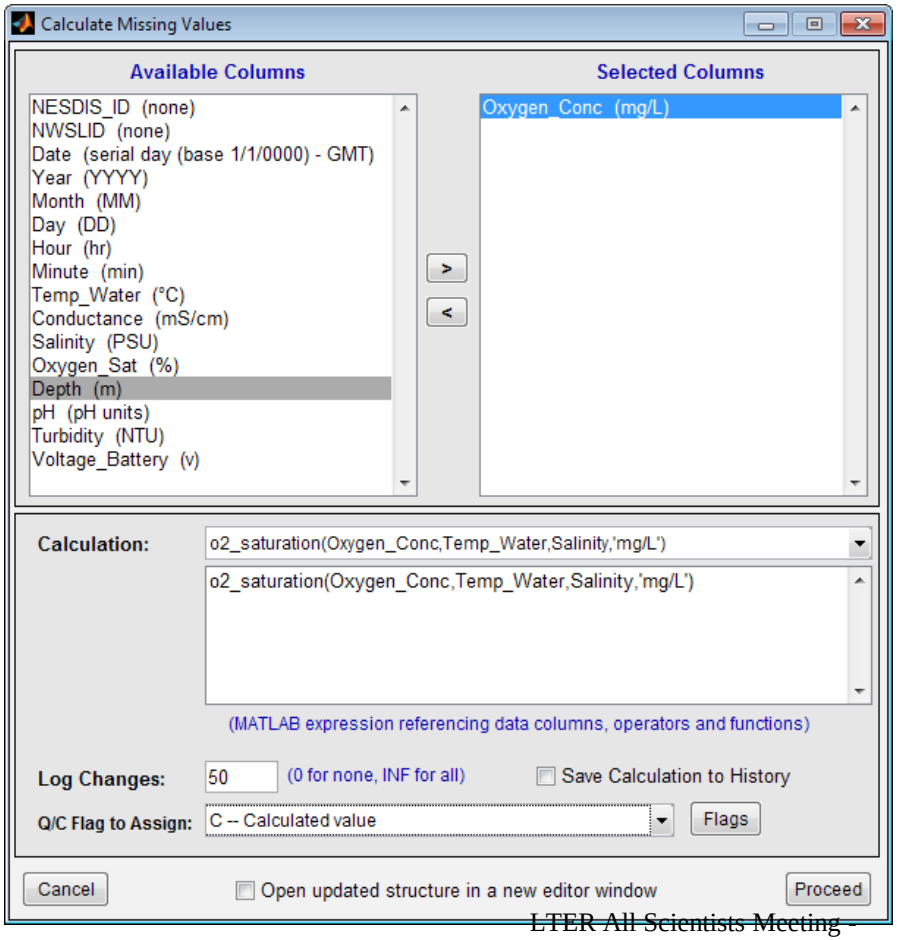
Automatic Assignment (Rules)

- Missing (NaN) values complicate rule evaluation
  - NaN can never equal anything, even another NaN (like RDBMS Null)
  - Aggregate statistics (mean, min, max, ...) return NaN if **any values** are missing
  - Compound Q/C criteria will always return false if any value is NaN, e.g. col_Salinity>0&col_Depth>1&col_Temp>10&col_Temp<35='Q' will never assign a flag for a row where Salinity, Depth or Temp value = NaN
  - No warning will be produced if NaN prevents flag assignment (valid condition)
- Best practices for NaNs
  - Always include basic, single-variable rules for limit checks when applicable (don't rely on multi-column rules)
  - Use no_nan() to remove NaNs from data before calculating mean, min, max, ...
  - Use nan2zero() to convert NaNs to 0 when rules involve totals

```
>> x = [2.1,7.25,1.2,-1,NaN,2.3]

x =
    2.1000   7.2500   1.2000  -1.0000    NaN    2.3000

>> idx = x == NaN

idx =
     0      0      0      0      0      0      0

>> idx = isnan(x)

idx =
     0      0      0      0      0      1      0

>> mean(x)

ans =
   NaN

>> mean(no_nan(x))

ans =
    2.3700
```

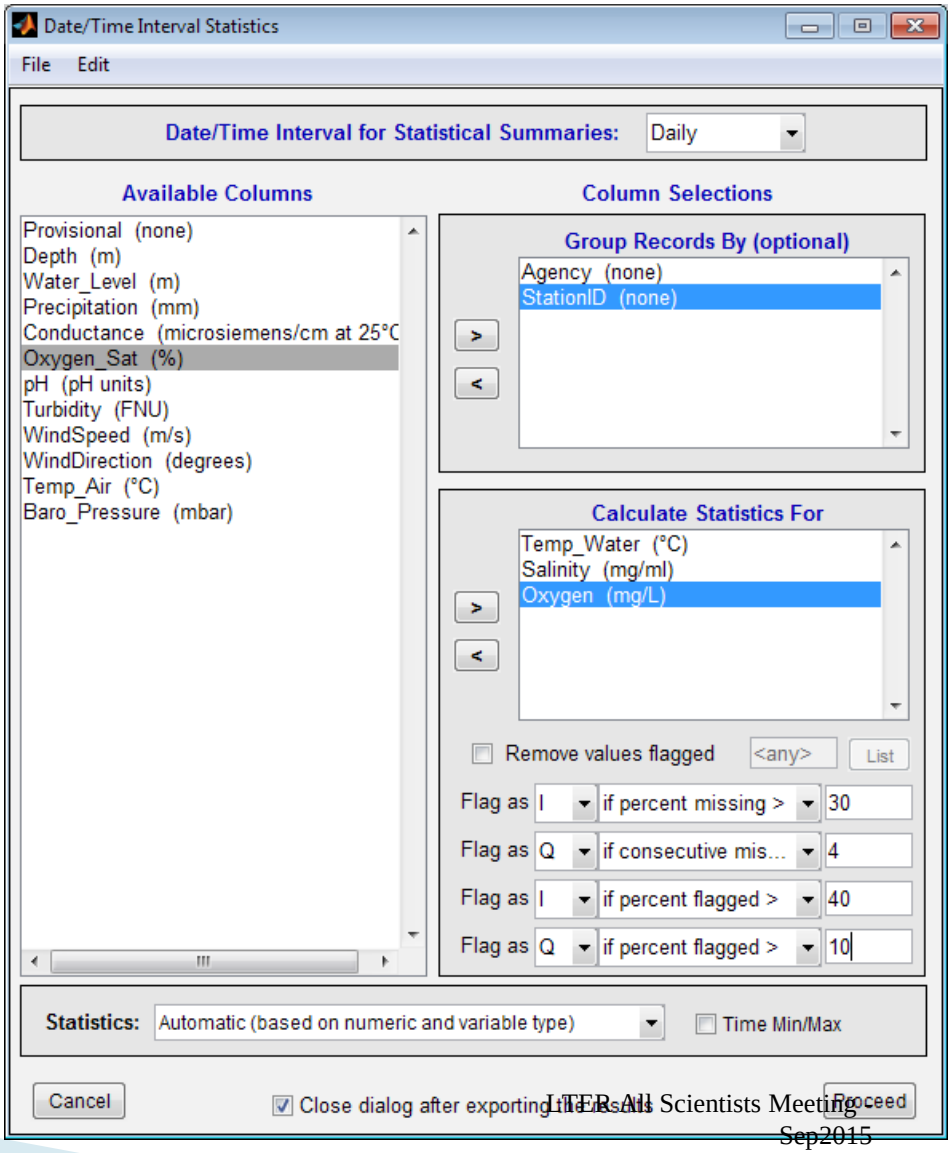
Flags for Revised/Calc'd Values

- Functions that calculate or revise values include options for assigning flags
  - Interpolated values – interp_missing()
  - Calculated values – add_calcexpr(), calc_missing()
  - Revised values – update_data()
- Useful for tracking data provenance and revisions



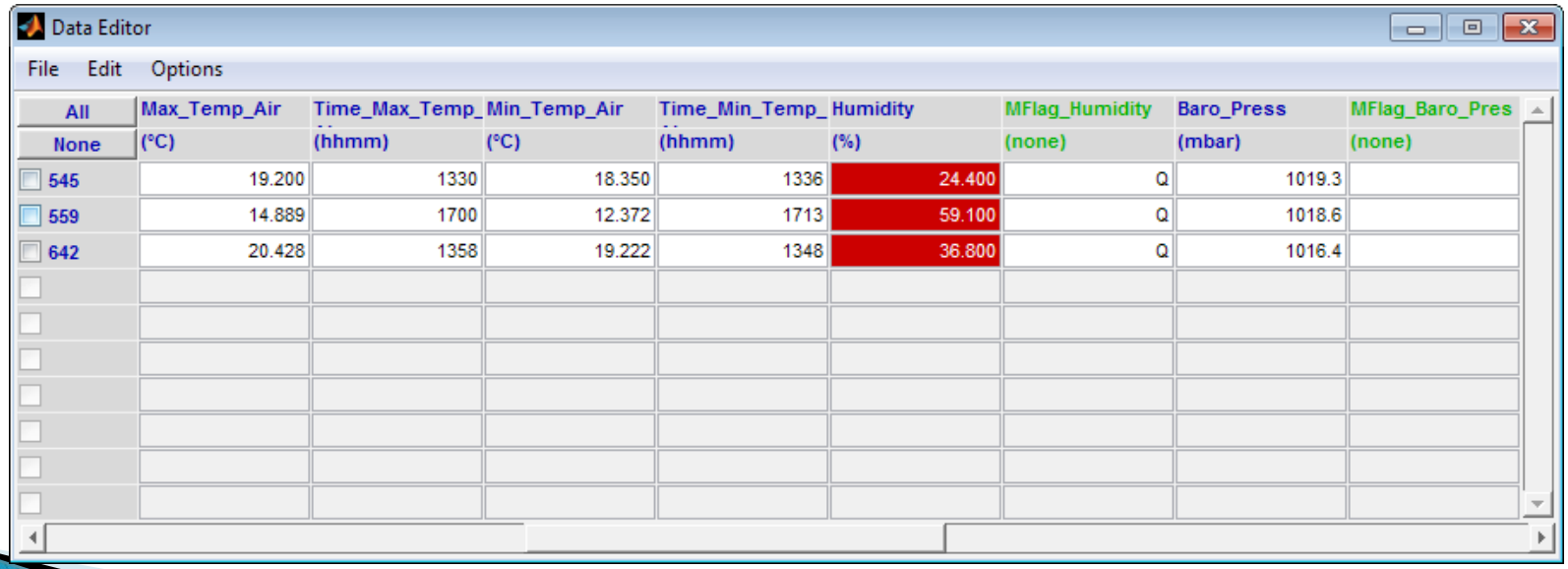
Flags for Summarized Data

- Functions that aggregate or bin data include options for generating Q/C criteria to flag derived columns
- Relevant metrics columns included automatically
  - Num_Missing_xxx
  - Pct_Missing_xxx
- Preserves info about quality and completeness of primary data
- Rules and flag assignments can be edited in derived data set using same tools as primary data set



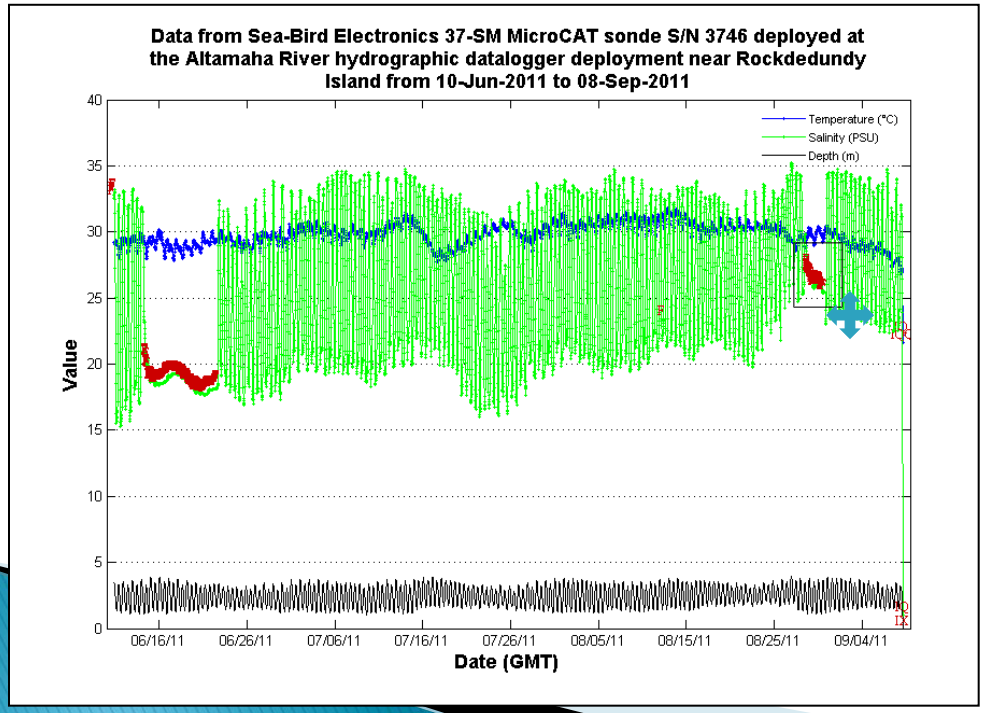
Manual Assignment (Grid)

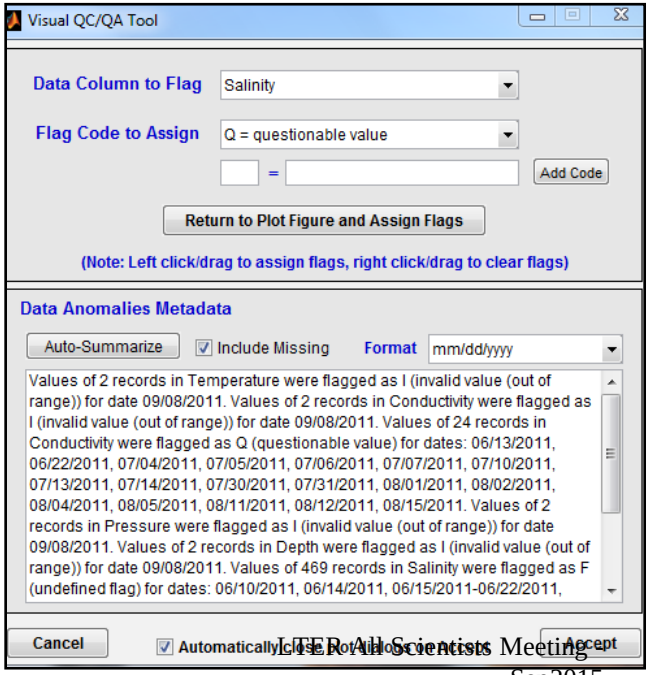
- Flags can be manually edited in the data grid
  - Useful for fine-tuning assignments
  - Can add and remove flags
  - Can filter view to hone in on flags or values
  - Any edits “lock” rules to prevent overwriting revisions



Graphical Assignment

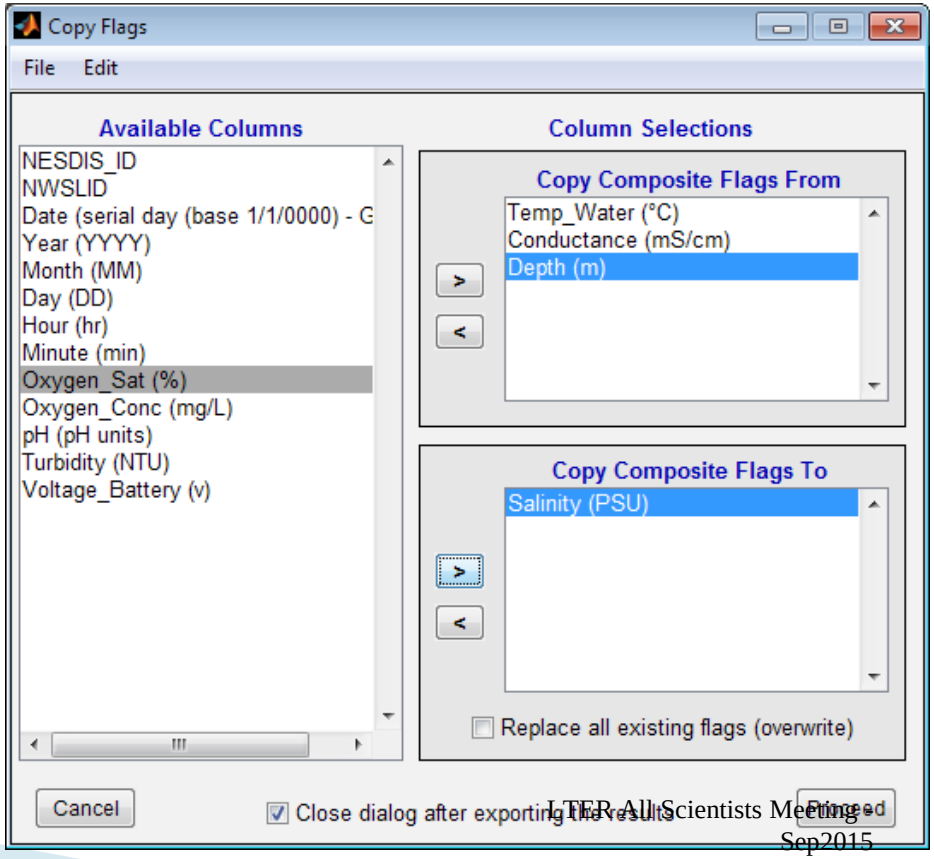
- Visual Q/C tool can be invoked from interactive data plots
  - Actions variable-specific to prevent inadvertent flagging of wrong values
  - Can zoom/pan to isolate points to flag
  - Left-click/drag to assign, right-click/drag to clear
- Anomaly reports can be auto-generated and edited to describe rationale in metadata





Copying Flags

- Flags can be copied from 1+ columns to 1+ other columns (many:many cardinality)
- Useful for propagating flags to dependent columns
  - After manual editing
  - To avoid complex dependency checks
- Can add to or over-write flags on target column(s)
- Can use GUI form or copyflags() function from command line



Text Columns to Flags

- Flags imported as text columns can be converted to intrinsic toolbox flags
  - Single and multi-character flags supported
  - Multi-character flags require mapping (/settings/flap_mapping.mat)
- Flag columns must have “Flag_” prefix and name matching corresponding data column (Salinity, Flag_Salinity)
- Flags can be added to or overwrite existing flags
- Can be used to cache manual flag assignments before restoring automatic evaluation
  - Instantiate flags as columns
  - Edit manual flags as necessary
  - Unlock flags and revise Q/C criteria as necessary
  - Convert text columns to flags, adding to new automatically-assigned flags

Specialized Flag Assignment Func's

- daterange2flags()
  - Assigns flag to 1 or more columns based on date ranges
  - Accepts array of start/end dates (discontinuous)
  - Useful for flagging known outages or maintenance periods
  - Command-line only
- codes2criteria()
  - Generates Q/C criteria for coded columns based on code definitions in the metadata
  - Useful for catching typos and undefined codes
  - Command-line or Data Editor menu command

Managing Qualifiers

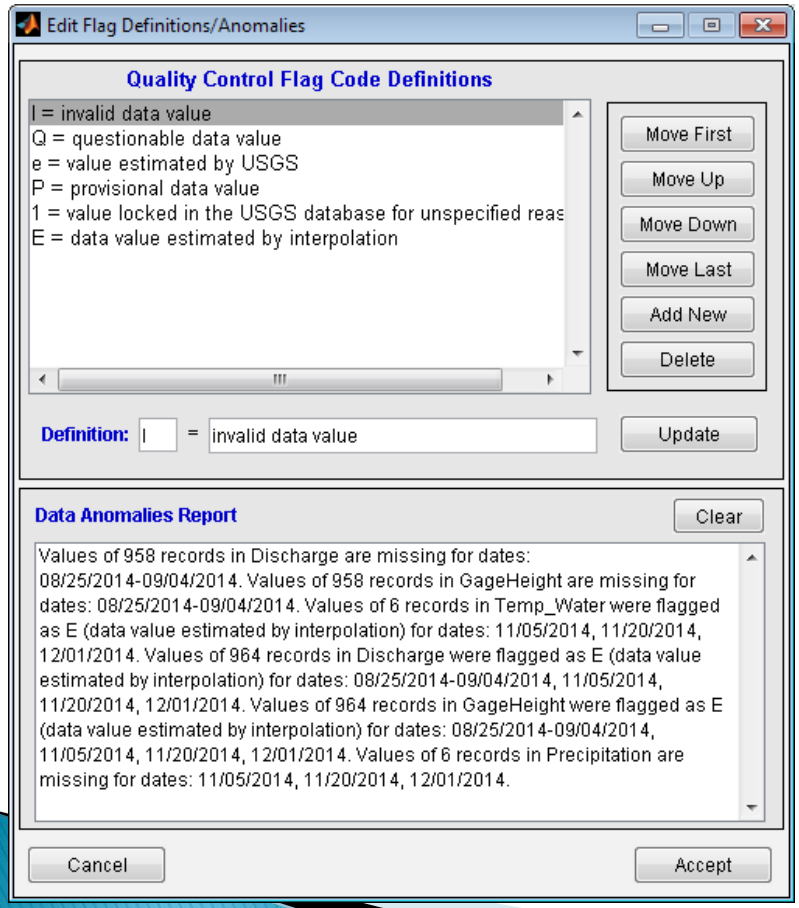
- Qualifiers can be cleared using the same approaches
  - Revise Q/C criteria limits or remove rules
  - Clear flags manually or graphically on plots (right-click)
  - Copy flags from other columns using the overwrite option
- Criteria can be locked/unlocked to manage auto assignment
  - Locking adds the token “manual” to criteria (but preserves other rules)
  - Unlocking removes “manual”, triggers recalculation
  - Any manually-assigned flags cleared when criteria unlocked!
- Bulk operations also supported
  - Clear all flags in selected column(s) and lock rules
  - Revise flag codes using search/replace

Managing Qualified Values

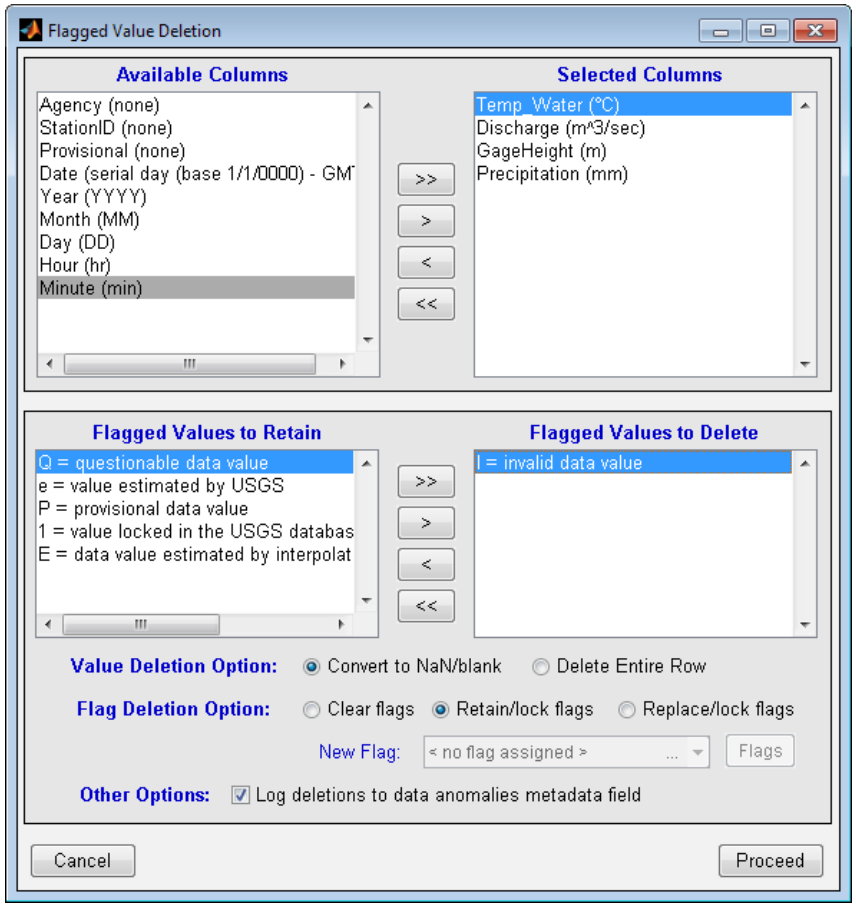
- Data values and qualifier flags paired and managed together transparently
  - Flags move with data when sorting rows/columns, merging, joining data
  - Flag column present even if no criteria defined or flags are assigned
  - Revising data value triggers criteria evaluation (unless locked)
- Data never automatically altered/deleted based on flags
  - Flags regarded as value-level metadata
  - Separation of data, flags permits flexible handling in workflows, archives
- Data analysis, plotting, export tools provide options for managing flagged values “on the fly”
  - Retain, document/display flags with values
  - Delete all or selected flagged values
  - Ignore flags

Managing Qualified Values

- Can document flagged/missing values in metadata



- Can selectively delete flagged values, rows permanently



Q/C Strategy Recommendations

- Define limit check rules for all measured variables
  - Sensor reading outside max/min specs
  - Impossible values (e.g. negative count, fraction over 100%, zero mass)
  - Improbable values based on historical data, experience (e.g. >3 SD over mean)
- Define set-based rules to check coded values (flag_inlist, ...)
- Define multi-column dependency rules for related variables
  - Redundant measurements comparable (e.g. air temp)
  - Suitable conditions when measurements made (e.g. good water depth, above freezing, suitable wind speed)
  - Reasonable time of day for diurnal variables (e.g. PAR, solar rad day/night)
  - Readings not recorded during extreme events (e.g. precip, wind)
- Define rules to check for expected disruptions or maintenance
  - Sensors disconnected or out of water for cleaning
  - Stuck/fouled/blocked sensors

Q/C Strategy Recommendations

- Define pattern check rules to identify possible contamination
  - Value changes too rapid (flag_valuechange, flag_nsigma)
  - Too little value change over time (flag_novaluechange)
  - Short-duration spikes/dips (flag_valuechange, flag_percentchange)
  - Long-duration maintenance events (flag_well_pumping)
- Save baseline Q/C rules in metadata template for re-use
- Review/refine automatic flag assignments on data plots
- Propagate flags to dependent/calculated columns to reflect edits on primary measurements
- Generate anomalies report and edit to include descriptions of rationale for manual revisions

Demo/Exercises

- Import or load a sample data set
- Define flags and rules in Q/C Criteria editor
  - Add and define one or more flags using 'Flag' button
  - Define limit check rules using primary form controls
  - Define multi-column rules using 'Add/Edit Custom Criteria'
  - Define algorithmic rules using 'Add/Edit QC Flag Function'
  - Try to implement all of the syntax examples from slides 9-10
  - Save the metadata as a template for re-use
- Refine flags on a data plot
  - Add single flags and drag to flag a range of values
  - Clear flags
- Copy flags from multiple columns to another column
- Unlock flags to restore automatic calculation
- Delete values assigned a specific flag
- Interpolate missing values and assign a flag to the imputed values

Core QA/QC Functions

addflags	Adds a character flag to specified records in one or more columns of a GCE Data Structure syntax: [s2, msg] = addflags(s, cols, rows, flag, flagdef)
clearflags	Clears specified flags from a GCE Data Structure for display or export purposes syntax: [s2, msg] = clearflags(s, flagchars, cols, lockopt, metaopt)
codes2criteria	Generates QA/QC criteria for coded columns in a GCE Data Structure based on code definitions syntax: [s2, msg] = codes2criteria(s, cols, flagcode)
cols2flags	Converts values in specified text columns of a GCE Data Structure to QA/QC flags syntax: [s2, msg] = cols2flags(s, flagcols, datacols, overwrite, delete, prefix)
cols2flags_mapped	Converts data set columns to QA/QC flags after mapping multi-character flags to single character syntax: [s2, msg] = cols2flags_mapped(s, flagset_name, flagcols, datacols, overwrite, delete)
copyflags	Copies composite flags from one or more columns and adds to or replaces the existing flag arrays syntax: [s2, msg] = copyflags(s, flagcols, datacols, opt)
cullflags	Deletes all records from a GCE Data Structure containing any values assigned specified flags syntax: [s2, msg] = cullflags(s, flagchars, cols, metaopt, logsize)
dataflag	Evaluates Q/C criteria or assigns user-specified flags to generate or update Q/C flag arrays syntax: [s2, msg, flagerrors] = dataflag(s, cols, manual_flags)
daterange2flags	Assigns Q/C flags by date range and locks flags to prevent automatic recalculation syntax: [s2, msg] = daterange2flags(s, datecol, dates, cols, flag)
get_flagdefs	Retrieves definitions for selected QA/QC flags from GCE Data Structure metadata syntax: flagdefs = get_flagdefs(s, flags)
harvest_check	Generates a harvest check email based on user-specified thresholds for missing and flagged values syntax: msg = harvest_check(s, days, missing, flagged, daily_flagged, wrap)
nullflags	Converts values in a GCE Data Structure assigned specified flags to NaN/empty syntax: [s2, msg] = nullflags(s, flagchars, cols, metaopt, clearflags, newflag, logsize)

QA/QC GUI Applications

ui_clearflags	GCE Data Toolbox dialog for selective deletion of QA/QC flags or flagged values, or selective conversion of flags to columns syntax: ui_clearflags(op, s, mode, h_cb, cb)
ui_copyflags	GCE Data Toolbox dialog for copying composite flags from one or more data columns syntax: ui_copyflags(op, s, h_cb, cb)
ui_flagdefs	QA/QC flag definition and data anomalies editor dialog called by 'ui_editor'. syntax: ui_flagdefs(op, meta, h_cb, cb)
ui_flagfunction	GUI dialog called by 'ui_qccriteria' for adding custom function calls to a Q/C criteria string syntax: ui_flagfunction
ui_flagpicker	Adds a Q/C flag picker popupmenu and edit button to a GUI figure at a specified position syntax: ui_flagpicker(op, s, pos, h, cb, enable)
ui_manual_qc	Opens a GCE Data Structure in a data grid to allow data values and Q/C flags to be viewed and edited syntax: ui_manual_qc(op, s, cols, h, cb, colwid)
ui_qccriteria	QA/QC criteria editor dialog called by 'ui_editor' and 'ui_template' syntax: ui_qccriteria(op, s, col, flagdefs, h_cb, cb)
ui_querybuilder	GUI dialog for building row restriction queries to subselect data from a GCE Data Structure syntax: ui_querybuilder(op, val)
ui_string_replace	Dialog called by 'ui_editor' for searching and replace text values or flags in a GCE Data Structure syntax: ui_string_replace(op, s, col, target, h_cb, cb)
ui_visualqc	Dialog for assigning and clearing QC/QA flags visually by clicking on data points with the mouse. syntax: ui_visualqc(op, qc_data)

QA/QC Functions

flag_locks	Locks or unlocks Q/C flag criteria for specified columns in a GCE-LTER data structure syntax: [s2, msg] = flag_locks(s, lock_option, cols)
flag_replace	Performs string replacement for flags of one or more columns in a GCE Data Structure syntax: [s2, msg] = flag_replace(s, cols, oldstring, newstring, matchtype, caseopt)
flags2cols	Converts Q/C flags in a GCE Data Structure to coded string or integer columns in the data set syntax: [s2, msg] = flags2cols(s, flagcols, clearopt, missing, pos, encode, prefix, firstflag)
flags2cols_selected	Converts selected Q/C flag information in specified columns of a GCE Data Structure to coded string columns syntax: [s2, msg] = flags2cols_selected(s, flags, cols, encode, emptycols, prefix)
flag_ctd_soak_period	Returns an index indicating records collected during the pre-deployment soaking period of a CTD cast syntax: Iflag = flag_ctd_soak_period(vals, windowsize, maxdepth)
flag_daterange	Returns an index of date/time values that are within a specified time of day for time-based QA/QC flagging syntax: Iflag = flag_daterange(datetime, daterange, dateformat)
flag_inarray	Returns an index of numeric values that are present in a specified array syntax: Iflag = flag_inarray(vals, valuearray, tolerance)
flag_inlist	Returns an index of string values that are present in a specified list or file syntax: Iflag = flag_inlist(vals, valuelist, caseopt)
flag_locationcoords	Returns an index of location codes with coordinates that differ by more the specified tolerance from reference coordinates syntax: Iflag = flag_locationcoords(location, longitude, latitude, tolerance, caseoption, ref_file)
flag_locationnames	Returns an index of location code values that are not present in the geographic database syntax: Iflag = flag_locationnames(locations, caseopt, emptyopt)

QA/QC Functions (cont.)

flag_notinarray	Returns an index of numeric values that are not present in a specified array syntax: Iflag = flag_notinarray(vals, valuearray, tolerance)
flag_notinlist	Returns an index of string values that are not present in a specified list or file syntax: Iflag = flag_notinlist(vals, valuelist, caseopt, emptyopt)
flag_novaluechange	Returns an index of values that do not differ from the mean of preceeding values syntax: Iflag = flag_novaluechange(vals, lowlimit, highlimit, framesize, iterations)
flag_nsigma	Returns an index of values above or below the mean of preceeding values by the specified number of standard deviations syntax: Iflag = flag_nsigma(vals, lowlimit, highlimit, framesize, iterations)
flag_o2saturation	Returns an index of DO concentrations that are above or below specified saturation limits syntax: Iflag = flag_o2saturation(o2_conc, temp, sal, maxsat, minsat, units)
flag_percentchange	Returns an index of values above/below the mean of preceeding values by specified percentage syntax: Iflag = flag_percentchange(vals, lowlimit, highlimit, framesize, iterations)
flag_sitenames	Returns an index of site code values that are not present in the geographic database syntax: Iflag = flag_sitenames(sitecodes, caseopt, emptyopt)
flag_timeofday	Returns an index of date/time values that are within a specified time of day syntax: Iflag = flag_timeofday(datetime, timerange, dateformat)
flag_total	Returns an index of values that exceed a limit when totalled with a specified number of preceding values syntax: Iflag = flag_total(vals, highlimit, framesize, iterations)
flag_valuechange	Returns an index of values above or below the mean of preceeding values by a limit syntax: Iflag = flag_valuechange(vals, lowlimit, highlimit, framesize, iterations)
flag_well_pumping	Returns an index indicating records collected during and following well pumping events based on negative spikes in pressure syntax: Iflag = flag_well_pumping(vals, windowsize, threshold)