UCODE USAGE CHECKLIST

__ Create a forward model
    __ that converges __ that runs completely in batch mode

__ Create a fn.uni file with observations and weights

__ Create an fn.ext file that extracts the simulated equivalents for fn.uni observations

__ Create a simple fn.pre file that substitutes one parameter value directly

__ Execute UCODE PHASE 1

__ Check that all of the extracted simulated equivalents are correct
    __ fn._ot __ fn._ck

__ Confirm that Paths are correct in:
    UCODE.batch_file
    APPLICATION MODEL.batch_file
    fn.uni path to MRDRIVE & APPLICATION MODELS

__ Create a list of alternative models

FOR EACH ALTERNATIVE MODEL

__ Decide which parameters to estimate

    __ Later this section may be iterated to consider subsets of this alternative model
        involving various combinations of parameters to be estimated (the same
        model setup with different combinations of parameters can be viewed as
        alternative models, or as subsets of one alternative)

__ Create a fn.pre file, and as necessary a fn.fnc file that substitutes the parameter
    values into the application codes

__ Execute UCODE PHASE 1

__ Check that all of the substituted vales are correct
    Files create from *.tpl s often *.sub
    Application model output files

__ Check that all of the extracted simulated equivalents are correct
    __ fn._ot __ fn._ck

__ Execute UCODE PHASE 2 or 22

- If the application model runs fairly rapidly, use phase 22.
- Phase 22 takes twice as long as phase 2, but provides correlation information as well as sensitivity information.
- If the application model takes a long time to run, one may wish to evaluate sensitivities and decide if some of the parameters should be omitted from early phases of the regression before proceeding

__ Evaluate the sensitivities and determine if:

-accuracy depends on:
- number of accurate significant figures in extracted simulated values (depending on the computer accuracy & use of double precision in the application model, use of more than 6 or 7 significant digits may be meaningless)
- magnitude of the simulated values
- magnitude of the substituted parameter values
- size of the parameter perturbations, for nonlinear parameters
-possible improvement significant figures (e.g., change in datum, scaled concentrations)
-determining appropriate perturbation size:
too small perturbations may result in : negligible differences in extracted values,
or   differences that are obscured by round-off error
too large may yield: inaccurate sensitivities for nonlinear parameters
-zero sensitivity:
-     may have physical meaning
-     may indicate extracted perturbed and unperturbed values are identical, given the number of significant figures, or that the application model did not execute
-**FOR A PARAMETER:**
- If <u>many other sensitivities are nonzero</u>, observation is not very important<u>, NO corrective action</u> needed
- If <u>all sensitivities are zero, corrective action</u> is needed.
- If <u>many sensitivities are zero, corrective action MAY OR MAY NOT be needed</u>
Five possible corrective actions:
1) smaller solver convergence criteria can be specified in the application codes;
2) the extracted values can be printed with more significant figures in the application model output file if the values are calculated with sufficient accuracy;
3) the datum of the problem can be changed or a normalization can be applied;
4) the perturbation for the parameter can be increased;
5) the methods for coping with insensitive parameters discussed later can be employed.
- Reconsider the model construction
- Modify the defined parameters
- Eliminate observations or prior information, if biased
- Adjust weights either for groups of, or individual, observations

__ Evaluate sensitivities and correlations and decide which parameters to continue estimating (recall a 2 order of magnitude span on CSS is about the limit), making notes for other combinations to try later and regarding which parameters to include for later evaluations of predictions

__ Execute UCODE PHASE 3

AT THIS STAGE, IT MAY TAKE A LOT OF TIME TO ATTAIN CONVERGENCE
This is not only reasonable and to be expected, it is also the KEY
BENEFICIAL TASK one undertakes when using regression to calibrate a
model. This is the step where one learns about the available data and the
system, and builds a representative model of quantified quality.
If the regression is not converging:

1. CHECK THE ACCURACY OF THE SENSITIVITIES
2. REMEMBER AND USE THE GUIDELINES:

    1. APPLY PRINCIPLE OF PARSIMONY
    2. USE BROAD RANGE OF INFORMATION TO CONSTRAIN
    3. MAINTAIN A WELL POSED (will converge), COMPREHENSIVE (greatest level of complexity
        that data will support) PROBLEM
      * define parameters based on the need to represent the system
      * include as many aspects of the problem and parameters as possible
      * use guideline 2 to attain reasonable simplicity
      * use Composite Scaled Sensitivities and Parameter Correlation Coefficients to define
        parameters and decide which to estimate
    4. INCLUDE MANY TYPES OF DATA AS OBSERVATIONS
    5. USE PRIOR INFORMATION CAREFULLY
      * begin with none
      * exclude insensitive parameters early and include them later
      * do not use prior to force unrealistic estimates to realistic values (if the data contain
        substantial information on the parameter, then this is likely a model or data problem;
        often exemplified by confidence intervals that do not contain reasonable values)
    6. ASSIGN WEIGHTS REFLECTING MEASUREMENT ERRORS
    7. ENCOURAGE CONVERGENCE BY MAKING THE MODEL MORE ACCURATE
      * even when stats are desirable, sometimes the model won't converge; then work to make the
        model more accurately represent the system
    8. EVALUATE MODEL FIT
      * utilize statistical and graphical measures of fit to improve the model

ANALYZE THE REGRESSION RESULTS

__ CHECK REGRESSION PERFORMANCE MEASURES:

Marquardt Parameter	Non-zero values indicate an ill-conditioned problem.
Parameter That Changed the Most	The parameter for which the maximum fractional change occurs. If the regression does not converge, the parameters listed here are likely to be contributing to the problem.
The Amount of Change	The magnitude of change

__ CHECK FIT AND RESIDUAL STATISTICS:

Table of observations, simulated values, residuals, and weighted residuals	Residuals are calculated as the observations minus the simulated values. Use this table to investigate model fit for individual observations.
Maximum weighted residual Minimum weighted residual	The maximum weighted residual indicates where the worst fit occurs relative to the expected fit, and often reveals gross errors. The minimum provides a little context by which to judge the maximum value.
Average weighted residual	An average weighted residual near zero is needed for an unbiased model fit (usually satisfied if regression converges).
# Residuals >= 0. # residuals < 0.	The number of positive and negative residuals indicates whether the model fit is consistently low or high. Preferably, the two values are about equal.
Number of runs	Number of sequences of residuals with the same sign (+ or -). Too few or too many runs could indicate model bias. The related statistic is printed and interpreted in *fn._ot*.
Least-squares Obj Func (dep.var. Only) (w/parameters)	Weighted least-squares objective function value. Given randomly distributed residuals and the same observations and weight matrix, a lower value of the least-squares objective function indicates a closer model fit to the data.
Calculated error Variance	Given randomly distributed residuals, smaller values are desirable. Values less than 1.0 (within user calculated confidence intervals: ns^2/X_U^2; ns^2/X_L^2) indicate that the model generally fits the data better than is consistent with the variances used to weight the observations and prior information, values greater than 1.0 indicate that the fit is worse. A more intuitive measure of model fit is: (s)*(statistics used to calculate the weights)
Standard error of the regression	The square root of the calculated error variance, and the same comments apply.
Correlation coefficient w/prior	R Correlation between weighted observed or prior information and simulated values. Correlation coefficient values below about 0.9 indicate poor model fit.
Max Like Obj Func AIC BIC	The maximum likelihood objective function, and the AIC and BIC statistics. Given randomly distributed residuals, lower values indicate better fitting models.
Ordered weighted Residuals	The weighted residuals are ordered smallest to largest.
Correlation between Ordered weighted residuals and normal order statistics	R_N^2 Values above the critical values printed in *fn._ot* indicate independent, normal weighted residuals, and that the points of file *fn._nm* are likely to fall on a straight line.

__ USE GRAPHICAL ANALYSIS TO EVALUATE FIT AND RESIDUAL STATISTICS:

fn._os	Observed versus simulated values	Ideally points lie along a line with a slope of 1.0. Uneven spreading along the length of the line does not necessarily indicate problems because the values are not weighted.
fn._ww	Weighted observed versus weighted simulated values.	Ideally the points lie along a line with a slope of 1.0. A different slope or uneven spreading along the length of the line may indicate problems.
fn._ws	Weighted residuals versus weighted simulated values. Traditionally, weighted simulated values are on the x axis.	Ideally the points are evenly distributed above and below the zero weighted residual axis, which indicates random weighted residuals. Uneven spreading along the zero axis may indicate problems.
fn._r	The residuals listed in this file can be plotted against any independent variable of interest.	Possible displays include plotting values from a single location against time on an x-y graph, on maps, on three-dimensional images of a contaminant plume, and on nested maps representing different times. Useful to display model fit, but use of unweighted residuals means that large values may not indicate problems
fn._w	The weighted residuals listed can be plotted as suggested for *fn._r*	The plotted values should be random, which can be tested using a runs test. Individual extreme values and areas of consistent negative or positive values are likely to indicate problems. They should be closely examined and the model corrected if possible
fn._nm	Normal probability graph of the weighted residuals. The probability values are transformed so that they plot on an arithmetic scale.	Ideally the weighted residuals fall along a straight line. If not, possibilities include: (1)The apparent nonrandomness results from limited number of values, which can be tested using *fn._rd,* or from the regression itself, tested with *fn._rg*, or (2) problems are indicated (often a poor conceptual model)
fn._rd	Normal probability graph of random numbers.	Demonstrates the variation from a straight line caused by the limited number of plotted values. If these sets of normal deviates exhibit similar deviations from a straight line as the weighted residuals of the model, the nonlinearity is due to too few observations.
fn._rg	Normal probability graph of correlated random numbers.	Demonstrates the variation from a straight line caused by the limited number of weighted residuals and by the regression fitting of the data. If these sets of normal deviates exhibit similar deviations from a straight line as the weighted residuals of the model, the nonlinearity is likely due to regression-induced correlation. If the deviations are not similar. It is likely that the conceptual model is incorrect.

IF THE FIT IS UNACCEPTABLE CONSIDER:
    __ Model Error
    __ Data Error
    __ Weighting errors

__ USE PARAMETER STATISTICS TO LEARN OF THE OPTIMAL PARAMETER
      VALUES; and EVALUATE THE QUALITY OF THE CALIBRATION:

Dimensionless scaled sensitivities (scaled by b*(wt**.5))	Indicates the importance of an observation to the estimation of a parameter or, conversely, the sensitivity of the simulated equivalent of the observation to the parameter. Identify values that are determined by one or very few observations.
Composite scaled sensitivities ((sum of the squared values)/nd)**.5	Indicates the information content of all of the observations for the estimation of a parameter. Printed at the end of the scaled sensitivity table. Values less than 0.01 times the largest value indicate parameters with much less information, and that the regression is likely to have trouble converging.
Parameter covariance matrix	The diagonal terms of this matrix are variances, the off-diagonal terms are covariances. These values are used to calculate the statistics listed below.
Parameter values	When parameter estimation converges, these are the optimized parameter values. Compare these values (and their confidence intervals) to field observations. Unreasonable optimal parameter values indicate a problem with the observations or the model.
Parameter standard deviations	Standard Deviations on optimized parameter values indicate the precision with which the values are estimated.
Parameter coefficients of variation	Provides a dimensionless measure of the precision with which the parameters are estimated which can be used to compare the precision of parameters with different dimensions.
Parameter 95% linear individual confidence Intervals	Given normally distributed residuals, reasonable optimized parameter values, a satisfactory model fit, and a linear model, linear confidence intervals are likely to reflect the uncertainty of the optimal parameter values. Model linearity is tested using PHASE=33.
Parameter correlation coefficients	For any set of parameter values, absolute values larger than about 0.95 may indicate that two or more parameters cannot be uniquely estimated. Identify highly correlated parameters. Explore uniqueness by varying starting parameter values and checking for changes in optimized parameter values.

__ CONSIDER INCLUDING PARAMETERS THAT WERE PREVIOUSLY EXCLUDED
      FROM THE REGRESSION (perhaps with prior)

__ EVALUATE THE POTENTIAL FOR INCLUDING MORE ESTIMATED
      PARAMETERS
          - use sensitivities and correlations to identify characteristics for which the data
              hold substantial information and consider representing those parameters
              in greater detail

__ EVALUATE THE POTENTIAL FOR ADDITIONAL DATA
          - use scaled sensitivities & correlations to evaluate the value of potential types
              and locations of additional data to enhance the project

__ EXECUTE PHASE 33 TO EVALUATE LINEARITY OF THE MODEL /
      RELIABILITY OF THE LINEAR CONFIDENCE INTERVALS:
          - use the discussion at the bottom of fn._33 for evaluation

__ PREPARE TO EXECUTE PHASE 44 TO CALCULATE PREDICTIONS AND THEIR ASSOCIATED CONFIDENCE/PREDICTION INTERVALS:

__ Setup and ensure that the predictive version of the application code properly executes

__ Confirm that the edited versions of the temp.*44 files are saved as fn.*44 and are correct with regard to substituted parameter values and extracted simulated equivalents

__ EXECUTE PHASE 44

__ DETERMINE the type(s) of intervals appropriate for the problem (individual, combined, or simultaneous)

__ Consider insensitive & correlated parameters
    __ if previously omitted, repeat PHASE44 and include them (perhaps with prior)
    __ if currently included, repeat PHASE 44 without them (note you will also have to rerun PHASE 3 without them)

__ PREPARE TO EXECUTE PHASE 45 TO CALCULATE PREDICTED DIFFERENCES AND THEIR ASSOCIATED CONFIDENCE/PREDICTION INTERVALS:

__ Setup and ensure that the base case version of the application code properly executes

__ Confirm that the edited versions of the temp.*45 files are saved as fn.*45 and are correct with regard to substituted parameter values and extracted simulated equivalents

__ EXECUTE PHASE 45

__ DETERMINE the type(s) of intervals appropriate for the problem (individual, combined, or simultaneous)
__ Consider insensitive & correlated parameters

    __ if previously omitted, repeat PHASE45 and include them (perhaps with prior)
    __ if currently included, repeat PHASE 45 without them (note you will also have to rerun PHASE 44 without them)

__ CONSIDER THE CALIBRATION FROM THE PERSPECTIVE OF THE DESIRED PREDICTIONS

* evaluate all models and parameters using prediction scaled sensitivities, confidence intervals, composite scaled sensitivities and correlation coefficients

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		PRECISION OF PARAMETER ESTIMATE	
		POOR Small CSS Large Coef of Var Large Confid Int.	**GOOD** Large CSS Small Coef of Var Small Confid Int
IMPORTANCE OF PARAMETER TO PREDICTIONS OF INTEREST	**NOT IMPORTANT** Small PSS	*ACCEPTABLE*	*ACCEPTABLE*
	IMPORTANT Large PSS	*IMPROVE ESTIMATION OF PARAMETER & ASSOCIATED FEATURES*	*ACCEPTABLE*

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		UNIQUENESS OF PARAMETER ESTIMATE	
		POOR Absolute Value Of some Correl Coef for this Parameter Using only Calibration Data are near 1	**GOOD** Absolute Value Of ALL Correl Coef for this Parameter Using only Calibration Data are < 0.95
IMPORTANCE OF PARAMETER TO PREDICTIONS OF INTEREST	**NOT IMPORTANT** Same Parameter Pairs are Correlated	*ACCEPTABLE*	*ACCEPTABLE*
	IMPORTANT Previously Correlated Pairs Are Uncorrelated	*IMPROVE ESTIMATION OF PARAMETER & ASSOCIATED FEATURES*	*ACCEPTABLE*

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__ RETURN TO PAGE ONE AND CONSIDER ALTERNATIVE MODELS

* strive to find models that have:
    * better fit
    * more randomly distributed residuals
    * more realistic parameter values