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## NAME

UCODE\_2005 and six post-processors for universal inverse modeling, including sensitivity analysis, data needs assessment, calibration, prediction, and uncertainty analysis

## ABSTRACT

UCODE\_2005 and six post-processors are included in this distribution. These programs can be used with existing process models to perform sensitivity analysis, data needs assessment, calibration, prediction, and uncertainty analysis. Any process model or set of models can be used; the only requirements are that models have numerical (ASCII or text only) input and output files, that the numbers in these files have sufficient significant digits, that all required models can be run from a single batch file or script, and that simulated values are continuous functions of the parameter values. Process models can include pre-processors and post-processors as well as one or more models related to the processes of interest (physical, chemical, and so on), making UCODE\_2005 extremely powerful. An estimated parameter can be a quantity that appears in the input files of the process model(s), or a quantity used in an equation that produces a value that appears in the input files. In the latter situation, the equation is user-defined.

UCODE\_2005 can compare observations and simulated equivalents. The simulated equivalents can be any simulated value written in the process-model output files or can be calculated from simulated values with user-defined equations. The quantities can be model results, or dependent variables. For example, for ground-water models they can be heads, flows, concentrations, and so on. Prior, or direct, information on estimated parameters also can be considered. Statistics are calculated to quantify the comparison of observations and simulated equivalents, including a weighted least-squares objective function. In addition, data-exchange files are produced that facilitate graphical analysis.

UCODE\_2005 can be used fruitfully in model calibration through its sensitivity analysis capabilities and its ability to estimate parameter values that result in the best possible fit to the observations. Parameters are estimated using nonlinear regression: a weighted least-squares objective function is minimized with respect to the parameter values using a modified Gauss-Newton method or a double-dogleg technique. Sensitivities needed for the method can be read from files produced by process models that can calculate sensitivities, such as MODFLOW-2000, or can be calculated by UCODE\_2005 using a more general, but less accurate, forward- or central-difference perturbation technique. Problems resulting from inaccurate sensitivities and solutions related to the perturbation techniques are discussed in the report. Statistics are calculated and printed for use in (1) diagnosing inadequate data and identifying parameters that probably cannot be estimated; (2) evaluating estimated parameter values; and (3) evaluating how well the model represents the simulated processes.

Results from UCODE\_2005 and codes RESIDUAL\_ANALYSIS and RESIDUAL\_ANALYSIS\_ADV can be used to evaluate how accurately the model represents the processes it simulates. Results from LINEAR\_UNCERTAINTY can be used to quantify the uncertainty of model simulated values if the model is sufficiently linear. Results from MODEL\_LINEARITY and MODEL\_LINEARITY\_ADV can be used to evaluate model linearity and, thereby, the accuracy of the LINEAR\_UNCERTAINTY results. UCODE\_2005 can also be used to calculate nonlinear confidence and predictions intervals, which quantify the uncertainty of model

simulated values when the model is not linear. CORFAC\_PLUS can be used to produce factors that allow intervals to account for model intrinsic nonlinearity and small-scale variations in system characteristics that are not explicitly accounted for in the model or the observation weighting.

The six post-processing programs are independent of UCODE\_2005 and can use the results of other programs that produce the required data-exchange files.

UCODE\_2005 and the other six codes are intended for use on any computer operating system. The programs consist of algorithms programmed in Fortran 90/95, which efficiently performs numerical calculations. The model runs required to obtain perturbation sensitivities can be performed using multiple processors. The programs are constructed in a modular fashion using JUPITER API conventions and modules. For example, the data-exchange files and input blocks are JUPITER API conventions and many of those used by UCODE\_2005 are read or written by JUPITER API modules. UCODE-2005 includes capabilities likely to be required by many applications (programs) constructed using the JUPITER API, and can be used as a starting point for such programs.

HISTORY (the following list was reversed with release 1.014 to show the most recent changes first)

UCODE\_2005 Version 1.017 08/10/2009

- Updated ucode version # to 1.017
- The only change from 1.016 to 1.017 is that the Jupiter 1.3.0 version of pri.f90 was used with 1.016. The new prior module has corrected messages regarding prior that are only written when verbose>=3.

UCODE\_2005 Version 1.016 08/08/2009

- Updated ucode version # to 1.016
- Compiled with JUPITER API 1.3.1
- Data-exchange file name fn\_mv\_eig was changed to fn\_eig. This file contains eigenvalues and eigenvectors of the Variance-Covariance Matrix of the Parameters scaled by parameter values.
- A summary file is now printed when the trustregion option is selected.
- Messages were added to indicate fit-independent statistics, the total number of process model runs for a given analysis, and some guidance on reducing run time.
- Messages regarding final parameter values were clarified
- Model input files are now re-written at the end of all ucode modes so the appropriate, unperturbed parameter values are listed in the process model input files. Following an SOSSURFACE run the parameters are those of the final set of parameters considered in the SOSSURFACE analysis. Otherwise they are initial values if optimization is not performed, and optimized values for an optimization run and for subsequent more advanced analyses.
- A correction was made so that groups could be used to define information for observations and predictions when the LinearityAdv mode is used.
- A minor change was made to reg\_tr\_ucode.f90 to facilitate graceful closure when one starts with the optimal values as the starting values and uses the trustregion algorithm which is unable to find a lower sum-of-squared-weighted-residuals.
- A minor change was made to ucode\_mod.f90 to provide useful error messages and facilitate graceful closure when the input weight matrix is not positive definite.
- A correction was made such that model evaluation criteria MLOF, AIC, AICc, BIC, and KIC would use the SWSR from the optimal parameters in the case where optimal parameters were not found in the final iteration.
- Corrected text in an error message printed from REG\_GNMOD\_GEN
- A correction was made such that the proper values appear in

\_scgrpmodel in situations where some observations are not used.

UCODE\_2005 Version 1.015 03/19/2009

- Updated ucode version # to 1.015
- Compiled with JUPITER API 1.3.0
- Shortly after release of 1.014 a problem was found. Version 1.015 includes corrections related to calculation of CSS with prior, printing of confidence intervals in cases when some parameters are not adjustable, and substitution of optimal parameter values in application model input files using template files.
- If you are updating from a version older than 1.014, please read information about 1.014 below because substantial changes have been made.

UCODE\_2005 Version 1.014 03/09/2009

- Compiled with JUPITER API 1.3.0
- An updated version of the MicroSoft Visual Studio 2005, Intel Fortran Compiler was used for the windows executable of this version of ucode. Previously the Intel Fortran Compiler 9.1 was used, now Intel Fortran Compiler 11.0 is used. Its ability to cope with heap arrays has improved performance, particularly with regard to successfully completing residual analysis when a large number of parameters and/or observations are used. Note this program requires a full matrix with dimensions equal to number-of-observations by number-of-observations. The memory of many computers, even when paging memory is employed, is not sufficient to evaluate problems with very large numbers of observations.
- Updated ucode version # to 1.014
- Altered approach when parameters are omitted from the regression due to low relative sensitivity (using OmitInsensitive in the Reg\_GN\_Controls input block) or parameter constraint (using Constrain=yes in the Parameter\_Data block).
- Details of the altered approach:  
New option added to the UCODE\_CONTROL\_DATA block:
  - REACTIVATE = FINAL or STARTING or NO (Default=FINAL)  
Applies when parameters have been omitted from the regression because of insensitivity or reaching a constraint.
  - PREVIOUSLY if parameters had been omitted during the regression, then when the regression converged (or if stats\_on\_nonconverge=yes), the values of all parameters (including omitted parameters) were set to the values associated with the iteration having the lowest sum-of-squared-weighted-residuals. The final sensitivities and statistics were only generated for the parameters that were active at the end of the regression.
  - NOW if parameters have been omitted during the regression, then when the regression converges or if stats\_on\_nonconverge=yes, ucode proceeds as described below for REACTIVATE = FINAL. The user can change this by setting REACTIVATE to STARTING or NO in UCODE\_CONTROL\_DATA block.
  - If REACTIVATE = FINAL then when the regression converges or if stats\_on\_nonconverge=yes, all parameters (including omitted parameters) are set to the values associated with the iteration having the lowest sum-of-squared-weighted-residuals. The final sensitivities and statistics are generated for the parameters that were defined as adjustable at the start of the regression.
  - If REACTIVATE = STARTING then when the regression converges or if stats\_on\_nonconverge=yes, all parameters that were active in the iteration with the lowest sum-of-squared-weighted-residuals are set to the values associated with the iteration having the lowest sum-of-squared-weighted-residuals and omitted parameters are set to their starting values. The final sensitivities and statistics are generated for the parameters that were defined as adjustable at the start of the regression.

- \* This method has the advantage of using values for omitted parameters that are more likely to be in the middle of their expected range. \* However, the use of a mixed set of parameter values (i.e. starting values for the omitted parameters and altered values for the other parameters) could result in a set of parameters that produce a poor model fit. It is advisable to repeat the regression with the omitted parameters set to adjustable=no. To bring this to the attention of the user UCODE prints warning messages if the resulting sum-of-squared-weighted-residuals is larger than the lowest sum-of-squared-weighted-residuals identified during the regression.
- If REACTIVATE = NO then when the regression converges or if stats\_on\_nonconverge=yes, all parameters (including omitted parameters) are set to the values associated with the iteration having the lowest sum-of-squared-weighted-residuals. The final sensitivities and statistics are generated only for the parameters that were active for the iteration with the lowest sum-of-squared-weighted-residuals.
- In conjunction with the above change of approach, an additional line was added to the \_dm file reporting: NUMBER ESTIMATED PARAMETERS IN LOWEST SUM OF SQUARES ITERATION:
- Also in conjunction with that change, messages in the #uout file explain the process as it pertains to a specific run of a regression. Also warnings are printed at the end of the #uout file, the \_summary file, and the command window output.
- Corrected calculation of the % of the objective function represented by smallest and largest residuals. The objective function values for the second to the last iteration was being used rather than the value from the last iteration.
- Corrected printing of data exchange files when prediction=yes and sensitivity=no. The residual files from the regression \_os, \_r, \_w, \_ws, and \_ww were being over written with the prediction information. Now those are unchanged and the prediction files \_dmp, \_gmp, \_p, \_pv, and \_paoptp (if there are new prior for the prediction mode) are written.
- Corrected printing of the eigenvectors of the Variance-Covariance Matrix of the Parameters scaled by parameter values. The column headings are now sequential numbers instead of parameter names.
- Added a data-exchange file containing eigenvalues and eigenvectors of the Variance-Covariance Matrix of the Parameters scaled by parameter values. The file name is fn.\_mv\_eig (later note: this was changed to fn.\_eig in 1.016).
- Added a data-exchange file containing the decomposition of the CSS (with prior if used in the regression) using SVD of the XT<sub>W</sub>X matrix scaled by parameter values and the number of observations plus the number of prior information equations. The file name is fn.\_sc\_svd. The resulting stacked version of the CSS in a bar chart provides some indication of parameter correlation.
- Clarified message related to the inability of ucode to write the \_b1 file for cases with extremely large parameter confidence intervals
- Corrected a problem for which an error message related to writing of derived parameters to final template files was printed to the screen after completion of all other tasks and after printing of the successful completion message.
- Corrected a problem in which a parameter that was specified as constrain=no would be flagged with a "!" when its value was outside of the constraint bounds. This occurred if at least one other parameter was defined as constrain=yes. Also added the "-" in prediction mode for parameters for prediction. Calculated results are unaffected.
- Corrected a problem for which the Kashyup statistic could not be calculated for cases with omitted parameters that included prior information.
- Omitted printing of CSS to the screen and the fn.#upred file when prediction=yes, and instead included a note referring

- the user to the `_sp*` files as described in Chapter 14 of the UCODE\_2005 documentation.
- Corrected garbled labels of names of parameters for predictions in underscore files.
  - Now the optimal (rather than initial) parameters are printed at the start of advanced phase "#" output files.
  - Omitted printing of some warning messages that were not relevant to the task. For example there is no longer a warning that default values for regression controls are used in prediction mode.
  - In UCODE\_2005 and all auxiliary codes: changed references to "underscore" files in error messages to "data-exchange"
  - Corfac\_Plus: Updated version #, compiled with Jupiter 1.3.0.
  - Linear\_Uncertainty: Updated version #, compiled with Jupiter 1.3.0, added parameter labels that were missing for parameters for prediction.
  - Residual\_Analysis\_Adv: Updated version #, compiled with Jupiter 1.3.0, corrected calculation of mean and standard deviation for simulated weighted residuals for some cases involving omitted and non-adjustable parameters.
  - Made CDUM, IDUM, RDUM global variables in `ucode_mod.90`
  - Model\_Linearity: Updated version #, compiled with Jupiter 1.3.0.
  - Model\_Linearity\_Adv: Updated version #, compiled with Jupiter 1.3.0, corrected a label in `#modlinadv_conf` that indicated weights were being read when sensitivities were being read, corrected parameters used for calculation of nonlinearity measures for some cases involving omitted and non-adjustable parameters.

UCODE\_2005 Version 1.013 08/12/2008

- Updated version # to 1.013
- Support for nearly all of the UCODE\_2005 data-exchange files is now available in GW\_Chart, freeware available from [http://water.usgs.gov/nrp/gwsoftware/GW\\_Chart/GW\\_Chart.html](http://water.usgs.gov/nrp/gwsoftware/GW_Chart/GW_Chart.html).
- Corrected error for the case when the final parameters did not yield the lowest sum-of-squared residuals. In that situation ucode was printing information related to parameters from the final iteration rather than those that yielded the lowest sum-of-squared residuals. This can affect UCODE\_2005 output files with filename extensions `#uout`, `_b1`, `_b2`, `_dm`, `_linp`, `_mc`, `_mv`, `_nm`, `_os`, `_pc`, `_r`, `_s1`, `_sc`, `_sd`, `_so`, `_sppp`, `_sppr`, `_spsp`, `_spsr`, `_spu`, `_su`, `_w`, `_ws`, `_ww`, and `_wt` (if keyword `WtOSConstant`>0, see page 85 of the documentation); Residual\_Analysis output files with extensions `_rb`, `_rc`, `_rd`, and `_rg`; and Residual\_Analysis\_ADV output file with extension `_rdadv`. This correction affects example `ex1a` in appendix A of the documentation in that the values in some of the files listed above are slightly different.
- Corrected error in which the flag for calculating nonlinear intervals on a parameter in the `parameter_data` block was ignored for mode `NonlinearIntervals=yes` in the `UCODE_CONTROL_DATA` block.
- Added a final substitution of the template files so they contain the optimal values. Prior to this, the template files contained values perturbed for sensitivity calculations.
- To allow multiple runs to be used to calculate nonlinear intervals (as often is needed because of lengthy runs and convergence problems), new files with date/time stamps are produced for files with extensions `_intconf`, `_intconfpar`, `_intpred`, and `_intpredpar` to create, for example, `ucode_rootname--2008_06_21--22.17._intconf`. For each UCODE\_2005 run, files with extensions `_intconf`, `_intconfpar`, `_intpred`, and `_intpredpar` are still produced. As before, they contain the intervals calculated in the most recent run. To obtain a full list of interval limits, values from the time-stamped files may need to be moved into these files. The nonlinear intervals can now be plotted in graph form

- using GW\_Chart.
- Corrected an error in which an additional forward&der run was executed for the trustregion option when derivatives were read from process model output
- Corrected value of uncertainty associated with prior information on "parameters for prediction" (See note for UCODE\_2005 version 1.009). Previously the variance on these parameters was multiplied by the cev of the regression, but now the variance is used directly without multiplication.
- Previously parameters that were omitted from the regression due to parameter constraints were marked with a !. Now parameters that are omitted due to insensitivity are also marked with a !.
- Added an underscore file \_scgrp that reports composite scaled sensitivities and the two observations with the largest sensitivities for each observation group.
- Modified ucode such that regressions with parameters omitted due to insensitivity or parameter value constraints could be used for advanced evaluations (e.g. predictive uncertainty, nonlinear intervals) without rerunning the regression with those parameters as adjustable=no. The uncertainty measures include the uncertainty associated with the "parameters for prediction".
- increased number of significant figures printed in \_pasub to match those printed in \_paopt. Format was changed from 1PE15.7 to 1PE25.16.
- increased number of significant figures printed in #uout for SUM OF SQUARED, WEIGHTED RESIDUALS. Format was changed from G12.5 to G15.7.
- unused subroutine UCODE\_DEF\_WRITEITER was deleted from ucode\_mod.f90
- removed write statements that are no longer needed from ucode\_2005.f90
- Updated Corfac\_Plus to version 1.005. Corrected reading of prior for "parameters for prediction" (See note for UCODE\_2005 version 1.009) in the case where parameters had been omitted from the regression due to insensitivity or constraint. This problem caused corfac\_plus to fail in this situation.
- Updated Linear\_Uncertainty to version 1.006. Increased format for writing the numbers of items at the start of the output to accomodate more observations.
- Updated Model\_Linearity\_Adv to version 1.004 to use results from projects that include parameters for prediction.

UCODE\_2005 Version 1.012 02/05/2008

- Updated version # to 1.012
- Compiled with JUPITER API 1.2.3
- Added option to run prediction=yes with sensitivities=no to facilitate testing of the predictive mode setup
- The above change required that sensitivities be set to yes in the file 05.in of folder ex1a
- Corrected format error for writing large numbers of predictions
- Corrected further error in which \_mvp was not written properly for prediction=yes mode.
- In the calculation of the hookstep Marquardt parameter, the algorithm now uses a scaled Hessian and unscaled Marquardt parameter. This improves robustness on ill-conditioned Hessians.
- Corrected calculation of  $\ln|F|$ , log determinant of the Fisher Information Matrix. Now  $\ln(|XTwX|/(SOSWR/n))$  is printed. This results in a change in the order of variables in the subroutine REG\_GNMOD\_EVA\_MLOFSTATS. This only changes values printed for "LN DETERMINANT of Fisher Information Matrix" with and without prior. The value printed for KIC is not affected.
- Corrected condition in which underscore files for residuals

- were not written for sensitivities=no optimize=no dataexchange=yes.
- Corrected condition for which \_xyzt file was not written because unused observation names were not included in the .xyzt file. Now only used observations need to be listed in the .xyzt file in order for \_xyzt to be written.
- Cleaned up coding in UTLUCODE\_CHECK\_PRI. This did not affect functionality.
- Improved error checking and messaging for definition of prior.
- Corfac\_plus was edited. The version number was updated to 1.004.
  - there is now a default for Read\_cov. The default is no.
  - the default for RegressionUsedTrueCov was changed to yes
- Residual Analysis was edited so that one line of the code that was longer than 80 characters is now wrapped and thus does not exceed 80 characters.
- the documentation pdf was updated to match the version distributed on the USGS Publication Warehouse web site. Differences between this pdf and the previously distributed pdf are:
 

Page(s)	Change from previous to current version
xiv	Missing page number for table 38 added
30-39	Different pagination caused by moving text from after to before table 3
44	Sentence added at end of last paragraph.
63-64	MAXSTEP description revised
154	Definition for NP added to header

UCODE\_2005 Version 1.011 10/10/2007

- Updated version # to 1.011
- Adjusted formats for \_sc because labels and some numbers ran together
- Corrected error where parameters were not substituted properly for the base case of a prediction=yes analysis.
- Adjusted job definition so that runs with Forward&Der run the application code only once.
- Corrected error in which \_paoptp was not read properly for prediction=yes mode.
- Corrected error in which \_mvp was not written properly for prediction=yes mode.
- Clarified some of the statements printed to the screen during execution of ucode
- Modified Residual\_Analysis and updated to version 1.005 to print a message and terminate when the number of observations exceeds 10,000 because the NxN matrix is too large.

UCODE\_2005 Version 1.010 08/16/2007

- Updated version # to 1.010
- Compiled with JUPITER API 1.2.1
- Modified such to provide normal termination for cases in which there are fewer observations than parameters but only sensitivity calculations (not optimization) are requested. In this situation parameter variance cannot be calculated and related statistics are not printed. If this occurs when optimization is requested, the message:  
CONSIDER WHETHER TOO MANY OBSERVATIONS HAVE BEEN OMITTED  
has been changed to  
TOO FEW OBSERVATIONS GIVEN THE NUMBER OF PARAMETERS

UCODE\_2005 Version 1.009 07/12/2007

- Updated version # to 1.009
- Compiled with JUPITER API 1.2.1
- Updated to accommodate the use of parameters in predictive mode that were not included in the calibration. This allows the user to specify uncertainty for a parameter that influences predictive uncertainty but cannot be estimate in

the calibration mode. For example the addition of effective porosity for an advective travel time prediction when the calibration considers only head and flow observations which do not contain information about effective porosity. This change includes a number of new input blocks which are described in the supplemental pdf:

"Additional\_Input\_Blocks\_ucode\_2005.pdf".

- Updated input files for ex1b to use the capability to add parameters for prediction.
- Corrected maximum record length on data-exchange files with long lines in ucode and associated codes. In some cases the length was not sufficient to write the entire line and the execution would terminate.
- Modified format of header lines in b\* files so parameter and observation names line up with their values
- Heading banners for warnings were changed from !'s to \*'s
- Added a feature to edit prior information equations in the case where a log-transformed parameter appears as the only term of a prior equation but is not included in the parentheses of a log10 function. If such a parameter occurs in any form other than log10(param-name) or param-name alone, an error message is written and the code terminates.
  
- Updated Corfac\_Plus to version 1.003. This version considers parameters that are included for the predictive mode. The level of verbose required to echo input was increased from 3 to 4 in order to avoid echoing at the default value of verbose. In addition, a trailer was added indicating the time of completion and the time required to execute.
  
- Updated Linear\_Uncertainty to version 1.005. This version considers parameters that are included for the predictive mode. In addition, a trailer was added indicating the time of completion and the time required to execute.
  
- Updated Model\_Linearity to version 1.005. Increased maximum record length for reading b1 and b2. Modified output format for final table to improve readability. In addition, a trailer was added indicating the time of completion and the time required to execute.
  
- Corrected Model\_Linearity\_Adv and updated to version 1.003 to properly consider cases in which some parameters are not adjustable in the regression. This version considers parameters that are included for the predictive mode. In addition, a trailer was added indicating the time of completion and the time required to execute.
  
- Corrected Residual\_Analysis and updated to version 1.004 to use new api to read supri. In addition, a trailer was added indicating the time of completion and the time required to execute.
  
- Corrected Residual\_Analysis\_Adv and updated to version 1.002 to use new api to read supri. In addition, a trailer was added indicating the time of completion and the time required to execute.

UCODE\_2005 Version 1.008 was a temporary version that was not released

UCODE\_2005 Version 1.007

- updated version # to 1.007
- k of Kashyap's measure is now NPE, the number of parameters estimated for the process model rather than NPE+1 as is used for other model criteria, where the addition of one reflects the estimation of sigma-squared
- subroutine UTLUCODE\_INVERT was modified to scale the matrix before inverting it and unscale the inverted matrix before returning it. This makes matrix inversion possible for difficult problem in which elements of the matrix differ by

- many orders of magnitude and in most cases prevents the error  
Error: Failed in UTLUCODE\_INVERT
- added test to determine if upperconstraint>lowerconstraint for parameters with constrain=yes, program terminates and indicates the parameters for which this is not met
  - extension of the range of DOF in UTL\_CHISQ was accomplished by calling UTLUCODE\_CHISQ which allows for appropriate intervals to be calculated on cev when many observations are included in the regression
  - Model\_Linearity was corrected to only print the prior weight matrix if prior information are included in the model being evaluated. In addition this print was altered so it will only occur when verbose>4. Version of Model\_Linearity was updated to 1.002
  - Printing of Residual\_analysis was modified to accomodate cases with more than 99 parameters by allowing 4 spaces for each parameter and printing strips of 10 parameters at a time. Version of Residual\_Analysis was updated to 1.002
  - Summary of the progress of the regression is now printed at the end of \*.#uout when the regression does not converge even if Stats\_on\_nonconverge=no.
  - The same summary information is printed after each iteration to a file named \*.\_summary. This information is available to quickly evaluate the progress of the regression should it terminate prematurely.

UCODE\_2005 Version 1.006 was a temporary version that was not released

UCODE\_2005 Version 1.005

- updated version # to 1.005
  - added version checking for compatibility of UCODE source and Jupiter API
  - compiled with JUPITER API 1.1.0
  - using JUPITER API 1.100 allows up to 2 billion observations previous limit was 44721
  - corrected error related to SOSSURFACE when only one parameter was evaluated, parameter value now varies over the indicated range
  - corrected error that led to printing of zero for derived predictions and variance in \_p and \_pv
  - corrected error that at times led to problems with damping when parameters were constrained
  - included a check for conditions that at times led to continual estimation of the same values when parameters were constrained (this condition is likely to occur if parameters are over constrained)
  - added checking and adjustment of input that controls the value of the Marquardt parameter so as to avoid the potential for entering an infinite loop in the Gauss-Newton solution
  - extended message written to \*.#uout describing tasks accomplished when prediction=yes
  - Label STANDARD ERROR OF THE REGRESSION in #uout was changed to STANDARD ERROR so as to be applicable when calculated for a forward model execution.
  - Maximum Likelihood Objective Function is now reported as  

$$\text{MLOFO} = \text{NOBS} * \ln(\text{SWSR}/\text{NOBS})$$
 for Observations Only and  

$$\text{MLOFOP} = (\text{NOBS} + \text{NPR}) * \ln(\text{SWSRwPri}/(\text{NOBS} + \text{NPR}))$$
 for Obs & Prior  
 where:  

$$\text{SWSR} = \text{sum\_weighted\_squared\_residuals}$$
  

$$\text{NOBS} = \#\text{observations}$$
  

$$\text{SWSRwPri} = \text{sum\_weighted\_squared\_residuals including prior}$$
  

$$\text{NPR} = \text{number of prior observations}$$
- This change in the calculation of MLOF changes the values of model evaluation criteria. All criteria were affected by the same amount, so their relative rankings are not affected.
- calculation of the ln determinant of the Fisher Information Matrix was corrected from  $\ln|XTwX|$  to:  

$$\text{NPE} * \ln(\text{SWSR} / \text{NOBS}) + \ln |XTwX|$$
  

$$\text{NPE} = \#\text{ estimated\_parameters}$$
- When prior are included, the SWSR includes the residuals on prior information items and NOBS includes the number of

- prior information items.
- This change in the calculation of the Fisher Information Matrix changes the value of Kashyap's measure.
- Formula for calculating Kashyap's measure was corrected to use the normalized Fisher information matrix.
  - printing of model evaluation criteria was changed to include values only relative to MLOF, both without prior, and with prior if prior information equations are included in the parameter estimation.
  - changes were made to the `_dm` file:
    - 1) Maximum Likelihood Objective Function is now reported as describe above for the `#uout` file
    - 2) Values of the `ln` determinant of the Fisher Information Matrix and model evaluation criteria were corrected as described above for the `#uout` file
    - 3) Three lines were added. These contain: 1) the value of `ln` determinant of the Kashyap's measure (KIC) for observations only, 2) the Fisher Information Matrix for observations only. and 3) an indication of whether any of the final statistics were calculated with forward difference perturbation.
  - correction was made to ensure the final sum of squared weighted residuals is printed and used in calculation of the model measures

#### UCODE\_2005 Version 1.004

- updated version # to 1.004
- version numbers were incremented on all auxiliary codes that had been modified since first release in Feb 2006
- added write statements to indicate which version of the Jupiter API is used
- updated the API. Items known to be specific to `ucode_2005` functionality include:
  - UTL\_SSVD2 was revised so that when ITER equals 30, an error message is printed and UTL\_STOP is called to stop execution
  - write statements reformatted to print SCALEPVAL rather than BSCAL which is the name of SCALEPVAL in the code. This does not change the results or the numbers that are printed.
  - code was made consistent with input manual to allow SOSSurface to be not only yes or no, but also file. Error reporting related to that file was improved.
  - corrections were made to the trust region algorithm so that MODVALPREV is passed as an argument so its value is retained. Also a check was added to the hookstep to prevent an infinite loop.
  - a new feature was added to the trust region algorithm adding the option to not scale the least squares matrix. The keyword is:
 

```
SCALING = none (false, f, no, or n will work as well)
```

 Omitting scaling can, in some cases, improve performance of the regression.
- example files included a few prerelease parameters that are not part of `ucode`, these were altered or deleted. (TOL was changed to TOLPAR, TOLSOSR was changed to TOLSOSC, and FletcherReeves was deleted).
- A couple of errors were found in the examples files. 1) The `ex1a\02.in` and `03.in` file was modified to use the template file for the forward model. 2) For some cases, having only one outer pcg iteration was not enough to obtain convergence. So, the number of outer iterations was increased in `test-data-win\data-used-by-all\tc1.pcg`. These changes alter the details of the results but not their essence.
- the MODFLOW executable for the example problems was updated to version 1.17

#### UCODE\_2005 Version 1.003 08/13/2006

- updated version # to 1.003
- correction to use the absolute value of 1% of the starting parameter value as the default for ScalePval when it is not specified, because the value must be positive
- replaced STA\_UEV\_DX\_READ\_DM in `ucode_mod.f90` and

- reg\_gn\_ucode.f90 with UTLUCODE\_DX\_READ\_DM which is a modified version of STA\_UEV\_DX\_READ\_DM that echoes items of the \_dm file as they are read
- corrected error for which prior information plot symbol was always printed as 1 in some underscore files
  - added check to see if the simulated equivalents for subsequent Beale parameter sets are identical to the previous set, and write a warning to the screen, #umodlin, and #modlin if that is the case (occasionally there is a good reason for these being the same, but usually it is a failure of the process model for a given set of parameter values
  - corrected error that arose when derived predictions were used. UCODE\_2005 would fail if this error occurred.
  - nullified some pointers in all files which were identified as problems by some compilers and deleted some unused variables
  - corrected error that selected the second to the last iteration as the one with the lowest sum of squared residuals if model calculated sensitivities were being used. Note this results in slightly different results for the test problems.
  - corrected error that printed sum of squared residuals offset by one iteration in the penultimate summaries when intermediate printing was on. Also this output was slightly reformatted.
  - corrected error for which maximum fractional parameter change in regression space was used for convergence as well as for limiting change when maxchangerealm=regression
  - added the hookstep option to the trust region method. In order to use this the user needs to specify trustregion=hookstep in the REG\_GN\_CONTROLS input block. Descriptions of the hookstep method is provided by Dennis and Schnabel, in their book: "Numerical Methods for Nonlinear Optimization and Nonlinear Equations"
  - updated API modules, updating the modules corrected a bug that limited equations to 40 characters (the limit is now 2000)

changes were made to all source files for ucode and associated codes

- UCODE\_2005 Version 1.002 03/26/2006 - correction to nonlinear confidence limit feature to: avoid an unnecessary final calculation of sensitivities, print the correct set of parameter values, search for and print the values from the iteration closest to the goal, print warnings and suggestions when the result is far from the goal, and to provide a more readable output.
- correction to correct error when derived observations were used. UCODE\_2005 would fail if this error occurred.
  - updated API modules, notable is improvement in the parallel module
  - echo printing was added to repeat what is read when \_dm is read and verbose>4
  - a format was changed in linear\_uncertainty to add a missing "

changes were made to ucode\_2005.f90. ucode\_mod.f90  
reg\_gn\_ucode.f90 reg\_gn\_mod.f90 utlucode.f90 and sta.f90  
pll.f90 utl.f90 and linear\_uncertainty

- UCODE\_2005 Version 1.001 02/13/2006 - minor adjustment to sta.f90 to accommodate UNIX, distribution files are formatted for UNIX, an example make file is included for UNIX. Minor changes to documentation.

UCODE\_2005 Version 1.000 02/06/2006 - Initial release.

UCODE\_2005 Version history order of listing was reversed starting with version 1.014

#### DATA REQUIREMENTS

In order to use UCODE\_2005, the process model needs to be constructed and the main UCODE\_2005 input file needs to be created. Input data are read

from files.

#### SYSTEM REQUIREMENTS

UCODE 2005 is written primarily in Fortran 90. The code has been used on UNIX-based computers and personal computers running various forms of the Microsoft Windows operating system.

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