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LLNL-TR-503291

MicroCT: Automated Analysis of CT Reconstructed Data of Home Made Explosive Materials Using the Matlab MicroCT Analysis GUI

I. M. Seetho, W. D. Brown, J. S. Kallman, H. E. Martz, W. T. White

October 6, 2011

Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Lawrence Livermore National Laboratory Global Security Principal Directorate Image Database Development Project	Standard Operating Procedure	
	Doc. No. IDD-MCT-SOP-007	Rev. No. 0

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Concurrence MCT Technical Leader	Date
Approval IDD Project Principal Investigator	Date

Contents

1.0 Purpose and Scope

This Standard Operating Procedure (SOP) provides the specific procedural steps for analyzing reconstructed CT images obtained under the IDD Standard Operating Procedures for data acquisition [1] and MicroCT image reconstruction [2], per the *IDD Quality Assurance Plan for MicroCT Scanning* [3]. Although intended to apply primarily to MicroCT data acquired in the HEAFCAT Facility at LLNL, these procedures may also be applied to data acquired at Tyndall from the YXLON cabinet and at TSL from the HEXCAT system. This SOP also provides the procedural steps for preparing the tables and graphs to be used in the reporting of analytical results. This SOP applies to production work – for R&D there are two other semi-automated methods as given in [4, 5].

2.0 Precautions

There are no precautions from Integration Work Sheets or Facility Safety Plans and documents that are applicable to this work.

Work for this SOP is performed in project members' offices and does not present any high-risk safety situations. There are no operational safety boundaries such as set points or parameters that are applicable to this work.

3.0 Special Tools and Equipment

- Computer running Windows XP or above, with either Matlab version 2010a (or later) or the Matlab Compiler Runtime version 7.13 (or later) installed. Installations of Matlab require the inclusion of the image processing toolbox add-on.
- Automated MicroCT Analysis GUI version 1.2.1[1] or later -- at present all versions are backwards compatible (for an outline of the files included in the GUI, see Appendix A). The Matlab-based Automated MicroCT Analysis GUI includes a front-end graphical user interface used for facilitating the reduction and statistical characterization of CT reconstructed data, with add-on GUIs for viewing the resulting processed data and for comparing data across multiple tests for a form of similarity (see Appendix B). At each step in the data reduction process, this code writes resulting data to output files, which are outlined in section 5.2 of this SOP. The internal mathematical details of the software are discussed in Appendix C and the Automated MicroCT Analysis GUI mathematical reference [6]. Pre-use checks are outlined in Appendix D.
- Java Runtime Environment 6 or later.
- *watertosnake.jar.* This Java ARchive file contains class definitions and methods critical to the function of the analysis GUI.
- Microsoft Excel 2007 (or later).
- *chart_macros.xlsm.* This macro-enabled excel workbook is used to read in the output generated by the MicroCT GUI and generate plots of certain data.

[1] For data taken after July 1, 2011, version 1.3 should be used exclusively to remain consistent with LLNL.

4.0 Key Terms and Definitions

Experiment	The acquisition of MicroCT data, scanning a specimen with a specific x-ray source voltage (kV), with specific filtering medium and collimation parameters.
GUI	Graphical User Interface.
IDD	Image Database Development Program.
kV	kilovolts (thousands of volts).
LAC	Linear Attenuation Coefficient – a quantity characterizing how easily a material is penetrated by x-rays.
LMHU	Livermore-Modified Hounsfield Unit – Hounsfield units shifted such that at 160kV with an aluminum and copper filter, water has a mean LAC value of 1000, and air has a value of 0.
MicroCT	X-ray computed tomography using a system designed to scan small-quantity specimens.
QAP	Quality Assurance Plan.
QIP	Quality Implementing Procedure.
Reference materials	Six materials are used as comparison points to normalize and evaluate the quality of acquired specimen data values, in order to account for system and environment-generated variability.
Snakes/Active Contour Segmentation	Active contour methods used in segmenting images into component areas corresponding to discrete objects [7].
SOP	Standard Operating Procedure.
Specimen	The object to be x-rayed, consisting of a particular preparation of a sample of interest and the container holding the sample.
TAFRL/Tyndall	Tyndall Air Force Base Research Lab.
Test	The collection of experiments scanning a particular preparation of specimen.
TSL	Transportation Security Laboratory.
Watershed	A method for segmenting images into component areas corresponding to discrete objects [8].
$^{L}Z_{eff}$	Effective atomic number – an estimate of the average atomic number for a compound or mixture. The upper case L refers specifically to Livermore's method as given in [9].

μ The mean value of the LAC over a volume of interest for a given x-ray source voltage, filtration and collimation.

Note *Within this document, the adopted coordinate system is such that the x-axis is the horizontal axis in the slice image plane, the y-axis is the vertical axis in the slice image plane, and the z-axis traverses slices.*

5.0 Procedure

Notes *Assure applicable data and test dates are current and correct by comparing the dates provided in acquisition notes text file with the dates of scan and reconstruction files. The image files should have a filename structure "<specimen>_x.sdt" and "recobj_x.sdt," where* **specimen** *denotes the specimen name, and* **x** *is an integer value omitting leading zeros identifying the slice number of each scan file. The directory structure of the test directory will be outlined below in section 5.2.*

Stop the procedure immediately and notify the Technical Leader if there are any unusual discrepancies, failures, or abnormalities as noted within this document.

5.1 Preliminary Steps

This process begins when the Image Analyst is notified that data are available for processing and is given the location of the data to be analyzed. Note that these procedures apply only to the analysis of two-slit experiment data.

5.1.1 Verify the following:

5.1.1.1 The acquisition SOP has been followed (i.e., the data have been acquired with the dual-level carousel, the reference materials on the lower level of the carousel and the specimen(s) on the upper carousel, and every rotational view acquired includes either the reference materials or the specimen(s) in the field of view). This step should be completed in accordance with the directions outlined in the Data Acquisition and CT Reconstruction SOP documents.

5.1.1.2 The data has been acquired and reconstructed for at least the following two source-filtration and collimator settings:

a. 160 kV AlCu, 2 slits, known as "Exp1"
b. 100kV Al, 2 slits known as "Exp2"

5.1.1.3 If data has been acquired for the following optional source-filtration settings, it has also been reconstructed:

c. 160kV Al, 2 slits, known as "Exp3"
d. 300kV Cu or AlCu, 2 slits, known as "Exp4."
e. 160kV AlCu, 1 slit, known as "Exp1 Open"

f. 160kV Al, 1 slit, known as "Exp3 Open."

5.1.1.4 If files with mismatching dates are observed within an experiment set, stop work and notify the Technical Leader.

5.2 Data Analysis

5.2.1 Organize Data Files from Each Energy Spectrum

5.2.1.1 Copy all reconstruction files from each experiment of each test to be analyzed to the machine where they will be analyzed. For each experiment of each test present, both the image files (of the form *recobj_x.sdt*) and the corresponding settings files (of the form *recobj_x.spr*) should be present for every value of ***x***, where ***x*** is an integer value formatted to exclude leading 0's. Both sets of files must be present for proper operation of the Automated MicroCT Analysis GUI (failure to meet this requirement may result in premature termination of the analysis process).

5.2.1.2 Organize the data into a standard directory layout as follows: The Automated MicroCT Analysis GUI (version 1.2.1 or higher) requires that files be structured such that a test folder (the folder containing scan data of one specimen with references at all utilized energy levels and filtration settings) contains one subfolder for each experiment, in the format *Exp**X***… where ***X*** corresponds to the experiment number, identified above in subsection 5.1.1. Once organized, the file structure should appear as follows:

..\Datapath\materialID_batchID_YYMMDD\

—Exp1
—Exp2

5.2.1.3 Currently, multiple separate test reconstructions cannot be analyzed from the same test directory. If multiple reconstructions of the same data or multiple tests of the same specimen have been made, they should occupy different test directories.

For example, acquired data in the following layout should be separated into the canonical form shown in step 2 above:

..\Datapath\materialID_batchID_YYMMDD\

—Exp1
—Exp1_b
—Exp2
—Exp2_b

A proper separation should result in the following:

..\Datapath\material_batch1_YYMMDD \

—Exp1
—Exp2

..\Datapath\material_batch2_YYMMDD \

—Exp1 (originally "Exp1_b")
—Exp2 (originally "Exp2_b")

Notes *The original reconstruction image file indices have a jump in slice number between the specimen slices and the reference slices. This is a result of the physical separation between the two slits in the MicroCT array, where one slit allows illumination of the specimen and the other allows illumination of the references. The Matlab analysis script assumes that reconstruction files for specimen data have a slice number under 100, while reference reconstruction data have a slice number between 200 and 300, matching the output of the reconstruction step in the data analysis process, in order to make passing reconstruction step outputs to the analysis GUI as simple as possible.*

*The data files are numbered with consecutive integers during the reconstruction process such that the first file name is of the form recobj_**x**.sdt and the nth data file name is of the form recobj_**y**.sdt, where **y** = **x** + n − 1. The accompanying .spr files should be numbered identically. Leading zeros are omitted. If the files in the dataset undergoing reduction are not numbered in this convention, stop work and notify the Technical Leader.*

5.2.2 Run Data Analysis

5.2.2.1 Load the MicroCT GUI

If loading from source code:
To load the GUI, set Matlab's path to include the directory where micro_ct_gui_1_2_1.m is located.

a. To add this folder to the path, within Matlab go to **File→Set Path…**
b. Within the Set Path GUI window, click on **Add Folder…**
c. Find the location of the micro CT GUI files (this is left up to the user to store the software in a convenient location), select the folder and click OK.
d. Within the Set Path GUI window, click Close, and save changes if desired.
e. At the prompt, enter "micro_ct_gui_1_2_1," or "micro_ct_gui_1_3," depending on the version in use.[1]

If loading from the executable:
Find the directory in which the executable "MicroCT.exe" sits, and double-click to execute (this is left up to the user to store the software in a convenient location).

5.2.2.2 Assign a destination directory.

For setting the destination directory within the MicroCT GUI window, click on the "Destination Directory" Browse button near the top of the window. This selection should be any directory where you would like the reduced data to be placed.
When placed locally, response time for the software package is faster, and thus data reduction will complete more quickly. For each test folder analyzed, the GUI will generate a new folder

[1] For data taken after July 1, 2011, version 1.3 should be used exclusively to remain consistent with LLNL.

with the same name as the test folder within the destination directory. All reduced data will be saved within this new folder.

5.2.2.3 Assign the directory containing *watertosnake.jar*.

For setting this directory within the MicroCT GUI window, click on the "Java Archive Directory" Browse button near the top of the window. This file path must be present in order for the analysis of input data to proceed as this file defines several active contour (snakes) methods used in the analysis.

5.2.2.4 Using both the test plan directory browse and the single test browse functions, form a list of test folders to process.

In order for the GUI to accept a test directory for processing, Exp1 must be present, as this is used as a normalization reference (the procedure by which normalization is performed is outlined in Appendix A). Exp2 must also be present as the combination of high and low spectrum readings are used to compute effective atomic number. Exp3 and Exp4 are both optional scans, but will be analyzed automatically if present.
There are two ways to add a test folder to the processing list:

a. Setting a directory containing test folders by clicking the upper Browse button causes the GUI to search that folder for any directories that have a qualifying tree structure. The necessary qualification is the presence of Exp1 and Exp2, where both contain *recobj*.sdt* files in addition to corresponding *recobj*.spr* files.

Each valid test name will appear in the left-hand listbox. To add these to the processing list, select each individually within the listbox and click **Add**. Once added, a test name should appear within the right-side listbox.

b. Alternatively, clicking the Browse button between the two listboxes will allow the user to select an individual test folder. This test folder will be checked to ensure it contains at least Exp1 and Exp2, and if so, will be added to the queue.

If a test has been added that the user does not wish to process, that test may be selected in the "Data Reduction List" and removed by clicking **Remove**. Currently, any test can be represented only once in the processing list.

5.2.2.5 Click **Run Data Reduction**. Upon completion, the reduction process will post the message "data reduction for all materials is complete" (the run time averages between 15−20 minutes per test on an Intel Xeon 2.67-GHz PC).

Notes *The data reduction process saves reduced data in a file structure that mirrors the input format: a folder is generated with the same name as the test folder (which generally includes the name of the specimen and date of data acquisition) within the destination directory. Within this results folder, an experiment folder with the name format "Exp#" is generated for each present experiment. A summary .xls file is saved within the results folder, and data from each step in the reduction is saved within the corresponding experiment folders.*

There are two data formats for saved data during the data analysis process: Matlab-compatible .mat files, and ASCII text. The data files saved are:
a. Segmentation images (raw_material.mat)
b. Segmentation voxels (material.txt)
c. Cropped segmentation images (raw2_material.mat; no .txt equivalent)
d. Erosion images (erode_material.mat)
e. Erosion voxels (material_core.txt)
f. KDE values (kde_material.mat; no .txt equivalent)

ASCII text files are formatted with one line per voxel point. The ASCII line includes the x-position, y-position, and z-position voxel-value, in that order. The x, y, and z positions are integer values, while the voxels can be written in integer or floating-point format. All numeric values on each ASCII line are separated by spaces (data is space-delimited). These files are structured to be compatible with Jeffrey S. Kallman's Java analysis codes (see [4]*) and are not critical to the automated Matlab code analysis process.*

Matlab files for saved images contain 3-dimensional arrays representing the collection of slices of images corresponding to the save file type. Each contains two arrays: an array of values and a mask array. The arrays are oriented such that the first dimension represents the slice number.

5.3 Quality Assurance

5.3.1 QA Inspection of Images

5.3.1.1 Click on **Launch Viewer** within the micro_ct_gui window to go over the segmented, eroded, overlayed images, looking for any anomalies.

For each analysis run, the user should examine the resulting segmented images and erosions to determine that no qualitative errors have been made and the data quality is good. Conditions that should be noted include, but are not limited to:

a. Erroneous segmentation or erosion
b. The presence of visible streaks
c. Visible cupping or doming. If doming is observed, perform a lineout across the center of the object being observed, and note the approximate cup/dome-to-line value. If this value exceeds 10% of the mean LAC value of the entire object, notify the Technical Lead.

d. Mislabeling and mishandling of a reference (such as when they are not ordered properly in the carousel – see [10])
e. "Tuning fork" artifacts resulting from bad geometric information during reconstruction
f. Blurred Images

5.3.1.2 To view images from a test folder, within the micro_ct_viewer GUI window, click on Browse and select the test folder. Use the top pull-down menu to select the type of image. There are currently four types of images that micro_ct_viewer will display:

a. A segmented slice image that crops to include the segmented voxels plus 30 voxels in the image plane on all four sides
b. An erosion slice image over the same field of view as the corresponding segmented image (to allow for comparison)
c. An overlay slice image that displays the erosion region relative to the entire segmentation region by dimming discarded voxels by a factor of ½
d. Kernel density estimate plots

5.3.1.3 Use the second pull-down menu to select a material. Each of the references, as well as the test sample, can be selected.

Use the set of four pushbuttons to select the energy level and filtration settings. Only values corresponding to processed experiment values will be available for selection; the remaining pushbuttons will be inactive. Once all three selections are made, the appropriate list of slices will appear in the listbox. Select a slice to view its image.

While viewing a particular image type and material, clicking **Plot this Series** will generate a set of Matlab figures, one for each slice of the series.

View all sets of images and report any irregularities as described above in 5.3.1.1 to the Technical Lead.

5.4 Summarizing Results

5.4.1 Generate Excel Spreadsheet

5.4.1.1 The Matlab GUI generates an excel file with the reduced data displayed in Sheet 1. Open up this file, *test_name_characterization.xls,* and save as .xlsx. This is necessary because the **xlswrite** function in Matlab automatically generates an .xls file, while the .xlsx file format better supports additional used features (such as color-coded cells).

5.4.1.2 Open the chart macros spreadsheet *chart_macros.xlsm* and enable macros. Use the three chart macros (**$^{L}Z_{eff}$ vs μ_{high}**, **Low Range $^{L}Z_{eff}$ Fit**, and **High Range $^{L}Z_{eff}$ Fit**) to generate the appropriate plots. Format these plots as shown in the samples from the macros spreadsheet, replacing “specimen” with the appropriate name and date. The high-range fit R-value can be computed using the **R_high** macro. The low-range fit R-value is 1. The four macros are assigned to key combinations Ctrl-Shift-[Z,L,H,R]: Z for **$^{L}Z_{eff}$ vs μ_{high}**, L for **Low Range $^{L}Z_{eff}$ Fit**, H for **High Range $^{L}Z_{eff}$ Fit**, and R for **High Range Fit R-score**.

5.4.1.3 The kernel density estimates for the test sample at each scan energy are entered into Sheet 2, with each pair of data columns representing the experiments in numerical order (A:B for Exp1, F:G for Exp2, K:L for Exp3, and P:Q for Exp4). To generate a plot of voxel distribution KDEs:

a. After selecting each pair of columns, within Excel click **Insert→Scatter→Scatter with Smooth Lines**.
b. Cut and paste each chart onto the next until they are merged into a single chart, including all KDE curves. To do this, click to select a chart, type Ctrl-X to cut, click the next chart, and type Ctrl-V to paste. Continue this process until you have exactly one single aggregate KDE chart.
c. Right-click the chart and select **Edit Data**.
d. Provide the appropriate labels for each of the KDE curves (match from among "160kV AlCu" (exp1), "100kV Al" (exp2), "160kV Al" (exp3), and "300kV Cu" (exp4)).
e. Add a title and horizontal axis label matching the text style adopted in *chart_macros.xlsm*.
f. Copy the chart to the summary sheet (sheet 1). Generate another copy of the chart on the summary page as a semi-log plot to better emphasize the distribution tails. To convert to semi-log, right-click the vertical axis and select **Format Axis**. Select the **Logarithmic Scale** checkbox, set the minimum value to 1e-6, maximum value to 0.01, and "Horizontal axis crosses" value to 1e-6.

5.4.1.4 Change the name of the material in the "$^{L}Z_{eff}$ vs μ_{high}" plot on the summary page. The "Low Range $^{L}Z_{eff}$ Fit" and "High Range $^{L}Z_{eff}$ Fit" charts do not require the addition of the material name in the title.

Format the characterization spreadsheet using the "Summary" sheet of *chart_macros.xlsm* as a rough guideline.

5.4.1.5 Insert the appropriate images generated during the erosion process. From the microCT GUI window, click on **Launch Viewer**. From the viewer, select the test directory for which you are generating the current spreadsheet, and click **Generate Characterization Plots**. From each Matlab figure window, select **Edit→Copy Figure**, then paste the figure into the summary spreadsheet in the appropriate location.

5.4.1.6 Highlight certain data within the summary page according to the pattern observed in *chart_macros.xlsm*. Highlight the sample statistics and computed Z_{eff} on the summary page using green (from the Home tab within Excel). Highlight the water linear attenuation coefficient (LAC) at high energy with red.

5.4.2 Archive the Results on the Server

5.4.2.1 Create a subdirectory in a suitable location (for recent LLNL data acquisition, in the Analyses directory for the specimen; for TAFRL and TSL data acquisition, at the same level as the experiment subdirectories) with the name

a#a#_miscID_acqdate_analysis_**INIT_date**

where **a#a#** is the specimen name, **acqdate** is the date of data acquisition in the form yymmdd, **miscID** is any other identifying information that might be available (such as batch

number, set number if there were multiple data sets taken in a day, etc.), **INIT** are the initials of the person who analyzed the data, and **date** is the date the analysis took place.

5.4.2.2 Copy everything generated during the analysis (including the directory structure and Excel spreadsheets) into this subdirectory. Refer to the IDD Records Management QIP [11] for responsibilities in the handling of generated data.

5.5 Post-Procedure Checks and Notifications

5.5.1.1 Notify the IDD Records Librarian that the data are available for archival. Copy the IDD Technical Leads, PI, and Deputy Project Leader on the notification.

5.5.1.2 Contact the team member responsible for writing of reports once analyzed data are available on the server.

6.0 Records

Analysis results generated from this SOP shall be managed per the IDD Document Management QIP [12] and the IDD Project Data Management Plan [13].

7.0 Review Interval

This SOP shall be called for periodic review at an interval not to exceed 1 year from its previous issue.

8.0 Document Revision History

Date	Revision	Author	Responsible Manager	Comments
12/15/2010	0	Isaac Seetho	Harry Martz	
1/13/2011	0	Isaac Seetho	Harry Martz	Edit addressing various comments.
2/14/2011	0	Isaac Seetho	Harry Martz	Update for v 1.2.1 of GUI
3/20/2011	0	Isaac Seetho	Harry Martz	Edit addressing comments
4/5/2011	0	Isaac Seetho	Harry Martz	Added additional key terms
9/26/2011	0	Isaac Seetho	Harry Martz	Edit addressing comments.
10/04/2011	0	Isaac Seetho	Harry Martz	Edit addressing comments

9.0 References

1. *MicroCT: Acquisition of CT Data of Home Made Explosive Matierials*, IDD Standard Operating Procedure, IDD-MCT-SOP-003, latest revision.
2. *MicroCT: Reconstructing X-ray Computerized Tomographic Images from Data Acquired on LLNL MicroCT Systems*, IDD Standard Operating Procedure, IDD-MCT-SOP-004, latest revision.
3. Lawrence Livermore National Laboratory, *IDD Quality Assurance Plan for MicroCT Scanning*, IDD-MCT-QAP, latest revision, LLNL-AM-463479.
4. *MicroCT: Analysis of CT Reconstructed Data of Home Made Explosive Materials*, IDD Standard Operating Procedure, IDD-MCT-SOP-002, latest revision.
5. *MicroCT: Semi-Automated Analysis of CT Reconstructed Data of Home Made Explosive Materials Using the Matlab MicroCT Analysis GUI*, IDD Standard Operating Procedure, IDD-MCT-SOP-008, latest revision.

6. J. Kallman, I. Seetho, "A Description of MicroCT Data Analysis Techniques," LLNL-TR-XXXXX, Rev 0, January 26, 2011 (in development).
7. Doug P. Perrin and Christopher E. Smith, "Rethinking Classical Internal Forces for Active Contour Models," in *2001 IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, pp. II-615–II-620, 2001.
8. *K. Harris et. al.,* "Hybrid Image Segmentation Using Watersheds and Fast Region Merging," *IEEE Trans. Image Processing*, Vol. 7, No. 12, pp. 1684–99, December 1998.
9. Jeffrey S. Kallman, Daniel J. Schneberk, Harry E. Martz, Jr., *Two-energy Ratio Method to Determine Zeff from Reference Materials: A Comparison of an Explosive and a Simulant*, Version 3, Lawrence Livermore National Laboratory, LLNL-TR-491153, June 24, 2011.
10. Jerel A. Smith, Daniel J. Schneberk, Jeffrey S. Kallman, Harry E. Martz, Jr., David Hoey, *Documentation of the LLNL and Tyndall Micro-Computed-Tomography Systems*, Version 091216, Lawrence Livermore National Laboratory, LLNL-TR-421377, December 17, 2009.
11. *Records Management*, IDD Quality Implementing Procedure, IDD-QIP-002, latest revision.
12. *Document Management*, IDD Quality Implementing Procedure, IDD-QIP-001, latest revision.
13. *IDD Data Management Plan*, IDD-DAMA-Plan, latest revision.

Appendix A: Automated MicroCT Analysis GUI File Structure

In **source code** form, the Automated MicroCT Analysis GUI contains three types of Matlab files:

- **GUIDE Figure Files** (*micro_ct_gui_dlg.fig, kde_comp_dlg,fig, micro_ct_viewer_dlg.fig*)

  These files are generated automatically by the GUIDE GUI development toolbox within Matlab. These files specify graphical user interface layout and assign labels and types to all GUI elements. One file is required for each corresponding GUI window.

- **Dialog Box Control Files** (*micro_ct_gui_dlg.m, kde_comp_dlg.m, micro_ct_viewer_dlg.m*)

  These files are used to specify GUI functionality by supplying code connecting each GUI element with the corresponding callback functions.

- **Function Definition Files** (*micro_ct_gui_1_2_1.m or micro_ct_gui_1_3.m, kde_comp.m, micro_ct_viewer.m*)

  These files contain functional definitions for all Matlab callback functions, and define the state variables stored by the corresponding GUIs.

In **executable** form, the Automated MicroCT Analysis GUI contains the following file:

- ***MicroCT.exe***

  This is the main executable, which will run the Automated MicroCT Analysis GUI.

In addition, **both** versions of the analysis software contain the following files:

- ***watertosnake.jar***

  This file is a Java archive containing compiled code for each of the Java classes used by the Automated MicroCT Analysis GUI.

- ***chart_macros.xls***

  This is an Excel file containing macros used in the generation of the results Excel spreadsheet for each test material analyzed by the Automated MicroCT Analysis GUI.

Appendix B: GUI Operation and Capabilities

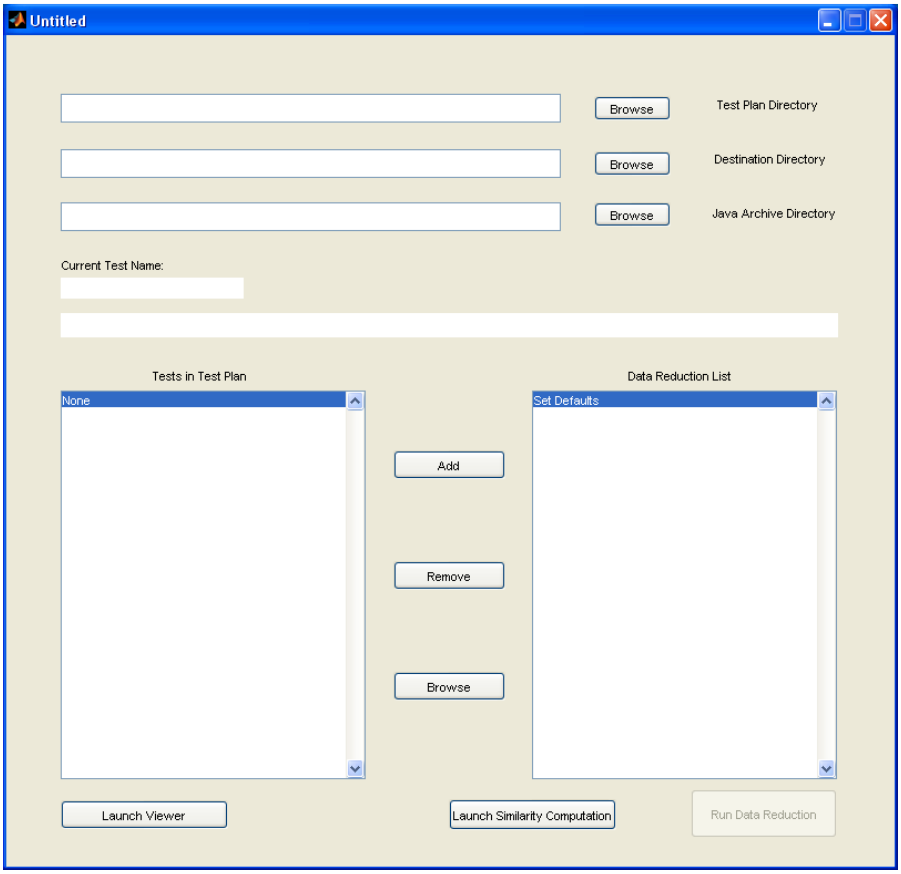

Figure 1. Initial graphical user interface of the Automated MicroCT Analysis program.

Main Automated MicroCT Analysis GUI Window

The main window of the Automated MicroCT Analysis GUI contains the following fields and functions:

- **Browse Test Plan Directory.** Clicking on this Browse button will bring up a browse window allowing the user to set a directory to scan for viable test folders. Any viable test folders found in this directory will be listed in the Test Plan Listbox in the lower left of the GUI window. Candidate test folders are checked against the layout requirements identified in subsection 5.2.1 of this SOP. Alternatively, the user can edit the text in the accompanying edit box manually. Any manually entered directory will be checked for existence. If the directory does not exist, the edit box will revert to its last valid value (includes the empty string).
- **Browse Destination Directory.** Clicking on this Browse button will bring up a browse window allowing the user to set the destination directory for saved data. The program generates a new subdirectory within the destination directory for each test reduced, and saves files in the format identified in subsection 5.2.2 of this SOP. Alternatively, the user can edit the text in the accompanying edit box manually. Any manually entered directory will be checked for existence. If the directory does not exist, the edit box will revert to its last valid value (includes the empty string).

- **Browse Java Archive Directory.** Clicking on this Browse button will bring up a browse window allowing the user to specify the Java archive directory where *watertosnake.jar* is located. This file is required for the data reduction process, so this directory must be set in order for data reduction to be run. Alternatively, the user can edit the text in the accompanying edit box manually. Any manually entered directory will be checked for *watertosnake.jar*. If the file is not found, the edit box will revert to its last valid value (includes the empty string).
- **Current Test and Operation Listing.** This text box cannot be edited, and will display the current step of the data reduction process as it proceeds.
- **Test Plan Listbox.** If the user specifies a Test Plan Directory, any valid test folders found in the directory will be displayed in this listbox.
- **Data Reduction Listbox.** If the user has added tests to be run through the data reduction process, they will be displayed in this listbox.
- **Add From Test Plan Listbox.** Clicking on a test in the Test Plan Listbox and then clicking the **Add** button will add the selected test to the Data Reduction Listbox.
- **Remove From Data Reduction Listbox.** Clicking on a test in the Data Reduction Listbox, and then clicking the **Remove** button will remove the selected test from the Data Reduction Listbox.
- **Browse for Test Data Folder.** Clicking on this Browse button will bring up a browse window allowing you to specify a test folder to add to the Data Reduction Listbox. Any folder selected will be checked for a directory structure matching that specified in subsection 5.2.1 of this SOP.
- **Launch Viewer.** Clicking on this button launches a separate Viewer GUI window.
- **Launch Similarity Computation GUI.** Clicking on this button launches a separate Similarity GUI window.
- **Run Data Reduction on Data Reduction List.** Clicking this button starts the data reduction process on the members of the Data Reduction Listbox. Note that the user must have specified a destination directory, found the location of *watertosnake.jar*; and specified a nonempty data reduction list in order for the **Run Data Reduction** button to become active.

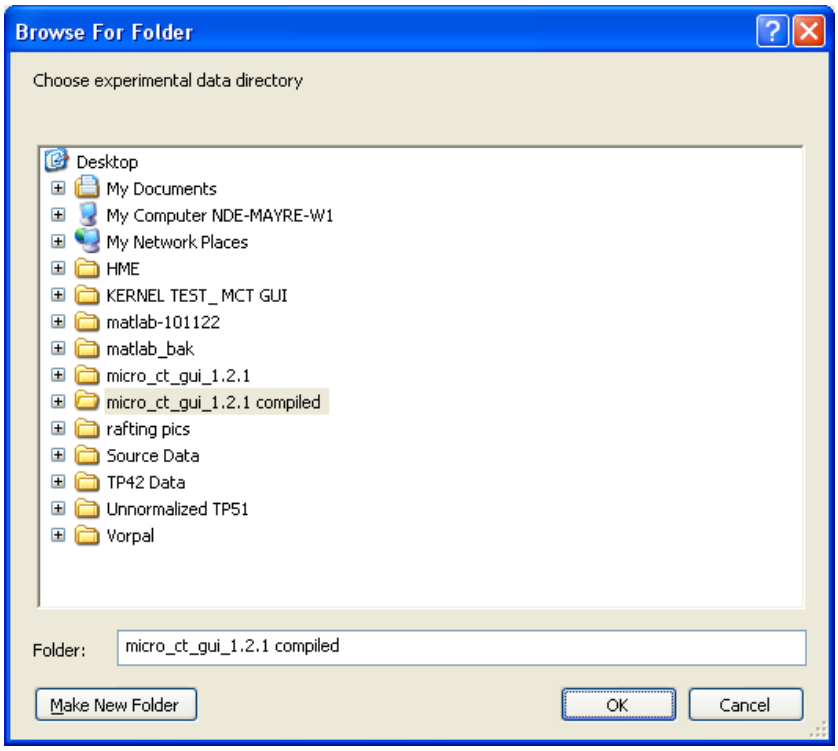

Figure 2. The dialog box that appears whenever a Browse button is selected.

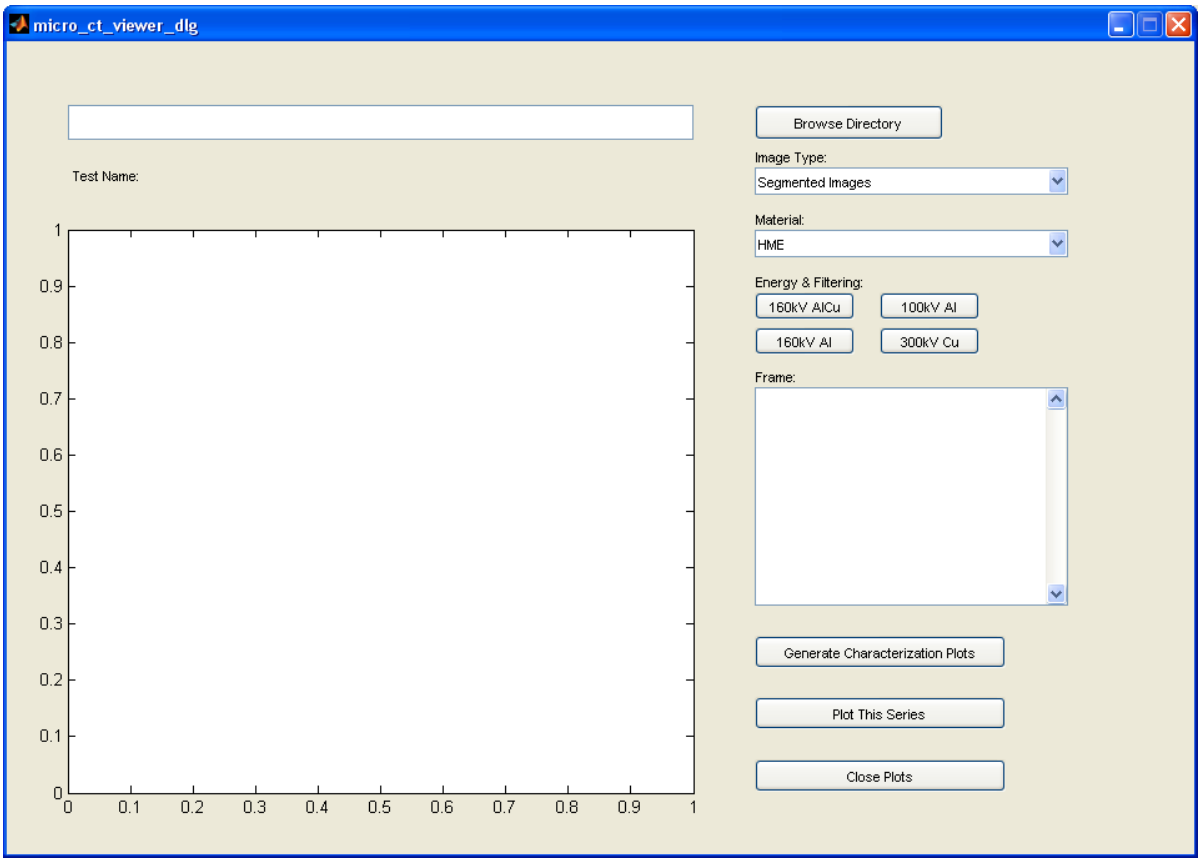

Figure 3. The Automated MicroCT Analysis Program Viewer GUI.

Automated MicroCT Analysis GUI Viewer Window

The viewer window of the Automated MicroCT Analysis GUI contains the following fields and controls:

- **Browse for Test Results Directory.** Clicking on this Browse Directory button will bring up a browse window allowing the user to specify the test results directory from which to display slice images. Alternatively, the user can edit the text in the accompanying edit box manually. Any entered directory will be checked for existence, as well as existence of data reduction results files generated by the GUI. These files should be structured within the directory according to the format specified in subsection 5.2.2 of this SOP. If no such files are found, the edit box will revert to its last valid value (includes the empty string).
- **Select Image Type.** Clicking on this pulldown menu when a valid results directory is specified allows the user to select from several different types of images to view:
    - Segmentation Images—Displays, for each slice, the voxels resulting from the segmentation process.
    - Erosion Images—Displays, for each slice, the voxels resulting from the erosion process.
    - Kernel Density Estimates—Displays, for each material and spectrum combination, a Kernel Density Estimate (KDE) of the erosion voxels for that material at that energy value. The process by which this KDE is obtained is described in Appendix C of this SOP.

  - Overlay Images—Displays, for each slice, the voxels from the erosion image scaled by a factor of 1, and the remaining voxels of the segmentation image scaled by a factor of 0.5. The boundary of the erosion voxels is marked by a white line. In images containing a container, a white circle marks the estimated container boundary.

For each of these images, the color map is gray and set such that the maximum voxel value corresponds to white while the minimum voxel value corresponds to black.

- **Select Material.** Clicking on this pulldown menu when a valid results directory is specified allows the user to select the material for which images should be displayed. “Aluminum, Delrin, Ethanol, Graphite, Teflon and Water” identify the corresponding reference materials. “Specimen” refers specifically to the main test sample (in some cases this may be the same material as one of the references).
- **Select Spectrum.** Only one of these buttons is active at any given time, and the toggle button selected (it should appear to be depressed in the GUI window) determines the spectrum value for which images will be displayed. The labels correspond to spectrum and filtering combinations specified in subsection 5.1 of this SOP.
- **Select Slice.** When an image type (excluding KDE), material, and spectrum value are selected, the listbox on the right side of the GUI will be populated with the slices corresponding to the selections. Clicking on one of these frames to select it within the listbox will plot the frame in the space on the left side of the GUI.
- **Generate Characterization Plots.** Selecting this option will generate all plots used in the writing of MicroCT reports. These include segmentation area plots, erosion area plots, overlay area plots, and plots of the differential of the erosion area (taken by the absolute value of subtracting each erosion voxel from the voxel to the right), for the specimen only, at all available spectra.
- **Plot Current Series.** Selecting this option will generate an individual Matlab figure window for each image slice listed in the listbox on the right side of the GUI, and plot each slice in the corresponding figure window.
- **Close Plots.** Selecting this option will close all open figure windows associated with the Automated MicroCT Analysis GUI.

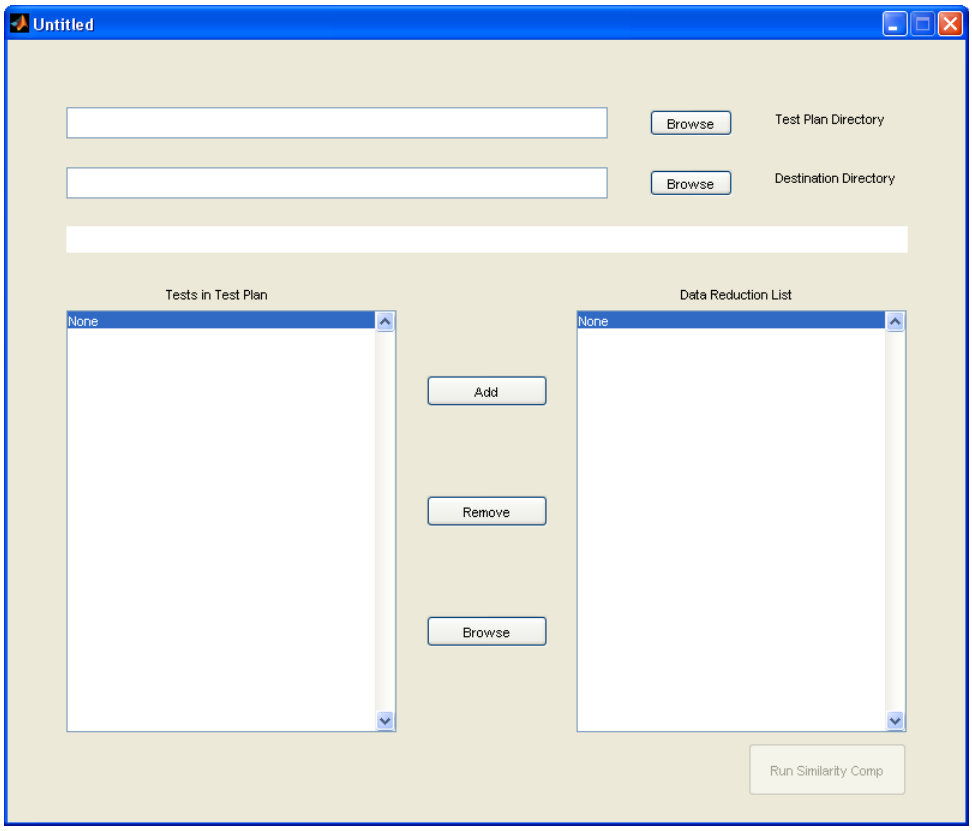

Figure 4. Similarity computation GUI window.

Similarity Computation GUI Window

The similarity computation window of the Automated MicroCT Analysis GUI contains the following fields and controls:

- **Browse Test Plan Directory (Data Reduction Results).** Clicking on this Browse button will bring up a browse window allowing the user to set a directory to scan for viable test folders. Any viable test folders found in this directory will be listed in the Test Plan Listbox in the lower left of the GUI window. Candidate test folders are checked against the layout requirements identified in subsection 5.2.2 of this document. Alternatively, the user can edit the text in the accompanying edit box manually. Any manually entered directory will be checked for existence. If the directory does not exist, the edit box will revert to its last valid value (includes the empty string).
- **Browse Destination Directory (KDE Results).** Clicking on this Browse button will bring up a browse window allowing the user to set the destination directory for save data. The program saves files in the .mat (Matlab) and .xls (Microsoft Excel) formats. Alternatively, the user can edit the text in the accompanying edit box manually. Any manually entered directory will be checked for existence. If the directory does not exist, the edit box will revert to its last valid value (includes the empty string).
- **Test Plan Listbox.** If the user specifies a Test Plan Directory, any valid test folders found in the directory will be displayed in this listbox.

- **Similarity Comparison Listbox.** If the user has added tests to be run through the data reduction process, they will be displayed in this listbox.
- **Add From Test Plan Listbox.** Clicking on a test in the Test Plan Listbox and then clicking the **Add** button will add the selected test to the Similarity Comparison Listbox.
- **Remove From Similarity Comparison Listbox.** Clicking on a test in the Similarity Comparison Listbox and then clicking the **Remove** button will remove the selected test from the Similarity Comparison Listbox.
- **Browse for Test Data Folder.** Clicking on this Browse button will bring up a browse window allowing you to specify a test folder to add to the Similarity Comparison Listbox. Any folder selected will be checked for a directory structure matching that specified in subsection 5.2.1 of this document.
- **Run Similarity Comparison.** Clicking on this button will start the similarity comparison process. The similarity comparison process will generate an Excel file in the destination directory containing similarity tables, with one sheet for each spectrum present. Similarity values are computed using the KDE distributions from each material at each spectrum. Similarity comparison requires:

    - The same material is being compared against itself
    - The two materials are scanned using the same spectrum
    - The two KDEs are obtained using data normalized to the same reference at the same spectrum

    Similarity is computed by summing the minima of two KDEs over the same domain set, multiplied by the granularity of the domain set. The domain set occupies the x-axis while the corresponding KDE values occupy the y-axis.

Appendix C: MicroCT Data Reduction Algorithm Overview

The Micro CT Matlab GUI breaks data analysis down into four main steps, as identified below. For greater mathematical detail, consult [6].

1. Segmentation

For each energy spectrum, the Matlab software generates a list of *recobj*.sdt* reconstruction files and partitions these files into two categories, specimen and reference, according to their file number (under 200 for specimen; between 200 and 300 for references). Within each subset, all files are loaded into a Matlab data array.

For each specimen subset, the Matlab software segments frame-by-frame, using one of two methods:

First, a watershed and graph aggregation process is applied to the leading frame until the image is classified into an “image” area and a “background” area. The boundary of this image area is used to generate points for an active contour, which is run through one cycle of updates as specified in [6]. A general discussion of watershed methods is found in [8]. Active contour methods are discussed in [7].

Second, a threshold mask is obtained using a threshold attenuation value of 0.01 (mm^{-1}) and applying it to a blurred version of the leading frame.

If the active contour mask does not match the threshold mask to within 4% by voxel count, the threshold mask is used and the active contour mask is discarded. Otherwise, the active contour mask is used.

Once the starting mask has been obtained, the outer perimeter of the mask is used to generate an active contour, which is allowed one cycle of updates per successive frame of the volume. After the active contour is allowed to update for each frame, the resulting segmentation area per frame is saved to a Matlab array identifying the segmentation region.

Reference materials are exclusively segmented using a watershed and graph aggregation process on the leading frame, using each of the six segmentation area boundaries corresponding to each reference to generate an active contour, and applying the active contours successively to each frame. References are subsequently identified within the reference mask by numbering each distinct mask region, computing the angular position of the center point of each region with respect to the center of the image frame, and using the largest angular gap between successive centroid values to identify material label ordering according to carousel specifications. In the coordinate system used, the angular values are in radians relative to the positive x-axis (directly to the right of the origin). At “high energy” (Exp1 as defined in section 5.1), expected attenuation values for the materials are ordered from highest to lowest as: aluminum, Teflon, graphite, Delrin, water, and ethanol. At “low energy” (Exp2 as defined in section 5.1), attenuation values are ordered as: aluminum, Teflon, Delrin, graphite, water, and ethanol. Note that the relative ordering of the Delrin and graphite reference materials changes with the source energy used. This ordering can be used to check that the segmentation region labels are correct.

The voxels resulting from the segmentation process are written to two separate files. The first is a Matlab data file of the form *raw_material.mat*, containing one three-dimensional matrix representing the mask and a second representing the segmented voxels. The second is *material.txt*, an ASCII format with one line per voxel, including x-position, y-position, z-position, and voxel value, in that order. Position values

are integer-valued, while voxel values may be integer- or floating-point-valued (non-normalized). This ASCII text file is space delimited, and is fully compatible with Jeff Kallman's **Eroder** and **SimTest** Java-based analysis software (see [4]).

2. Erosion

The erosion process first loads in the results of the segmentation from the appropriate .mat files and then performs a pre-erosion for all regions, removing two voxels in the segmentation region from the high-row-index side of each column in each frame. This pre-erosion is used to correct for an active contour function artifact, which leaves extra rows of data in the segmentation region. Additionally, the first frame and last two frames of each volume are discarded.[1] This discard is a carryover from analyses on initial datasets where these slices tended to contain artifacts and increased scatter due to proximity to the MicroCT system collimator.

After any necessary pre-erosion, the resulting mask then undergoes a morphological erosion with a square element of 3 × 3 voxels. The specimen undergoes 15 successive erosions. (Water and ethanol references undergo 13 successive erosions. Solid references undergo 4 successive erosions.) After erosion, each internal area is used for statistical computation.

Upon erosion, all eroded data from a single test folder is normalized by scaling with a scalar factor obtained from setting the mean value of eroded voxels from the reference material in Exp1 to its specified standard value. The current standard is to set eroded water in Exp1 to an average value of 1000.

The voxels resulting from the erosion process are written to two separate files. The first is a Matlab data file of the form *erode_material.mat*, containing one three-dimensional matrix representing the mask and a second representing the eroded voxels. The second file is *material_core.txt*, in ASCII format with one line per voxel, including x-position, y-position, z-position, and voxel value, in that order. Position values are integer-valued, while voxel values may be integer- or floating-point-valued. This ASCII text file is space delimited, and is fully compatible with Jeff Kallman's **SimTest** analysis software.

3. Kernel Density Estimation (KDE)

The microCT GUI uses the following KDE computation formulae:

$$KDE(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right), \text{ where}$$

$$K\left(\frac{x - x_i}{h}\right) = \frac{1}{\sqrt{2\pi}}\exp\left(\frac{(x - x_i)^2}{2h^2}\right), h = 0.9An^{-0.2}, A = \min\left(\sigma_x, IQR(x)\right)$$

In this computation, x represents attenuation values at which the KDE is computed, x_i represents individual voxel values, n represents the voxel count, σ_x is the variance of the voxel values, and IQR is the inter-quartile range of the voxel values, defined as the difference between the values of the first and third

[1] Beginning with data taken after July 1, 2011, the 1.3 version update should be used. This update of the GUI discards the first two frames and last two frames.

quartile. A quartile is one of three points dividing a data set into four equal groups. The first quartile cuts off the lowest 25% of data, while the third quartile cuts off the highest 25% of data. The second quartile is the median. The process by which the IQR is obtained is as follows:

1. Compute the median by sorting the elements of the set in numerical order and finding the central element. If no exact central element is found (if the set has even parity), take the average of the center-most two elements. Using this median value, divide the dataset into two equal halves, one set of values appearing before the median point in the ordered set, and one set of values appearing after the median point in the ordered set.
2. If the number of elements in the total set is even, compute the median for each half, where Q1 is the median of the lower half and Q3 is the median of the upper half. Then, IQR = Q3 − Q1.
3. If the number of elements in the set is odd, perform step 2 including the middle element of the whole set in each subset to obtain Q11 and Q31. Perform step 2 excluding the median element from each set to obtain Q12 and Q32. Then, IQR = ½(Q31 − Q11) + ½(Q32 − Q12).

For simplicity of running similarity comparisons across tests on saved data (such that KDEs do not need to be recomputed on a per-order basis), currently the GUI is set to compute KDE values indexed at the even integers of attenuation values on the LMHU scale.

The KDEs resulting from this computation are saved in the corresponding test directories at the destination directory location in files of the form *kde_material.mat*, containing the indexing attenuation values as well as the corresponding KDE values in Matlab array format.

4. Statistical Analysis

In generating the characterization Excel file, the GUI computes mean, differential entropy, and variance for 1st- and 2nd-order eroded data from the specimen and references. The GUI also uses the ratios of low/high energy mean LACs (treated as domain) and known effective atomic mass ($^{L}Z_{eff}$) values (treated as range) to generate quadratic regression curves for low- and high-range $^{L}Z_{eff}$ estimation.

Differential entropy is approximated from the KDE with the following formula:

$$E = -\sum p \log(p), \text{ where } p(x) = KDE(x) * \Delta x$$

For estimating Z_{eff}, two quadratic regression curves are computed, as follows:

1. Ethanol, Delrin and graphite have their LAC ratios and literature $^{L}Z_{eff}$ values combined into respective ordered pairs of the form (LAC ratio, $^{L}Z_{eff}$). These ordered pairs are used to generate a quadratic fit, as instructed by [9]. This is called the Low Range $^{L}Z_{eff}$ Fit curve, denoted as $\mathbf{f_L(x)}$.
2. Delrin, aluminum, teflon and water have their LAC ratios and literature $^{L}Z_{eff}$ values combined into respective ordered pairs of the form (LAC ratio, $^{L}Z_{eff}$). These ordered pairs are used to generate a second quadratic fit, as instructed by [9]. This is called the High Range $^{L}Z_{eff}$ Fit curve, denoted as $\mathbf{f_H(x)}$.

From these curves, an estimate for $^{L}Z_{eff}$ can be obtained by evaluating the appropriate $^{L}Z_{eff}$ value corresponding to the LAC ratio ($LACR_{spec}$) of the specimen, using the relationship between the specimen

LAC ratio and Delrin's LAC ratio as a decision point between the two quadratic fits. Taking the specimen LAC ratio, if it is less than Delrin's LAC ratio, find the value of the low-range quadratic fit function:

$Z_{eff} = f_L(LACR_{spec})$. Otherwise, $Z_{eff} = f_H(LACR_{spec})$

The statistical data are saved within the destination test directory, in a file of the form *test_name_characterization.xls*. They are also stored in struct format in the test directory, in a file named *analysis.mat*.

Appendix D: Validation Testing

When first installed, the user should verify that the Automated MicroCT Analysis GUI is functioning properly. Included in the program package should be a .zip archive file, *validation_datasheets.zip*, which includes analysis output files from all test cases. **If any of the test cases' output from the Automated MicroCT Analysis GUI do not match, do not use this program; consult the point of contact at LLNL.**

Table 1 identifies all test cases, as well as the correct slice ranges to use for each case. In each test case, run the Automated MicroCT Analysis GUI only on test folders containing the appropriate *recobj* files. These files have been filtered to exclude frames with defects or artifacts in accordance with the requirements presented in sections 5.2 and 5.3 of this SOP.

Table 1. List of slices to use in each test for validation of software.

Test Case	Exp1 Slices	Exp2 Slices	Exp3 Slices	Exp4 Slices
101026M1_Z5d	Specimen: 32-42 Ref: 228-238	Specimen: 32-42 Ref: 228-238	—	—
101026M2_Z3a	Specimen: 8-19 Ref: 208-219	Specimen: 8-21 Ref: 208-220	—	—
101105M1_Z5c	Specimen: 32-42 Ref: 228-238	Specimen: 32-42 Ref: 228-238	—	—
101109M1_Z4d	Specimen: 32-42 Ref: 228-238	Specimen: 32-42 Ref: 228-238	—	—
101123M2_Z1d	Specimen: 6-21 Ref: 207-221	Specimen: 6-21 Ref: 207-221	—	—
091105M1_Z1d	Specimen: 15-29 Ref: 217-231	Specimen: 11-26 Ref: 214-229	—	—
100322M1_Z5d	Specimen: 23-33 Ref: 219-229	Specimen: 23-33 Ref: 219-229	—	—
100330M1_Z4d	Specimen: 23-33 Ref: 219-229	Specimen: 23-33 Ref: 219-229	—	—
100810M1_Z5c	Specimen: 33-43 Ref: 229-239	Specimen: 33-43 Ref: 229-239	—	—
091117_Priority13_Z4C2	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233
091022_Priority13_Z1D1	Specimen: 53-63 Ref: 249-259	Specimen: 53-63 Ref: 249-259	Specimen: 53-63 Ref: 249-259	Specimen: 53-63 Ref: 249-259
091107_Priority13_Z5C2	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233	Specimen: 28-38 Ref: 223-233