LIBSSIM: SIMULATION OF LIBS SAMPLING ON ROCK SURFACES. P. A. Dobosh[1], E. A. Breves[2], M. D. Dyar[2], and M. McCanta[3].[1]Computer Science Dept., Mount Holyoke College, 50 College St., South Hadley, MA 01075, pdobosh@mtholyoke.edu.[2]Dept. of Astronomy, Mount Holyoke College, 50 College St., South Hadley, MA 01075, [3]Dept. of Geology, Tufts University, Lane Hall, Medford, MA 02155.

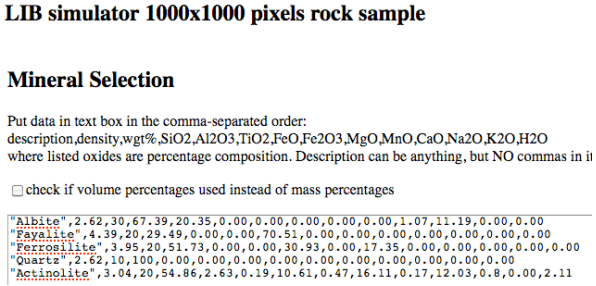
Introduction: ChemCam, a remote sensing instrument package including a Laser-Induced Breakdown Spectrometer (LIBS) and remote micro-imager (RMI), will provide geochemical analyses and context imaging as part of the Mars Science Laboratory (MSL) *Curiosity* rover payload. ChemCam has the innovative reconnaissance capability of obtaining near-complete chemical analyses on spot sizes ranging from ~175 μm to 500 μm at standoff distances of 1.5 m and 7 m. The laser can depth profile up to ~1 mm into a rock, and can be focused to extremely small spot sizes of less than 0.5 mm at 7 m stand-off distances. Single-spot analyses of locations on rocks and minerals will provide the first-ever *in situ* analyses of individual grains on the surface of Mars. However, valuable geological insights (for example, rock type) can also be obtained by considering multiple analyses of the same rock. The ChemCam science team is designing strategies for analysis of features at different scales [1] that must be informed by a better understanding of the effects of rock type, crystal size, and mineralogy. In the context of those three variables, this raises the question of how many different analysis spots are needed to represent the bulk composition of a rock or soil target. The question has also been addressed experimentally [2].

Therefore, the goal of this study was to build a model to simulate LIBS sampling from a rock or soil on Mars. Variables that are modeled here include the size of mineral grains in the rock relative to the size of the laser beam, the modes (volume percentages) of each phase, and their individual compositions.

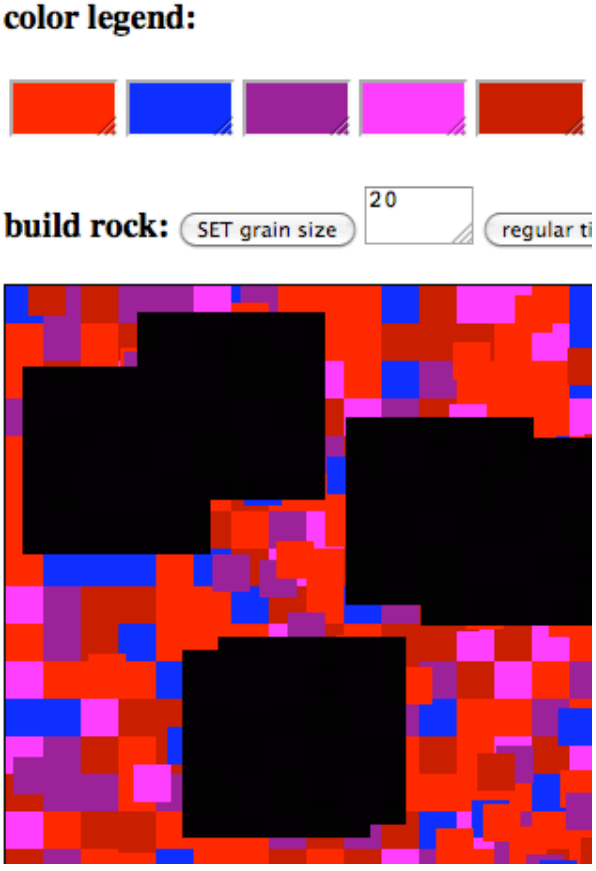
The model: The model is built around a 2-D 1000 × 1000 pixel image displayed on the web page. Two versions of the program are available. The teaching version builds rock slabs from a choice of minerals to which one can assign volume percentages. The research version is meant to allow direct input of the composition of a known rock sample, i.e., mass percentages of minerals with their oxide compositions.

Using the model: Both models require a sequence of steps, though the research version is more streamlined:

Choose the minerals: In the teaching version of the model the student can choose one mineral from each of eight classes. The desired volume percent of each choice is entered (as a whole number). The desired percentages are used to build a 100-element vector with the minerals proportionally represented and this vector is used in randomly selecting grains for the rock sample. In the research version, these data can be input by pasting in comma-separated values as shown below.



Build the rock slab: The user next chooses the grain size for the minerals, expressed in pixels ($n \times n$). A regular tiling is first done with randomly-chosen mineral grains laid out in a grid to cover the entire slab.

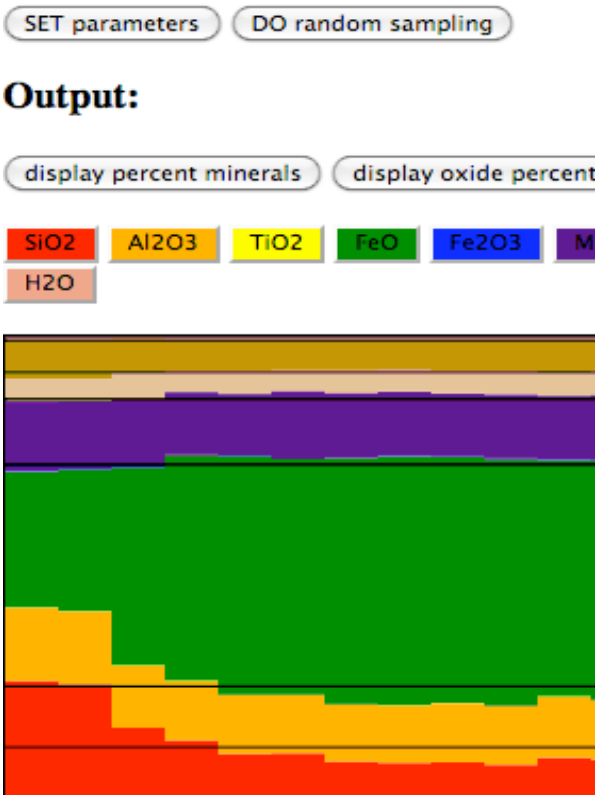


Additional random placements of 500 grains at a time can be added. The program then measures the actual

bulk composition by counting pixels. The color of each pixel is examined, with the green value coding the number of the mineral (0 through 7). The measured bulk composition is reported in text boxes above the slab image.

Set the sampling parameters: The user sets the beam size ($n \times n$ pixels), the number of sampling shots (50 max) and a further term that is a measure of how many layers the beam penetrates.

Take samples: The LIBS sampling is shown by black squares on the slab (see above). The square is not strictly black; it has the color rgb (0,*G*,0) where the green(*G*) is 0-7 indicating which mineral is at that pixel. Subsequent samples in the same area will still detect the mineral.



Display output: Two displays can be viewed by the user. One shows the measured mineral percentages accumulated across samples and the other the bulk oxide percentages as a function of the number of points sampled, which increases from left to right. The mineral results are displayed as percent volume composition while the oxides are mass percentages. A portion of the oxide display is shown here. The black horizontal lines indicate the "true" bulk composition of the rock as input by the user, and the magnitude of each color shows the amount of that element (as oxide) that would be calculated with increasing numbers of analyses (increasing from left to right).

Gather text output: To allow further measurement and computation, the results of the sampling are printed below the graphical output as a large volume of comma-separated text. This includes pixel counts for each mineral and each sample, cumulative mineral percentages and standard deviation for each mineral, actual oxide percentages and cumulative measured oxide percentage means and standard deviations. This output can be pasted into a text file for use in a spreadsheet or as input to other programs.

Results: The program outputs results that are qualitatively what was expected. For example, a representative bulk analysis of a rock with only a single mineral phase (e.g., sandstone) can be obtained with a single spot analysis. Rocks where the compositions of coexisting phases are similar (e.g., pyroxene, olivine, and basaltic glass) require fewer analyses that those with disparate phases (e.g. feldspar and pyroxene) regardless of grain size. Larger grain sizes require higher numbers of analyses to obtain representative bulk compositions. Predictions from this program tested using experimental rock data in [3], provide quantitative estimates of the number and distribution of analyses needed for analyses of real geological samples. A LIBSSIM version that mimics the ChemCam targeting pattern [1] is in development.

Javascript and Canvas: We have taken advantage of the increased capability of Javascript to perform computation [3] directly in the web page, i.e., without any server-side interaction. Each step happens as quickly as a press of the mouse button.

In addition to the speedup of Javascript, a graphical element, canvas [3], has been added to HTML5. The LIBSSIM web page contains a 1000 × 1000 pixel canvas object with each pixel color coded for the mineral at that pixel. The entire million pixels of the image can be rapidly scanned to determine the actual composition of the simulated rock and similarly each laser sample can be scanned.

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References: [1] Newsom, H. E., this conference. [2] Anderson, R. B., http://www.lpi.usra.edu/meetings/lpsc2011/pdf/1308.pdf [3] McCanta, M., this conference.
[4] https://wiki.mozilla.org/JavaScript:TraceMonkey
[5] http://www.w3.org/TR/html5/the-canvas-element.html.

Additional Information: The program can be found at: http://www.mtholyoke.edu/~pdobosh/libssim/lasersimR5.html