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Lunar Regolith Figures of Merit

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Agenda

- A quick review of Figures-of-Merit (FoM)
  - Composition
  - Size distribution
  - Shape
  - Density
- Software Implementation of FoM Algorithms
  - Components of the software
  - Inputs to the software
- Demonstration of the software

A Quick Review of Figures-of-Merit

Characterization of Lunar Regolith Simulant Materials

- A method is needed to specify simulant requirements and simulant suitability for a given purpose and to compare simulants to Lunar Regolith and other simulants.
- D. Rickman has postulated that a simulant may be characterized by the following four characteristics:
  - material composition
  - particle size distribution
  - particle shape
  - material density.
- This leads to the search for methods of specifying and comparing materials in terms of these four characteristics.

Figures of Merit (FoM)

- A FoM is conceptually an algorithm which computes a single number for quantifying the similarity or difference of a single characteristic of two materials and provides a clear measure of how well the materials match or compare.
- The two materials being compared are given the labels:
  - Reference Material
  - Simulant Material
- This labeling is arbitrary and does not factor into the FoM computation.
- Nominally one would consider the reference material to be an actual material one is trying to replicate or simulate. A reference material may however be completely hypothetical.
- A simulant is usually considered to be a material that replicates as much as possible (or to the degree specified) a reference material.
- However both materials may be simulants, which would allow for comparison of two simulants, or both may be actual lunar (or other material) samples, which would allow for comparison of these materials.
- FoMs may be used for:
  - comparing a simulant to actual regolith material.
  - comparing simulants from different vendors or production runs.
  - comparing different simulants to each other.
  - specification by stating the value a simulant's FoMs must attain to be suitable for a given application.
- FoMs have been constructed to lie between 0 and 1, with 0 indicating a poor or no match and 1 indicating a perfect match.

FoM Specifics

Four top level and several lower level characteristics for comparing materials have been defined for which FoMs may be computed.

- Modal Composition
  - Minerals
  - General
- Particle Size Distribution
- Particle Shape Distribution
  - Aspect Ratio
  - Angularity
- Density

Modal Composition

Two FoMs are computed for Modal Composition.

- Modal Composition – Minerals. Mineral composition includes only minerals.
  - Plagioclase
  - Olivine
  - Pyroxene
  - Spinel
  - Fe-Sulfide
  - Apatite
  - Native Iron
- Modal Composition – General. General composition is a more comprehensive composition definition and includes Mineral composition as one of its five top level classes.
  - Minerals
  - Lithic Fragments
  - Glasses
  - Agglutinates
  - Other (non-lunar materials and contaminants)
- The FoMs for Modal Composition are computed via the Discrete Category Function.

Size Distribution

- Size Distribution refers to the distribution of particle sizes.
- The FoM for Size Distribution is computed via the Relative Frequency Distribution Function.

Particle Shape

- It has been observed that particle shape is not homogenous for all the particles in a batch of material regardless of how shape is actually defined.
- The shape of the particles in a material follows a distribution of some sort. Shape is therefore a quantity which naturally may be described via a relative frequency distribution of a shape measure.
- Two Figures-of-Merit have been defined for Shape, involving two measures of shape:
  - Aspect Ratio, which quantifies the roundness or elongation of a particle.
  - Angularity, which quantifies the jaggedness or angularity of a particle.
- The FoMs for Shape Distribution are computed via the Relative Frequency Distribution Function.

Density

- Density refers to weight per unit volume of a material. However, for divided solids, those consisting of a collection of particles, the volume of a material will necessarily consist of particle volume, inter-particle void volume and internal pore volume.
- Therefore density is defined to refer to bulk density and any density measurements must be made over a sufficiently large enough sample so that the sample follows the particle size distribution of the material.
- Because bulk density is not an intrinsic property of a material, but depends in part on how a material is handled, we define the FoM for Density to include:
  - a minimum bulk density
  - a maximum bulk density
  - and the specific gravity of the material
- The FoM for Density is compute via the Discrete Category Function.

Software Implementation of FoM Algorithms

FoM Software

- The Figures-of-Merit software is a computer software implementation of the FoM algorithms and may be used to compute the FoMs.
- The Figures-of-Merit software only computes a set of numbers (the FoMs) which indicate how well a simulant material matches a reference material.
- It does not say anything about how well a simulant is suited for a particular application or purpose. The user of the software must make that determination.
- The Figures-of-Merit software does not contain any data; it is only a computational engine which computes FoMs from data supplied by a user.

Components of the Software

The software that implements the Figures-of-Merit consists of three parts:

- An input editor – we use Microsoft Excel for this purpose.
- A back end that computes the Figures-of-Merit – we use The MathWorks Matlab for this purpose.
- A front end with which the user interacts that opens and reads the Excel input files, performs checks on the inputs, and calls the Matlab routines for computation of the FoMs – this is custom code.

Example Discrete Category Function Input: Modal Composition - Minerals

Microsoft Excel - FOM rev 1.2.1b.xls

Modal Composition - Minerals

Short instructions	Size Range 1		Size Range 2		Size Range 3		Size Range 4		Size Range 5		Size Range 6		Size Range 7	
	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit	lower limit	upper limit
Enter Notes — Size														
Units	mm		mm		mm		mm		mm		mm		mm	
Sum of fractions (computed - must sum to unity)														
	fraction level 1	fraction level 2	fraction level 1	fraction level 2	fraction level 1	fraction level 2	fraction level 1	fraction level 2	fraction level 1	fraction level 2	fraction level 1	fraction level 2	fraction level 1	fraction level 2
Plagioclase														
fraction Albite														
fraction Anorthite														
Olivine														
fraction Forsterite														
fraction Fayalite														
Pyroxene														
fraction Clinopyroxene														
fraction Orthopyroxene														
(currently not used)														
Spinel														
fraction #1 material														
fraction #2 material														
fraction #3 material														
fraction #4 material														
fraction #5 material														
Fe-Sulfide														
Whitlockite *(currently not used)*														
Apatite														
Ilmenite														
Native Iron														

Legend

input fields

Notes

Short Instructions

For up to 8 Size Ranges (columns D-E; G-H; J-K; etc.), enter the following data (a Figure-of-Merit (FOM) will be computed for each Size Range):

1) The lower and upper limits of the size range (e.g. 0 - 100; 25 - 50).

2) The units for the sizes specified in step 1. Use the drop

Description | Modal Composition - Minerals | Modal Composition - General | Size Distribution | Shape - Aspect Ratio

Example Relative Frequency Distribution Function Input: Size Distribution

Microsoft Excel - FOM rev 1o.xls

Size Distribution

Sum of fractions (computed - must sum to 1)

Bins		Size validation	Bin Size Units	Bin Sizes	fraction
Bin 1	lower	(no data)	mm		
	upper	(no data)	mm		
Bin 2	lower				
	upper	(no data)	mm		
Bin 3	lower				
	upper	(no data)	mm		
Bin 4	lower				
	upper	(no data)	mm		
Bin 5	lower				
	upper	(no data)	mm		
Bin 6	lower				
	upper	(no data)	mm		
Bin 7	lower				
	upper	(no data)	mm		
Bin 8	lower				
	upper	(no data)	mm		
Bin 9	lower				
	upper	(no data)	mm		
Bin 10	lower				
	upper	(no data)	mm		
Bin 11	lower				
	upper	(no data)	mm		
Bin 12	lower				
	upper	(no data)	mm		
Bin 13	lower				
	upper	(no data)	mm		
Bin 14	lower				
	upper	(no data)	mm		
Bin 15	lower				
	upper	(no data)	mm		
Bin 16	lower				
	upper	(no data)	mm		

Short Instructions

For up to 16 Bins (rows 6-7; 8-9; 10-11; etc.) enter the following data:

1) The units for the sizes specified in step 2 (Bin Size). *Note: Units must be entered before Bin Size in order for proper validation to take place* (e.g. for Bin 1, units for lower bin size are entered into cell D6 and units for upper bin size are entered into cell D7; for Bin 2 and the others, only units for upper bin size need be entered, since the units for the lower size are the same as the units of the upper size of the previous bin.

2) The size of the upper end of a Bin (for Bin 1 a lower size must also be entered). Bins are treated as contiguous, so that the lower end of a Bin will be the upper end of the previous Bin (e.g. if Bin 1 spans the size range 50 to 100, 50 would be entered into cell E6 and 100 would be entered into cell E7. For Bin 2, and the others only the upper bin size need be entered, since the lower size is the same as the upper size of the previous bin.

3) The fraction of particles of the total in this size Bin. Enter the fraction for the Bin in the row associated with the Bin (e.g. fraction for Bin 1 is entered into cell F7; fraction for Bin 2 is entered into cell F9).

Note: The total of fractions for all Bins should sum to unity.

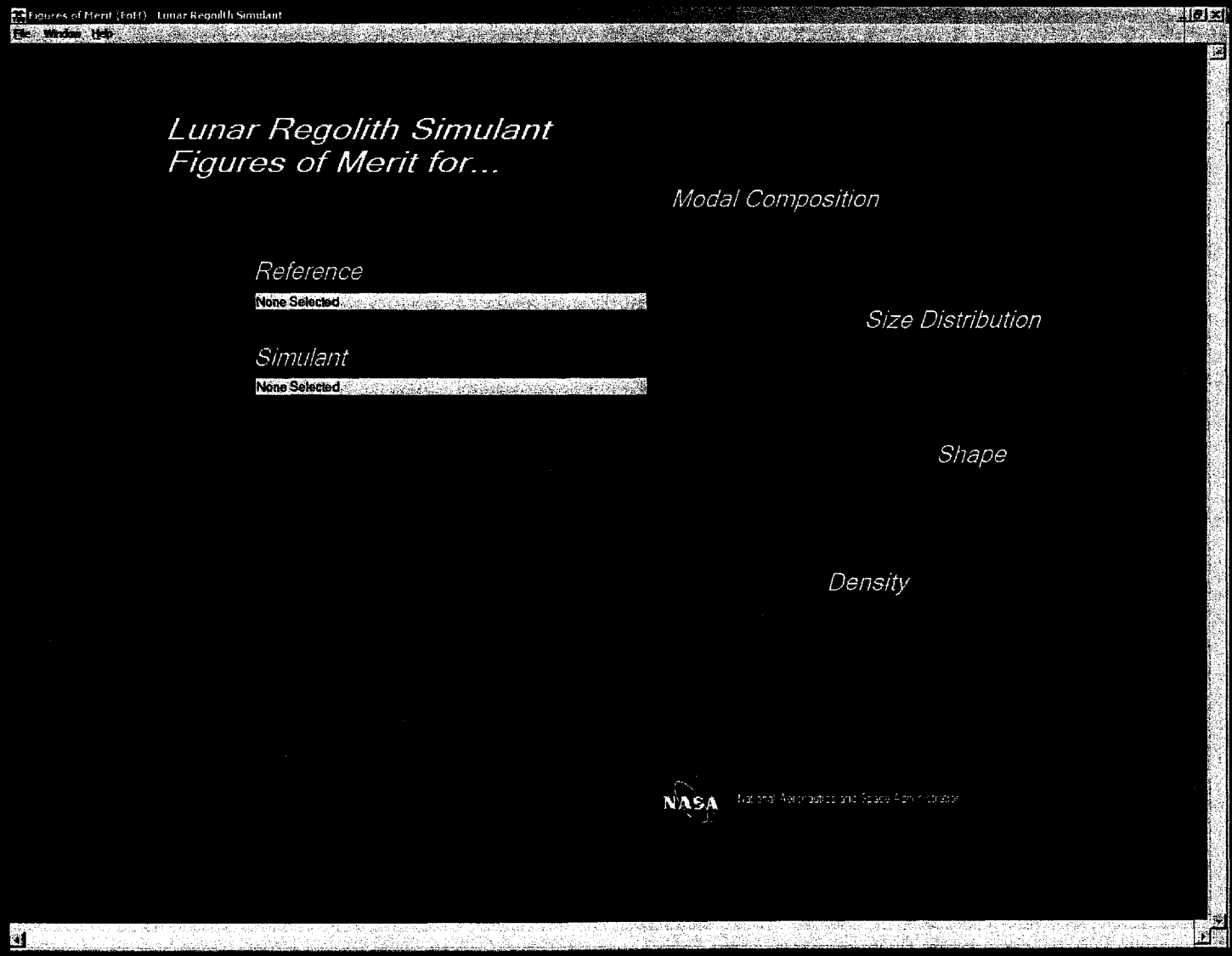
Note: Bin data must be entered in order of ascending bin size.

Legend: input fields

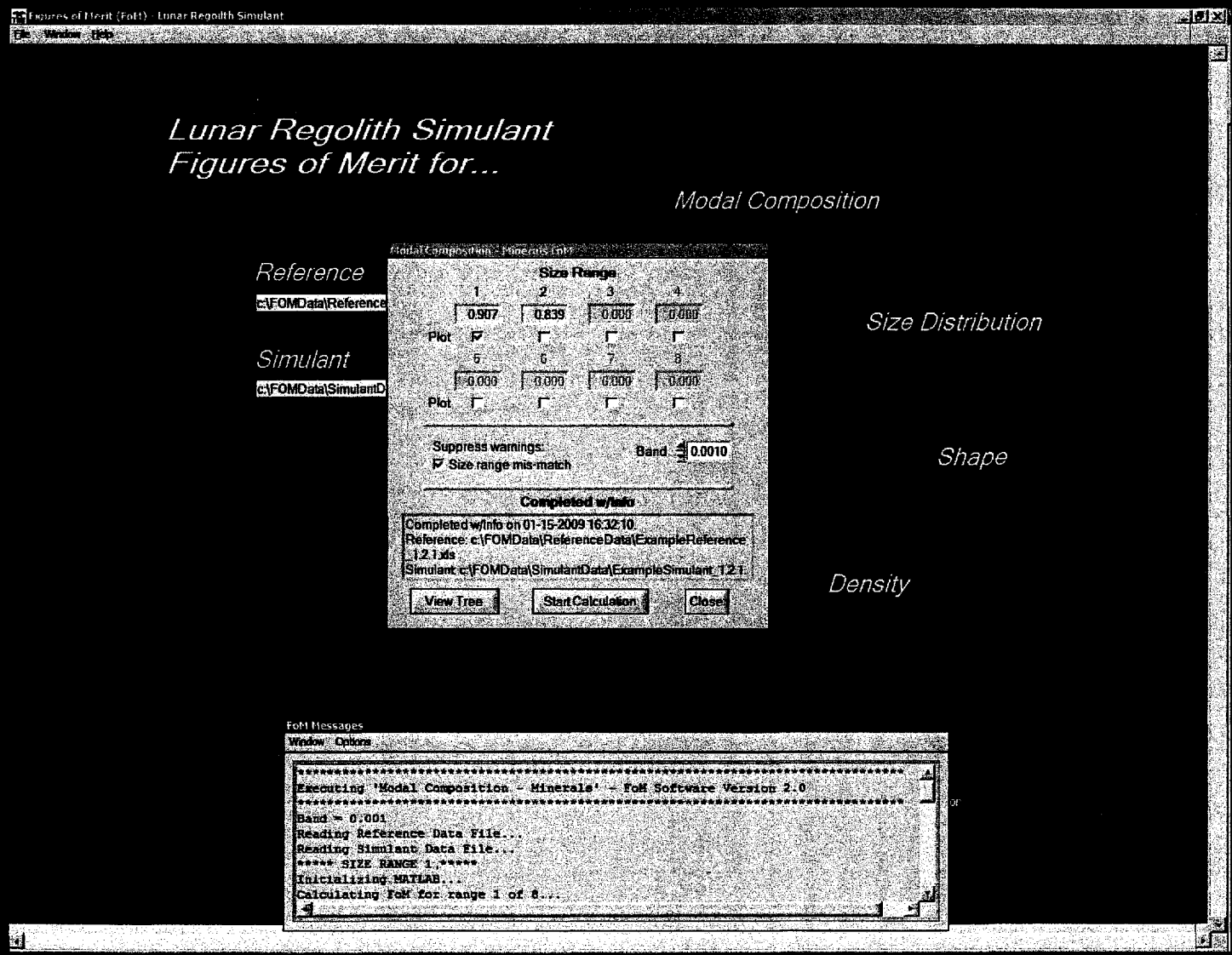
Notes

Description / Modal Composition - Minerals / Modal Composition - General / Size Distribution / Shape - Aspect Ratio

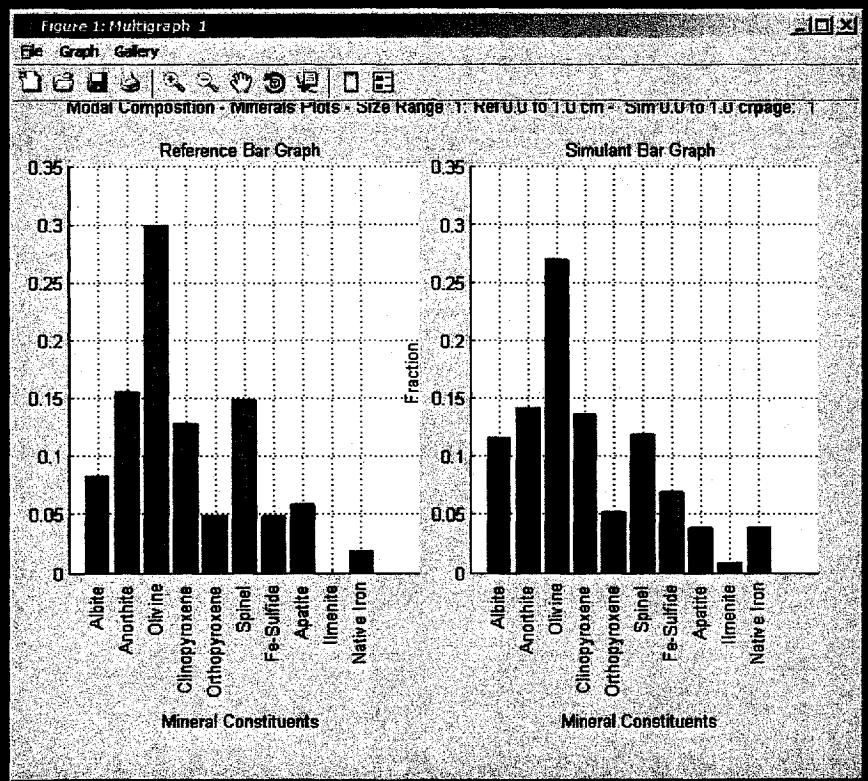
Fom Software Main Screen

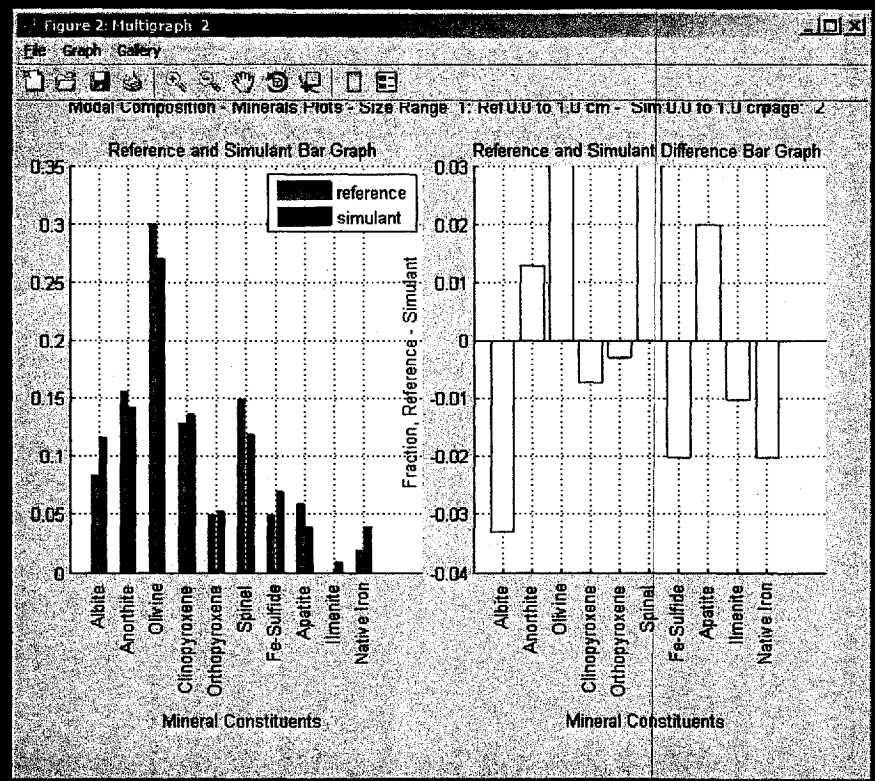


Example Discrete Category Function Screen Output: Modal Composition – Minerals

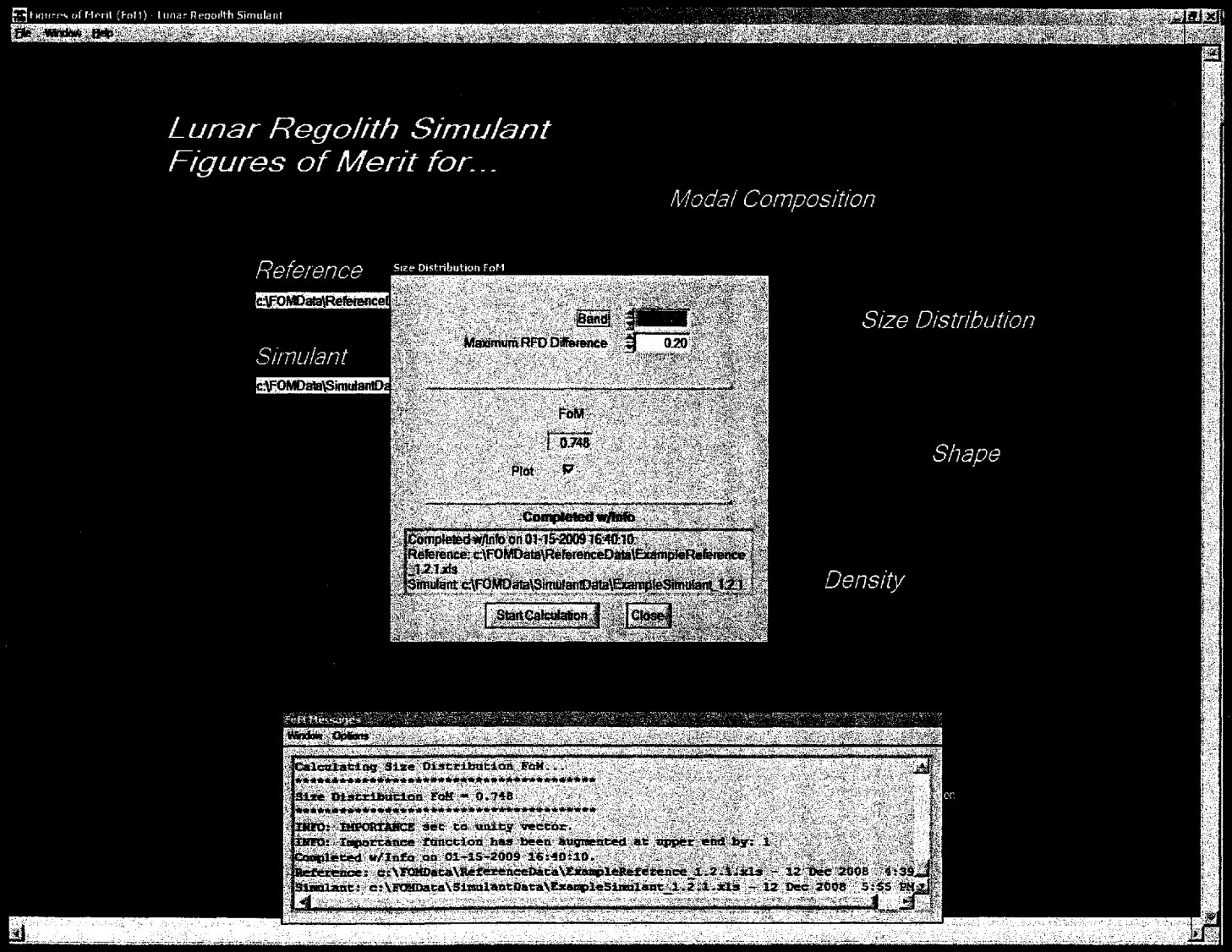


Example Discrete Category Function Graphics Output: Modal Composition – Minerals

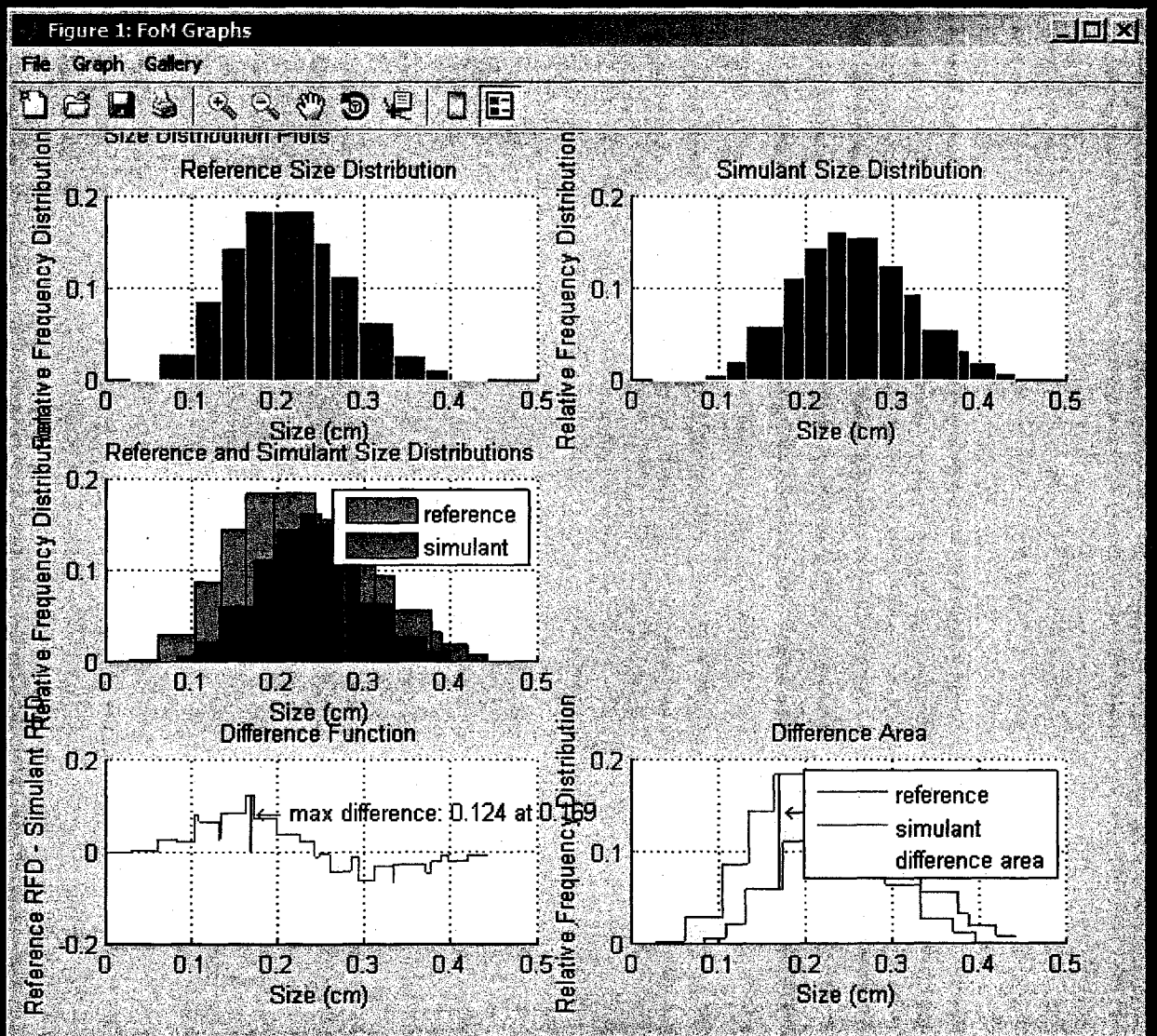




Example Relative Frequency Distribution Function Screen Output: Size Distribution



Example Relative Frequency Distribution Function Graphics Output: Size Distribution



Appendix Slides

Modal Composition FoM Interpretation

- The Figure-of-Merit for Modal Composition may be interpreted as:

"the fraction of material that is the same in both materials".

- As an example suppose you had a reference material and a simulant material consisting of:

Reference	Simulant
60 red marbles	40 red marbles,
30 green marbles	10 green marbles
10 blue marbles	50 blue marbles

- How do these compare? Well, the figure-of-merit would be 0.6.
- Now, of the red marbles, each material had at least 40, of the green marbles, each material had at least 10 and of the blue marbles each material had at least 10, so the two materials have 60 marbles in common out of 100 marbles, or, 0.6 of the marbles in each material are the same.

Other FoM Interpretations

- The Figure-of-Merit for Size Distribution may be interpreted as:

"the fraction of particle sizes that both materials have in common".

- The Figure-of-Merit for Shape Distribution may be interpreted as:

"the fraction of particle shapes that both materials have in common".

- The Figure-of-Merit for Density may be interpreted abstractly as:

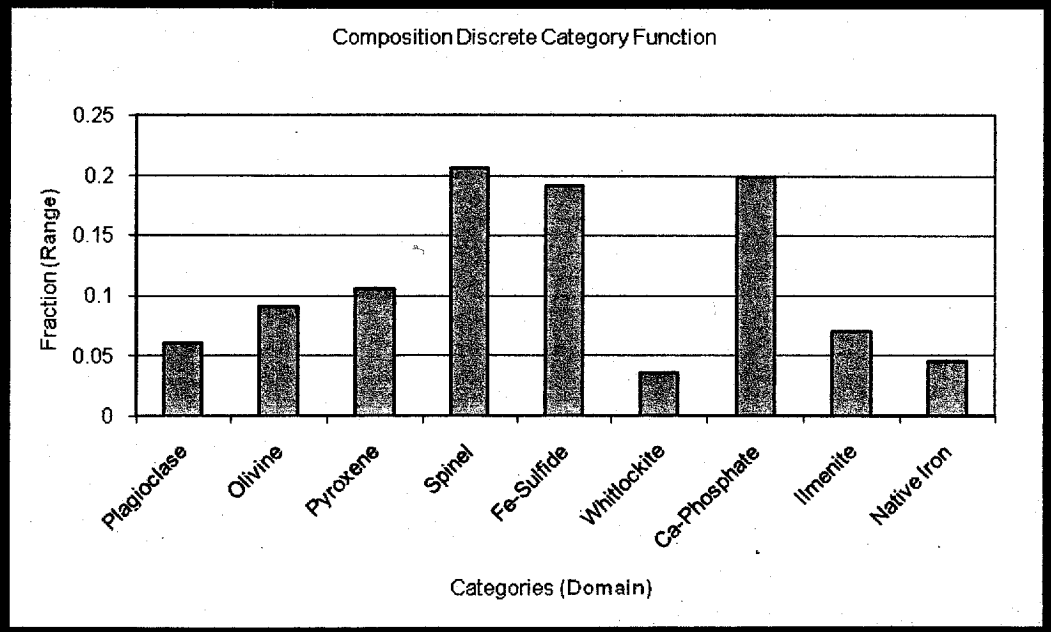
"the fraction of density that both materials have in common".

FoM Basics

- All FoMs are based on one of two methods for quantifying properties of materials.
- If a characteristic may be quantified by a collection of discrete categories, all of the same kind, then we may use a discrete category function to describe this characteristic. Discrete category functions may be plotted as bar charts.
- If a characteristic may be quantified by the distribution of a quantity, then we may use a relative frequency function to describe this characteristic. Relative frequency functions may also be plotted as bar charts.

Discrete Category Function

- A discrete category function is a function whose:
  - *Domain* (input, independent variable or argument) is a collection of discrete objects or categories all of the same "kind".
  - *Range* (output, dependent variable or value of the function) is the quantity, fraction, or other value for each of the elements in the domain.
- Discrete category functions may be plotted as bar charts showing the fraction or value of each of the categories.



Discrete Category Function FoM Preliminaries

- We may collect the domain and ranges into two vectors, one being a vector of categories, and the other being a vector of values for those categories, with a one to one correspondence between elements of the two vectors.
- We shall call the vector of categories the *category vector* and the vector of category values the *category value vector*.
  - Note that for category value vectors whose elements represent fractions of the categories, the sum of the elements of such vector must necessarily sum to unity (the sum of the fractional parts must equal the whole).

Category Vector

$$\begin{bmatrix} \textit{plagioclase} \\ \textit{olivine} \\ \vdots \\ \textit{native iron} \end{bmatrix}$$

Category Value Vector

$$\begin{bmatrix} 0.060 \\ 0.090 \\ \vdots \\ 0.045 \end{bmatrix}$$

Discrete Category Function FoM

The Figure-of-Merit for quantities described by a discrete category function is defined as 1 minus the L1 norm of the weighted difference between a reference category value vector (cvv) and a simulant category value vector scaled by the sum of the L1 norms of the weighted reference category value vector and the weighted simulant category value vector:

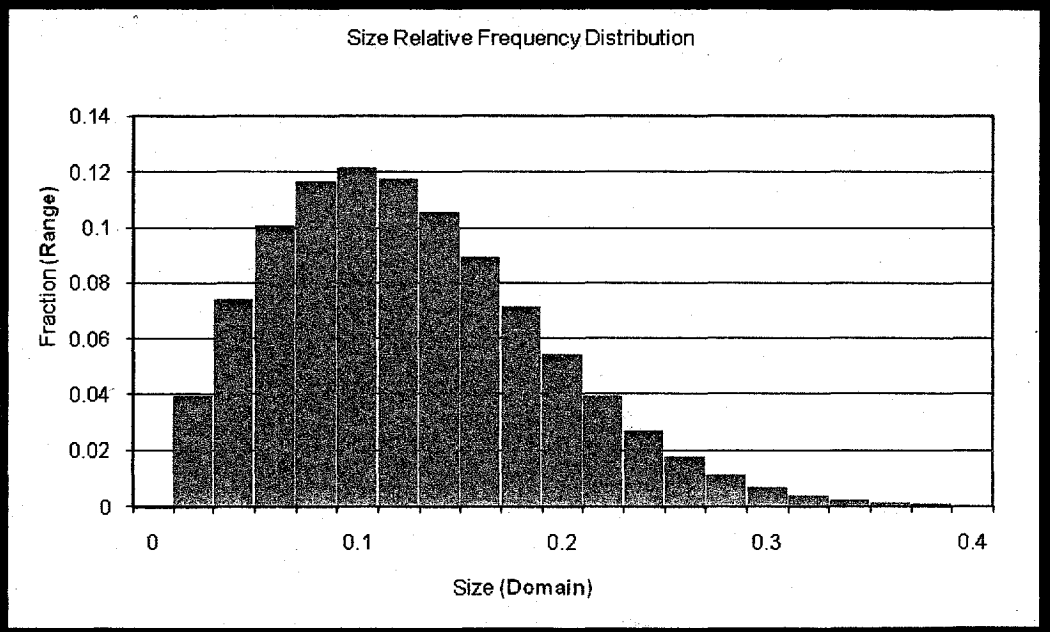
$$FoM = 1 - \frac{\left\| \mathbf{w}\left(\mathbf{cvv}^{reference} - \mathbf{cvv}^{simulant}\right) \right\|_1}{\left\| \mathbf{w}\,\mathbf{cvv}^{reference} \right\|_1 + \left\| \mathbf{w}\,\mathbf{cvv}^{simulant} \right\|_1}$$

$$= 1 - \frac{\sum_i w_i \left| \left(cvv_i^{reference} - cvv_i^{simulant} \right) \right|}{\sum_i w_i cvv_i^{reference} + \sum_i w_i cvv_i^{simulant}}$$

$$\left\| \mathbf{v} \right\|_1 = \sum_{i=1}^{n} \left| v_i \right| \textit{ denotes the } L1 \textit{ norm of vector } \mathbf{v}$$

Relative Frequency Distribution Function

- A relative frequency distribution (RFD) function is a function whose:
  - *Domain* (input, independent variable or argument) is a property that varies discretely over a set of values (also known as "bins").
  - *Range* (output, dependent variable or value of the function) is the quantity, fraction, or other value for bins in the domain.
- Relative frequency distribution functions may be plotted as a bar chart showing the distribution by fraction of a given property.



Relative Frequency Distribution Function Preliminaries

- Although a relative frequency function may be defined as a continuous function (continuous domain or input), for computational purposes we will work with discrete data.
- The discrete RFD's domain is defined by *n+1* values z_i, which define *n* contiguous bins, with the value of each bin (height of the bar chart bar) representing the fraction of particles between the lower and upper bin values constituting the range of the RFD.
- There is no requirement for the bin sizes to be of the same size across the RFD, and in fact variable bin sizes are allowed.
- Summation of the RFD range values between lower domain value z_j and upper domain value z_k yields the fraction of particles between z_j and z_k.
- Summation of the entire RFD range (from minimum to the maximum domain value) must necessarily equal unity (the sum of the factional parts must equal the whole).

Relative Frequency Function FoM

The Figure-of-Merit for a characteristic of a given reference and simulant that is quantified by a relative frequency distributions is defined as 1 minus the L1 norm of the weighted difference between a reference RFD and a simulant RFD scaled by the sum of the L1 norms of the weighted reference RFD and the weighted simulant RFD.

$$
\begin{aligned}
FoM &= 1 - \frac{\left\| w\left(RFD^{reference} - RFD^{simulant} \right) \right\|_1}{\left\| wRFD^{reference} \right\|_1 + \left\| wRFD^{simulant} \right\|_1} \\
&= 1 - \frac{\int w \left| RFD^{reference} - RFD^{simulant} \right|}{\int w \left| RFD^{reference} \right| + \int w \left| RFD^{simulant} \right|} \\
&= 1 - \frac{\sum_i w_i \left| \left(RFD_i^{reference} - RFD_i^{simulant} \right) width_i \right|}{\sum_i w_i RFD_i^{reference} width_i + \sum_i w_i RFD_i^{simulant} width_i}
\end{aligned}
$$