Testing a new sequential isofactorial simulation algorithm[1]

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Abstract

Existing geostatistical simulation approaches frequently rely on an assumption of Gaussianity or a computationally intense interpolation method to produce simulation realizations. These simulation methods encounter challenges in reflecting the attributes of sample data set exhibiting skewed distribution or non diffusive (clustered) properties. A new simulation algorithm has been developed, following the Sequential Isofactorial concept identified by Emery (2002). The simulation algorithm, referred to as the Sequential Isofactorial Algorithm ("SIA") allows for choice of a multivariate Gaussian or multivariate gamma based model to reflect a symmetrical or skewed distribution respectively. The SIA also incorporates a choice of destructuration coefficient reflecting varying degrees of clustering in the data (non diffusiveness in the multivariate distribution). Initial results from conditional simulation with the SIA utilizing a handful of conditioning data points suggest the results reflect the attributes of the chosen model, exhibiting the appropriate histogram, variogram and clustering. A comparison to sequential Gaussian simulation ("SGS") also creates an intuitive result, with the new algorithm showing greater variance in realizations. The SGS algorithm is constrained to produce a Gaussian local conditional cumulative distribution function with mean based on local conditioning data and variance independent on the sample values, only dependent on the spatial configuration of the information. The SIA (under a Gaussian diffusive model) also produces a Gaussian local CCDF with mean based on local conditioning data, however, the variance is dependent on the variance of the local conditioning data values.

1. Introduction

1.1. Mineral Resource Estimation and Traditional Simulation Techniques

Traditionally, the qualified person completing a Mineral Resource estimate applied kriging to arrive at a best estimate for mineral resource grade and tonnage. Kriging is a deterministic method unable to provide a relevant measure of uncertainty associated with its deterministic estimates. The qualified person would classify the mineral resource as measured, indicated, or inferred based on personal experience and industry association guidance related to drill hole spacing and deposit type.

Simulation provides a quantification of uncertainty in resource modelling. This allows an estimator to arrive at a quantitative view of how probable it is that a given block has a given value (e.g., probability that grade of block is above cut off). This probabilistic estimate of uncertainty can be carried through the

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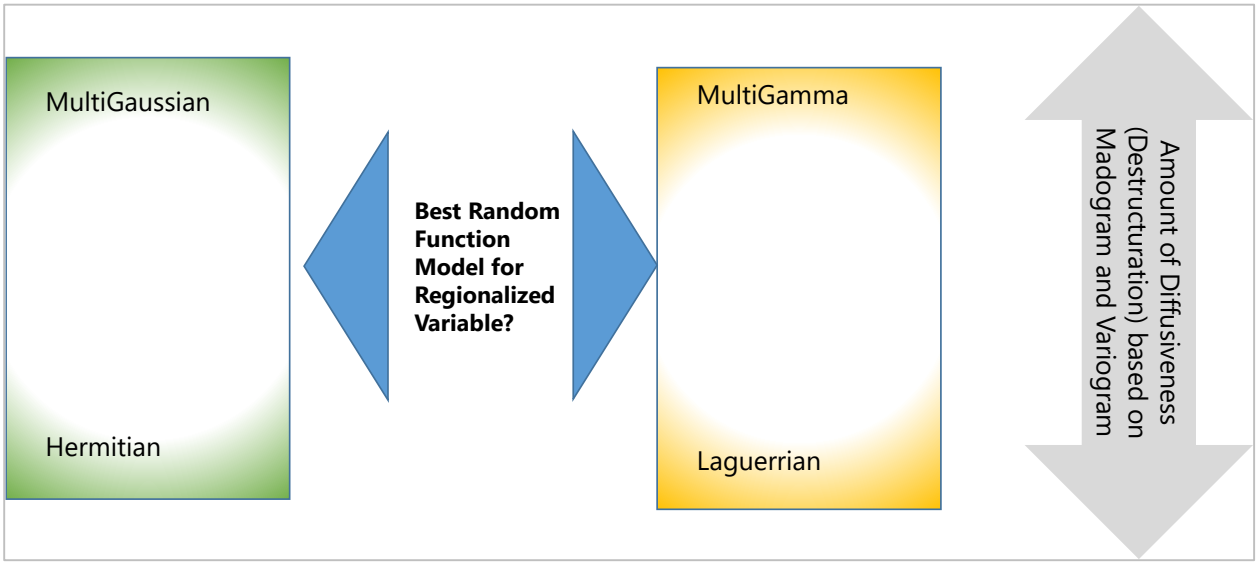
mine design and operation to make better decisions, understanding the range of possible operational and financial outcomes and associated likelihood.

Commonly applied simulation techniques include Sequential Gaussian Simulation and Sequential Indicator Simulation. Both these sequential simulation methods require a random draw from an estimated Conditional Cumulative Distribution Function ("CCDF") at unsampled locations. The CCDF, which is based on information in a neighborhood deemed to be relevant, reflects the probability that the unknown value at the location in question is below any value in its possible range. Simulation will not be successful if the CCDF is not accurate. Sequential Gaussian Simulation relies on the assumption that the regionalized variable under study is multiGaussian in nature. This is often not true. Simulation will also not be successful if it is not practical to implement. Sequential Indicator Simulation makes no assumption on the model of the variable under study but requires computation and modelling of many indicator variograms which makes it a cumbersome approach and challenging to implement in practice. Sequential Indicator Simulation also fails to account for cross correlation of indicator values at various thresholds, resulting in a sub-optimal model for the local CCDF (Emery and Ortiz, 2004; Machuca-Mory et al., 2008).

1.2. Context on Developed Simulation Isofactorial Algorithm

This broader research effort proposes to create a practical tool to choose either a multivariate Gamma or multivariate Gaussian random function model and associated parameters including level of destructuration based on observed properties of the available sample data. The "informed selection" of random function model, as shown in Figure 1 below can be applied in simulation of ore grades through the SIA. Importantly, this work will empirically test the relative success of this approach on partially sampled but known exhaustive data sets. Results will be compared against the exhaustive data set as well as simulation results obtained when traditional sequential Gaussian simulation is applied to the same sampled data set.

Figure 1: Illustration of Random Function Model Parameter Selection



1.3. Disjunctive Kriging to Model Gaussian or Gamma Local CCDF Functions

The Sequential Isofactorial Algorithm ("SIA") relies on disjunctive kriging based sequential simulation utilizing asymptotic polynomial expansions to model local conditional cumulative distribution functions ("CCDF's"). The polynomial expansion values calculated for sample values/locations can be used in conjunction with simple kriging to determine the transformed (e.g., normal score or "gamma score") value at an unsampled location. Disjunctive kriging is equivalent to simple co-kriging of the polynomial expansion terms. The specific polynomial expansions considered are orthogonal basis and the covariance between polynomials of different orders is zero. As a result, disjunctive kriging becomes simple kriging of the polynomial values for the transformed data values and then a linear weighted sum of the resulting polynomial values across orders. Disjunctive kriging is the equivalent of full indicator co-kriging but avoids the challenges of developing a workable model of co-regionalization for the indicator thresholds. This approach allows for the calculation of an expected value at an unsampled location based on statistical distance of nearby data points and reflecting the local conditioning data itself as embedded in the polynomial expansion terms at nearby sampled locations. The polynomial approximation technique can be used to define an expression for the local CCDF. Polynomial expansions may reflect a choice of multivariate random function family. The approach can be applied to sequentially simulate non multiGaussian data sets, such as multi-gamma data sets.

1.4. Randomizing Correlation Coefficient to Reflect Clustering of Values

Emery (2008) identified that the destructuration of grade (i.e., non diffusiveness of the random function model) can be reflected in simulation realizations by "randomizing" the correlation coefficient used in the disjunctive kriging process at each order of the polynomial expansion. Chiles and Delfiner (2012) provide a good overview of this technique. This approach takes the pure Gaussian and Gamma model and extends them to the more generalized "Hermitian" and "Laguerrian" models respectively. Without this adjustment, the Gaussian and Gamma models would be described as pure diffusive models. This diffusive property requires that the correlogram of the polynomials of order "p" are equal to the correlogram of the variable raised to the power p. Practically, the diffusive property means that sharp transitions (e.g., connectivity of extreme values) cannot be reflected in the model. In a diffusive model the transition between data points of different values will be gradual vs. abrupt. This is due to the higher order correlograms trending to zero as the power p increases (pure nugget). The incorporation of destructuration allows higher order terms to have greater weighting and, as a result, creates potential for sharper (non-diffuse) transitions, that appear in data sets as clustering of values.

2. Simulation Algorithm

2.1. Isofactorial Simulation

Polynomial expansion based disjunctive kriging can be used to define an expression for the local CCDF. This allows for the local CCDF to reflect the choice of bivariate random function family. Ortiz (2004) provides a good overview of fitting a finite function (any finite function is acceptable) with an expansion of Hermite Polynomials. A similar approach can be used to fit a finite function with an expansion of Laguerrian Polynomials.

The polynomials up to a selected order "N" are calculated at all sampled locations based on normal score or gamma score values. A variogram model is fitted to values. The covariance between polynomials of an

order N is based on the variogram with the resulting correlogram value raised to the power "N". Simple kriging is completed to solve for the numerical Hermitian or Laguerrian polynomial values of each order at the unsampled location.

For a given unsampled location we now have a set of numerical values for the polynomials at each order N. These polynomial values form the building blocks for the local CCDF at the unsampled location, effectively "coding" the information contained in the conditioning values (values and variance). The local CCDF is a weighted sum of these polynomial values. The weightings for each order polynomial in the CCDF are derived based on an expansion of the indicator function (i.e., probability value is less than or equal to a given threshold). The result is an equation for the CCDF value at an unsampled location as a function of the actual (but unknown) random variable value at that location.

2.2. Randomizing the Correlation Coefficient

The above procedure for disjunctive kriging considers only the case of no destructuration (i.e., diffusive models) as the correlograms of various orders are simply the correlogram raised to the power "N". This process can be adjusted to consider non-diffusive models. This is accomplished by a randomization of correlogram at higher orders using a beta distribution whose form is dictated by a specific scalar factor. As the scalar factor varies between zero and infinite, the model varies between the diffusive and non-diffusive (mosaic) case. In effect, as the model moves away from a pure diffusive model, greater weight is given to higher order expansions, resulting in a "tighter" local CCDF with less variance around its mean (i.e., sampling form the CCDF is more likely to yield a value closer to the local conditional mean and less informed by the broader background global mean). The incorporation of destructuration is accomplished by this change to the correlogram used in simple kriging of the polynomial values. The resulting numeric polynomial values kriged for a given unsampled location reflect both the underlying choice of bivariate family (i.e., Gaussian or Gamma) and a chosen amount of destructuration (clustering).

2.3. Sequential Simulation Algorithm

As described above, we can use the Isofactorial disjunctive kriging approach to create an equation for the local CCDF value as a function of the unknown underlying value. Sequential simulation draws a random number between zero and one and assumes this to be the CCDF value. Because the CCDF (by definition) is a monotonic function, a guess and check bounding algorithm was designed to iteratively determine the corresponding actual variable value that the CCDF random draw corresponds to (within a specified tolerance). The algorithm for solving the underlying value that corresponds to the randomly drawn CCDF value is described below.

1. Complete a random draw between one and zero for the simulated CCDF percentile value ("simulated percentile")
2. Based on range of known values (i.e., normal or gamma score values at sample locations) select a maximum and minimum possible value
3. For each of the maximum value, minimum value and midpoint value calculate the CCDF percentile using the modeled local CCDF function
4. Compare the simulated percentile value to the percentile value calculated at maximum, minimum and midpoint of the underlying normal or gamma scores

5. If simulated percentile value is within an acceptable tolerance of one of these percentile values, set the associated underlying normal score value as the simulated normal or gamma score value at that location, otherwise:
    a. Determine if the simulated CCDF value lies above or below the midpoint CCDF value, if above, set the minimum underlying value to the midpoint value, if below set the maximum underlying value to the midpoint value
    b. Go back to step 3 using this new minimum, maximum and midpoint value for the underlying
    c. Repeat until simulated percentile value is within acceptable tolerance of maximum, minimum or midpoint CCDF values and when it is set the simulated underlying value to the corresponding minimum, maximum or midpoint underlying value

Once the above algorithm is complete, we move (randomly) to the next unsampled location and repeat the algorithm considering both sampled locations and previously simulated locations in the neighborhood of the location being simulated.

3. Results

3.1. Examining Local CCDF Curves

A small five by three matrix was populated by randomly drawn values with three "unsampled" locations left blank in the array. This simple data set was used to check that modelled local CCDF curves were behaving in a manner that was intuitively expected. The results are shown below in figures 2, 3, 4 and 5.

Figure 2: CCDF Curves at Unsampled Points Demonstrating Impact of Conditioning Data

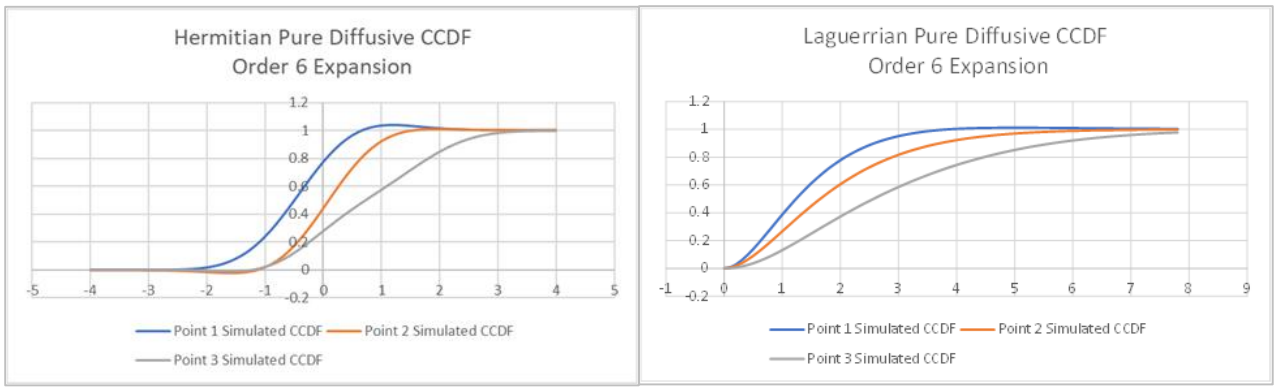


Figure 3: Illustration of CCDF Curves under Laguerrian cases with varying shape assumption.

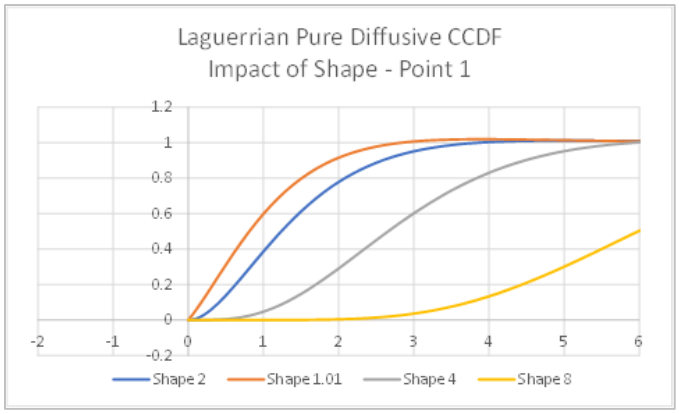


Figure 4: Illustration of CCDF Curves under Hermitian case with varying order of expansion

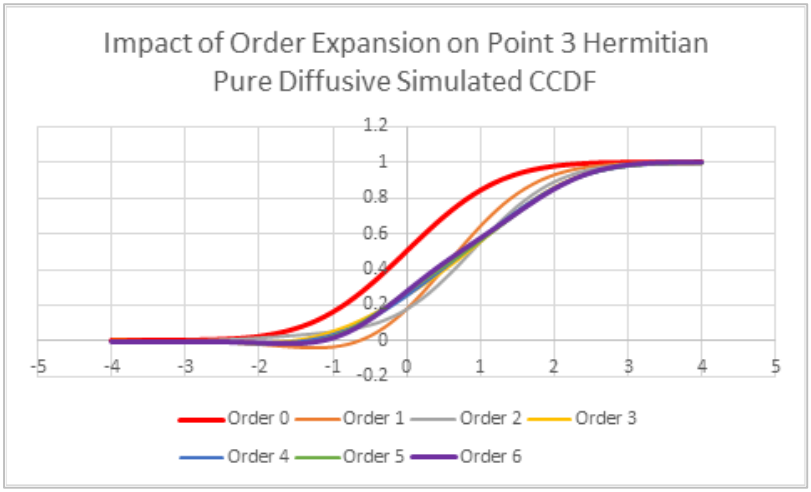
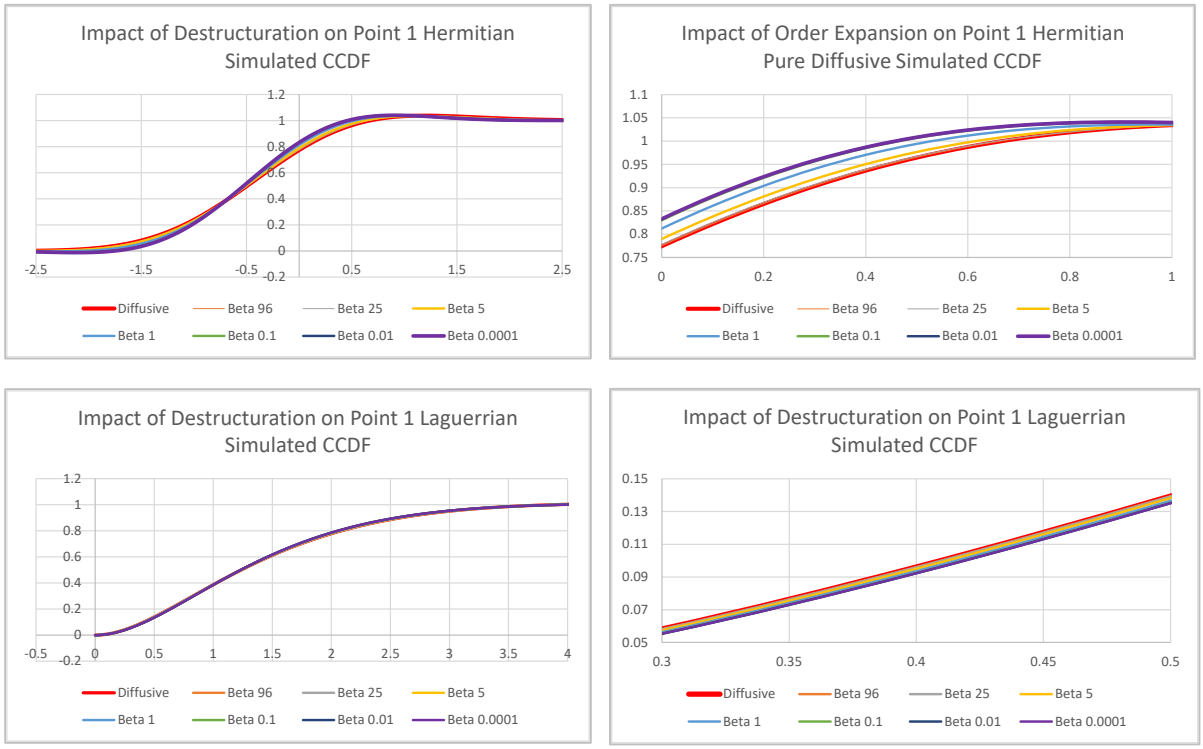


Figure 5: Illustration of CCDF curves at 1st simulated node under Hermitian and Laguerrian cases with varying destructuration



3.2. Comparison of SIA to Sequential Gaussian Simulation

Fifty simulation realizations on a 50x50 grid using the same conditioning data point were run with both Sequential Isofactorial Algorithm ("SIA") (Gaussian pure diffusive model) and traditional gslib SGSIM ("SGS").

- Single conditioning data point set at center of matrix of 0.2
- Lognormal reference distribution used resulting in normal score conditioning data point of ~-1.6 (based on lognormal percentile of 0.2 value)
- Spherical variogram with range of 8, nugget of 0.1
- Search radius of 12

While SIA results generally match those of SGS, SIA displays considerably greater variance than SGS, evidenced in variogram sills, conditional variance map and simulation realizations. This is driven by the fact that SGSIM is limited to a Gaussian CDF at any node, with variance obtained by simple kriging, hence independent of the sample values. In the SIA algorithm, the local CCDF's are built from the polynomial expansion. It is observed that the first term in the isofactorial expansion is the standard distribution, the second term adjusts for local mean, and subsequent terms adjust for the specific characteristics of the local conditioning data (e.g., a high variance in local conditioning data is reflected in the local CCDF curve being lower slope). The resulting variance of the CCDF depends on the particular sample values. Simulation results (in transformed normal score) are shown below in figure 6, 7, 8, 9 with SGSIM results on the left and SIA results on the right.

Figure 6: Comparison of SGS and SIA Realizations and Average (E-Type)

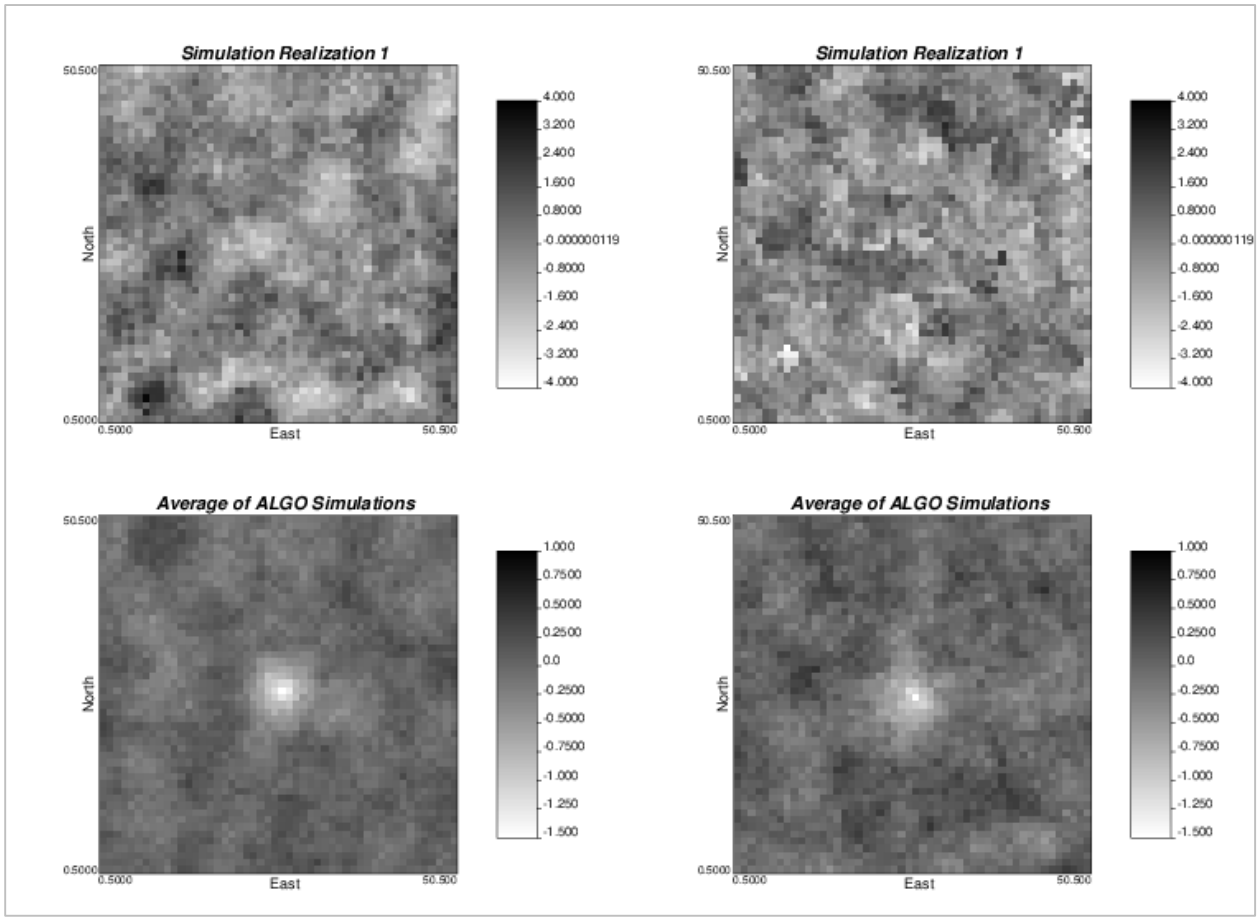


Figure 7: Comparison of SGS and SIA Conditional Variance

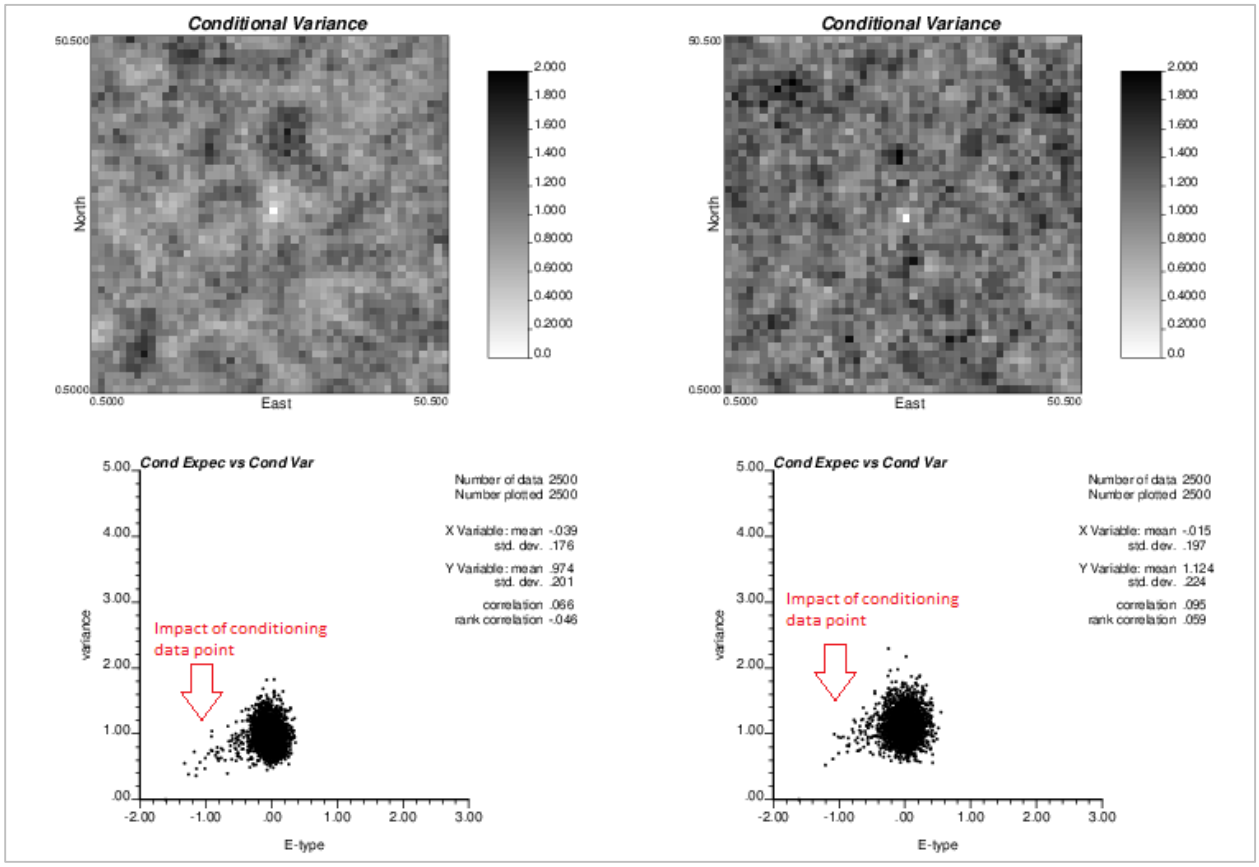


Figure 8: Comparison of SGS and SIA Experimental Variograms

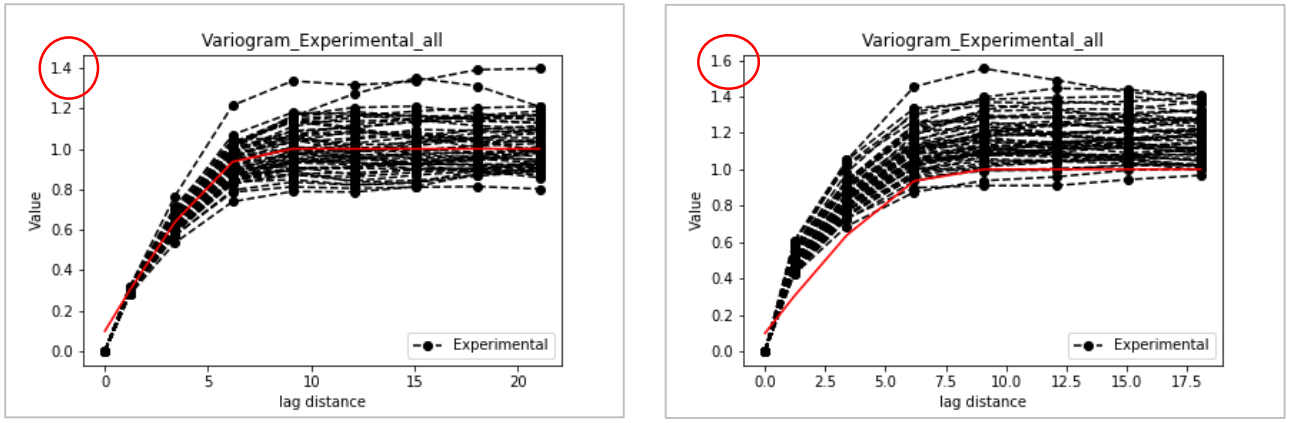
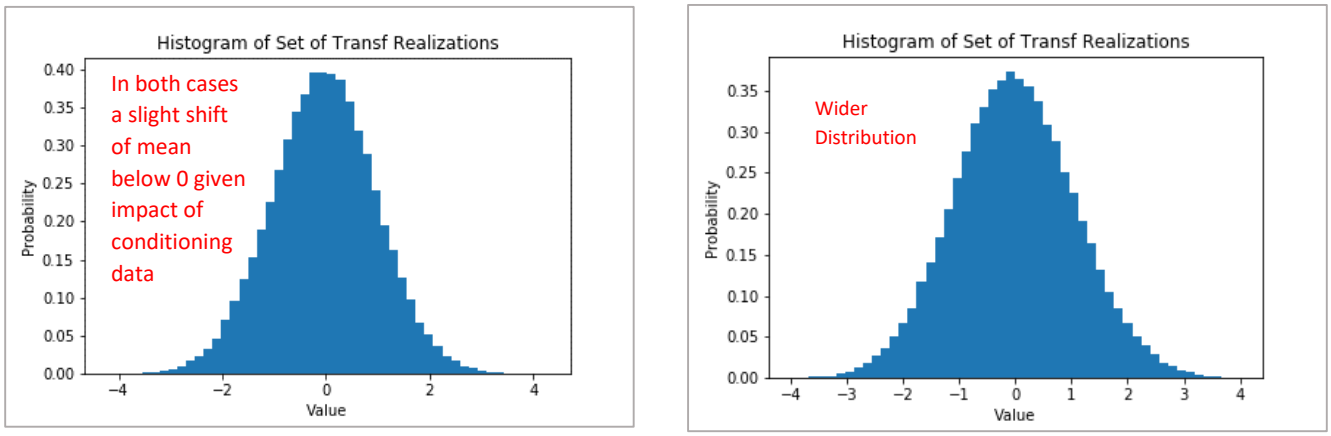


Figure 9: Comparison of SGS and SIA Histograms from Simulation Test



The simulation results back-transformed with lognormal reference distribution to be raw values are shown below with SGS results on the left and SIA results on the right in figures 10, 11 and 12.

Figure 10: Comparison of SGS and SIA Raw Realizations and Average (E-Type)

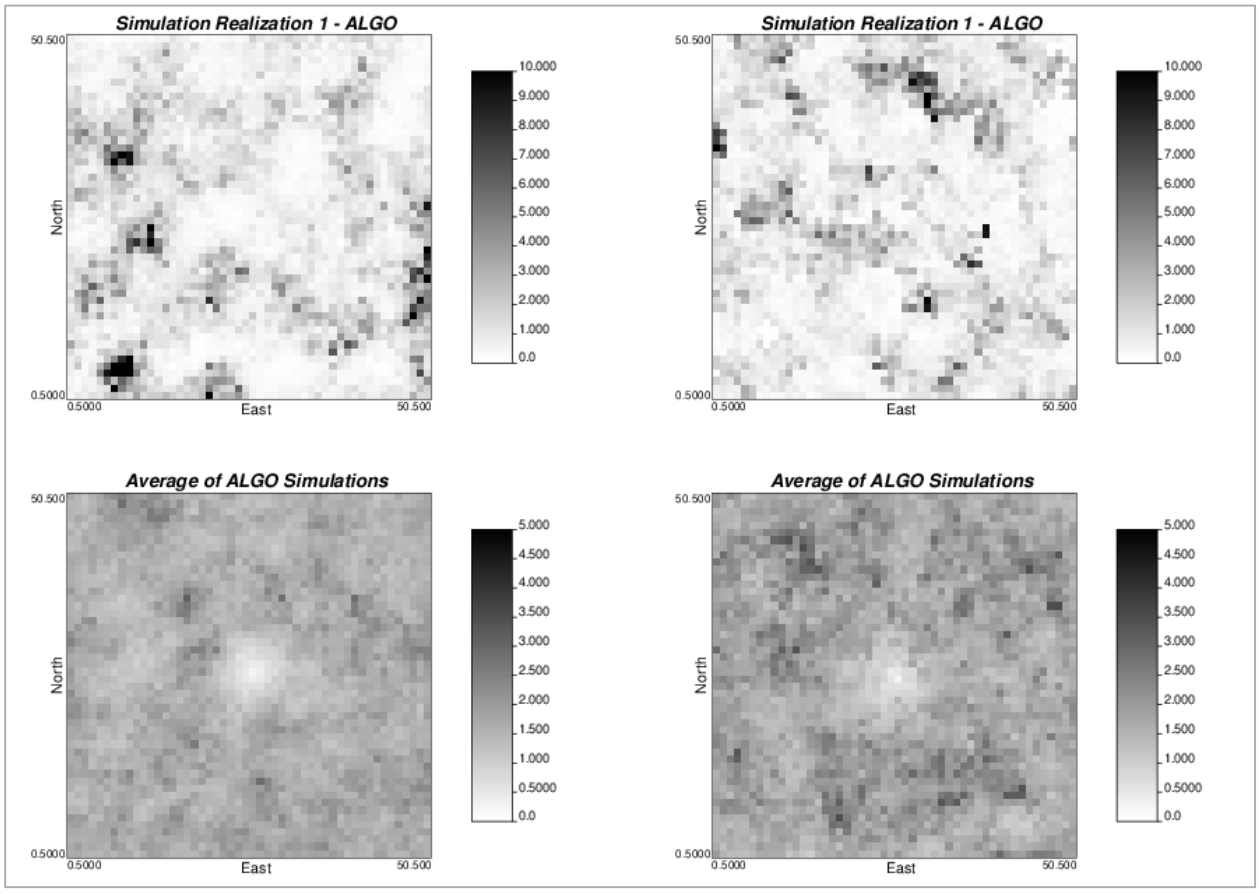


Figure 11: Comparison of SGS and SIA Raw Conditional Variance

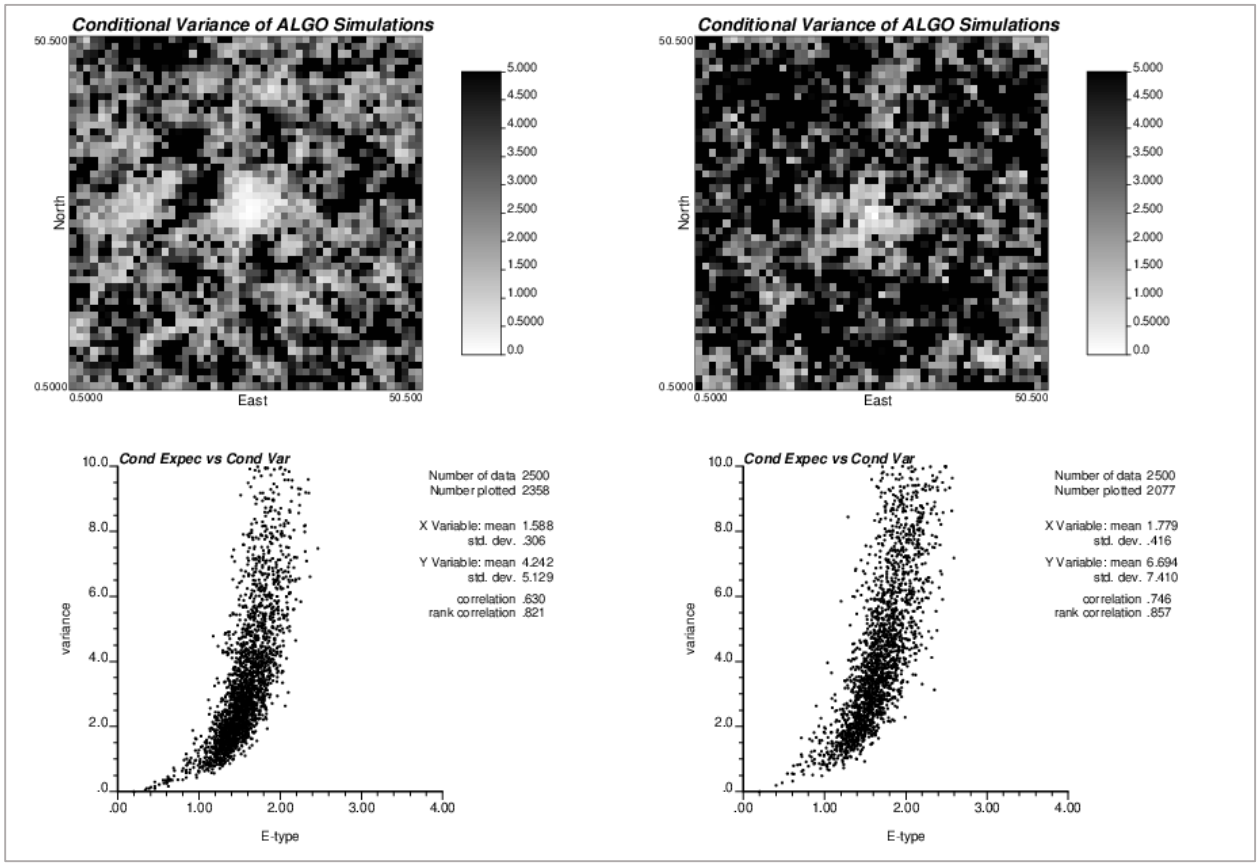
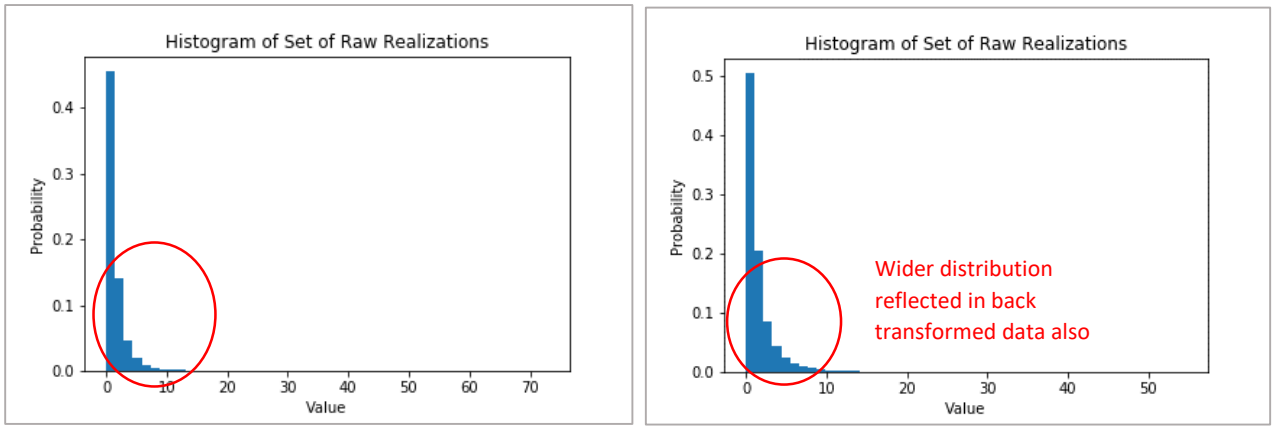


Figure 12: Comparison of SGS and SIA Raw Histograms



A second experiment was run using a larger variogram range. The results showed increased continuity in both SIA and SGS results as shown below.

Figure 13: Comparison of SGS and SIA Simulations with Increased Variogram Range; Realizations and Average (E-Type)

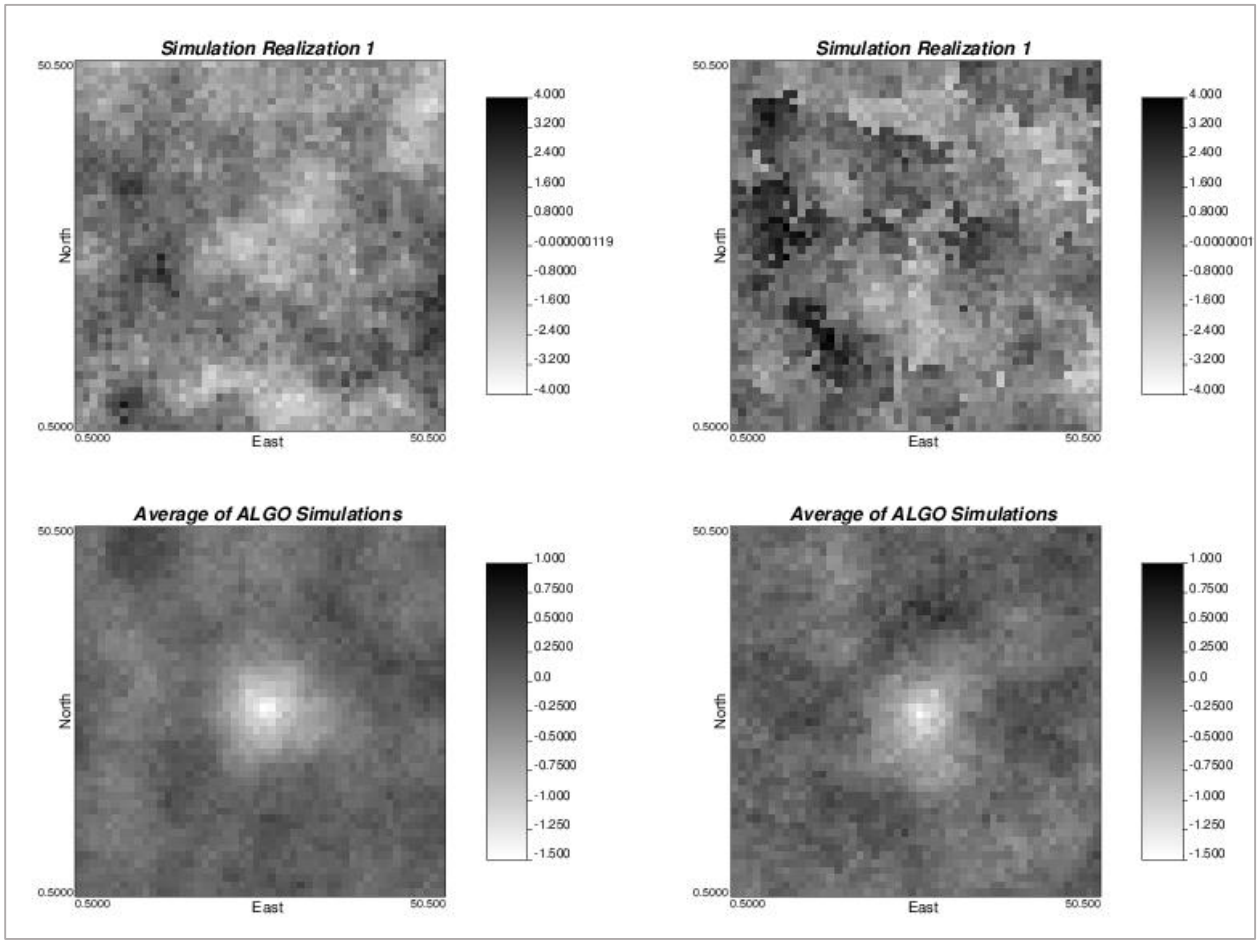
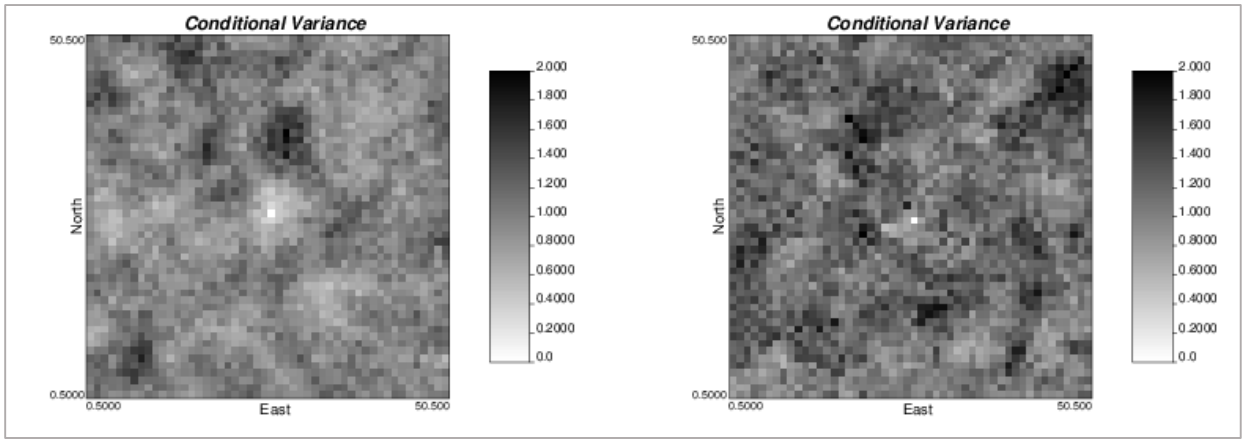


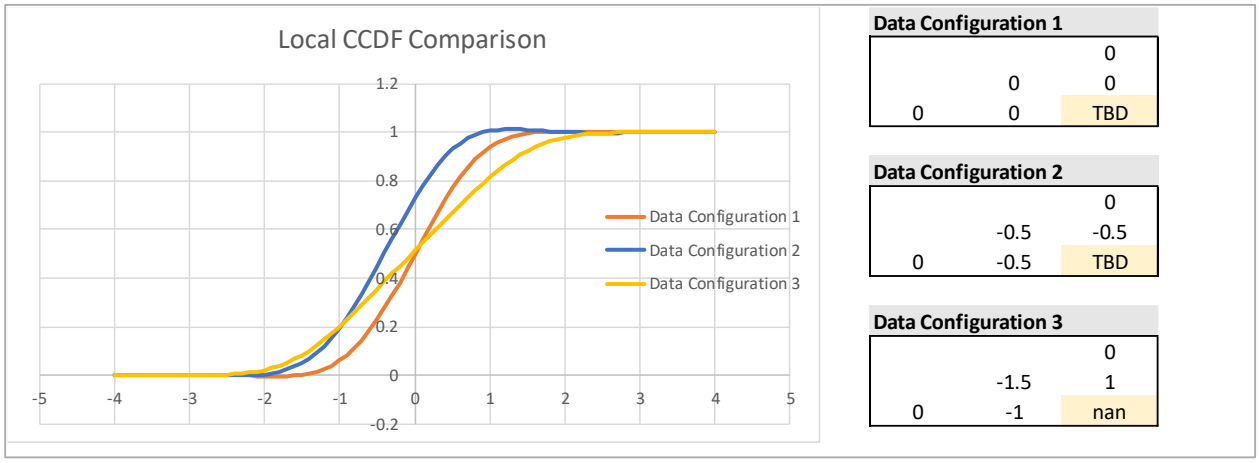
Figure 14: Comparison of SGS and SIA Simulations with Increased Variogram Range Conditional Variance



The cause of variability increases in the SIA realizations relative to the SGS realizations is described further. The local CCDF form under SIA is impacted by both the mean and the variance of the conditioning data. This is illustrated below using the SIA algorithm. First a local CCDF is created conditioned to a uniform set

of zero values, second a uniform value of negative 0.5 is used for all adjacent conditioning points (it can be seen below in figure 15 that SIA behaves like SGS and simply shifts the curve to the new mean). Finally, a curve with the same local mean as the first curve (0.0) but a much higher variance is shown to result from conditioning data with the same zero mean but much higher variance.

Figure 15: Comparison of SGS and SIA Simulations with Increased Variogram Range Conditional Variance



Data Configuration 1

		0
	0	0
0	0	TBD

Data Configuration 2

		0
	-0.5	-0.5
0	-0.5	TBD

Data Configuration 3

		0
	-1.5	1
0	-1	nan

3.3. Examining Variance in SIA Results

A further examination of the conditional variance relative to various model input parameters was conducted.

Base Results (50 x 50 grid)

- Variogram Range and search radius of 12
- Conditioning data point -1.6 normal score (0.2 lognormal)
- 50 simulations

Figure 16: Conditional variance of 50 x 50 simulation with single conditioning point showing gradual increase of conditional variance away from conditioning data point

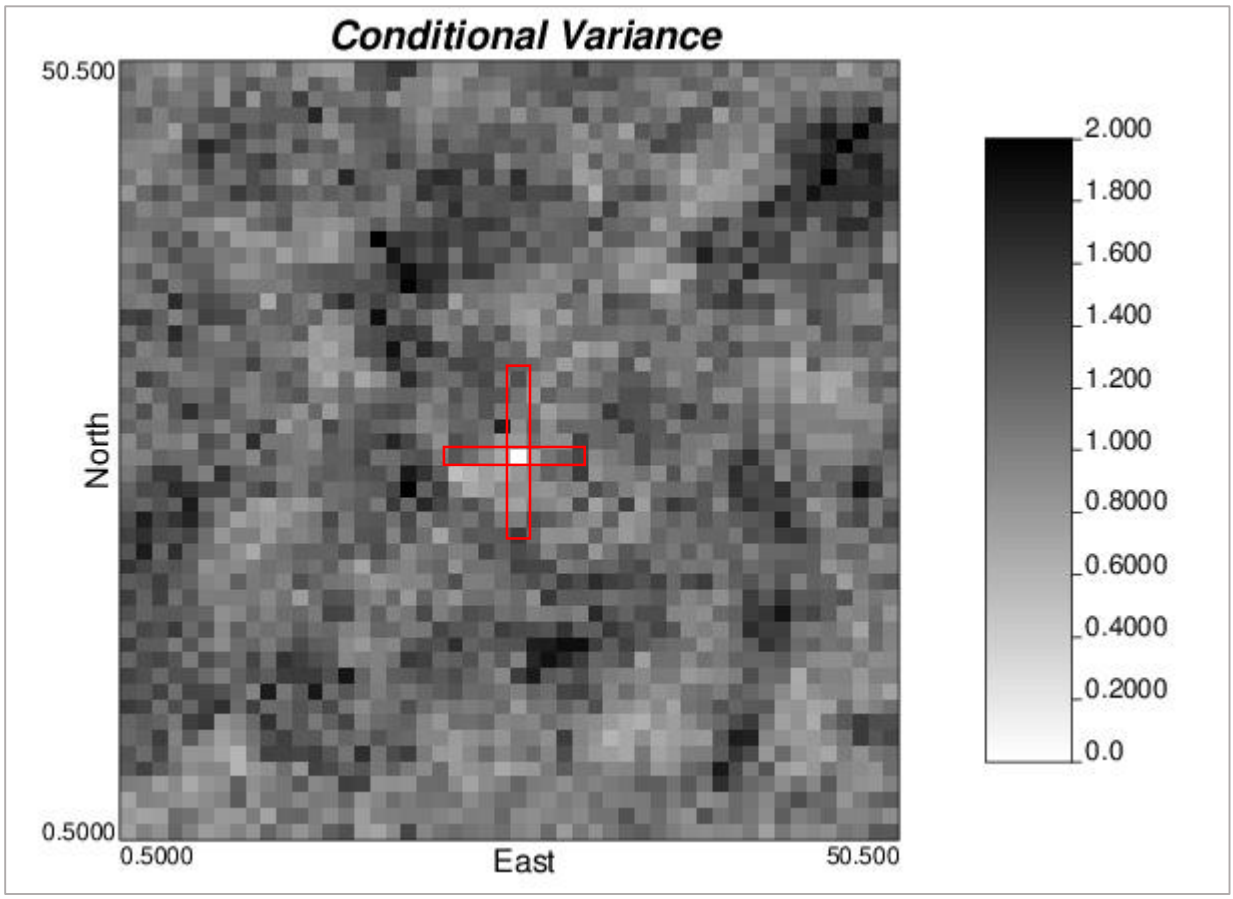
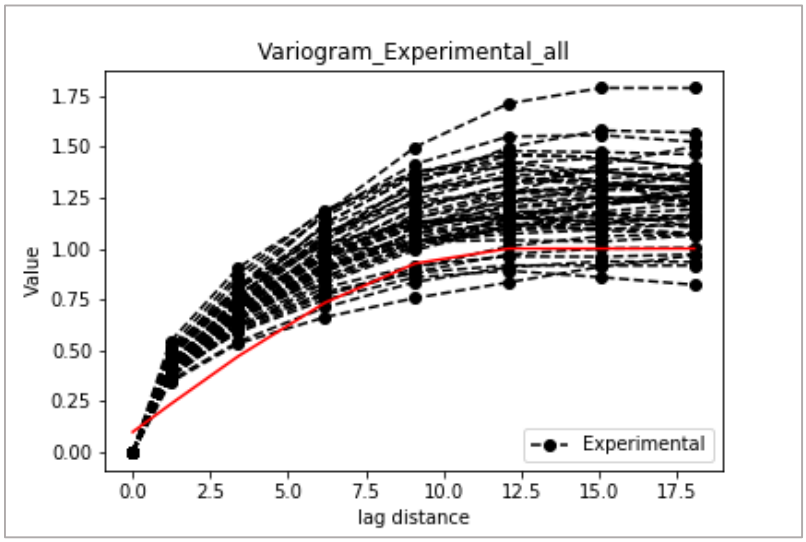


Figure 17: Experimental Variograms of 50 x 50 simulation with single conditioning point



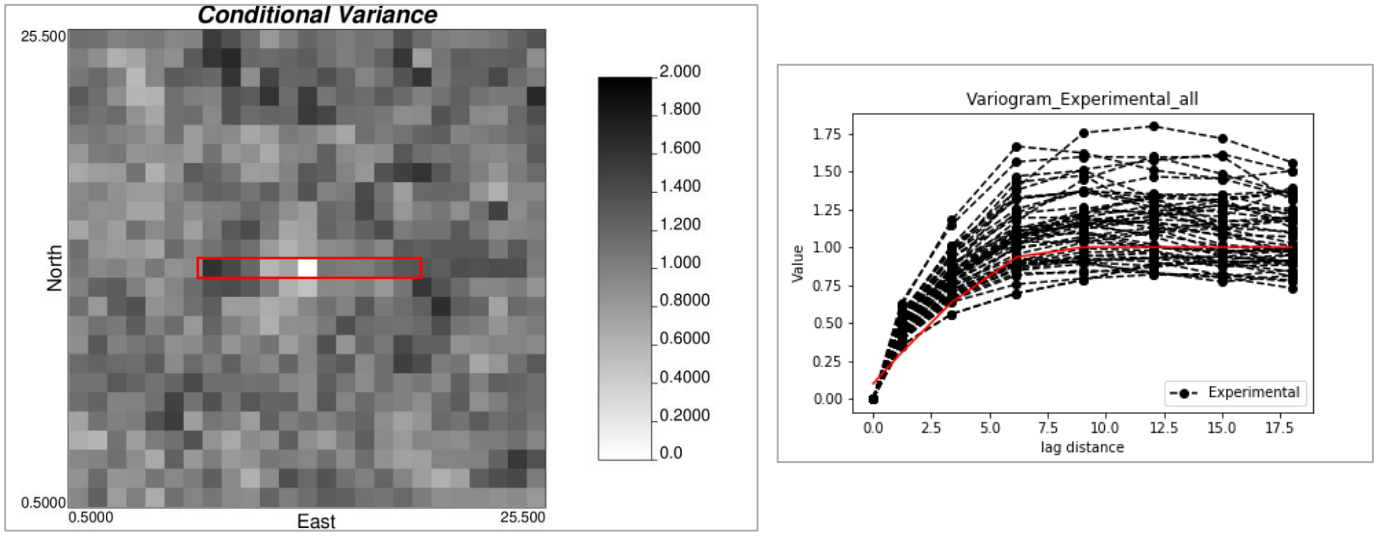
A number of other scenarios were examined on 25 x 25 grids to review impact of assumptions on variance as shown in map of conditional variance and experimental variograms for the set of realizations.

Hypothesis 1: less smooth conditional variance around the conditioning data point in SIA driven by the fact that starting with a low value creates greater dispersion of samples and a broader curve. This also drives higher overall variance in the realizations

Set Up 1

- Variogram Range and search radius of 8
- Conditioning data point -1.6 normal score (0.2 lognormal)
- 50 simulations

Figure 18: Conditional variance map and experimental variograms for set up 1

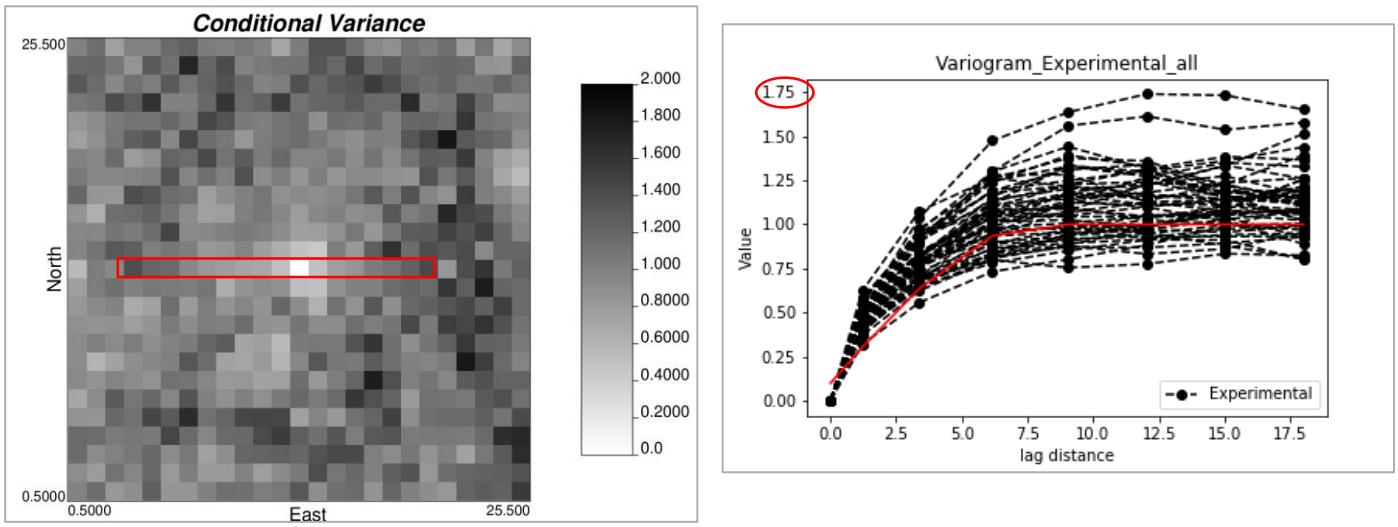


Set Up 2

- Variogram Range and search radius of 8
- Conditioning data point 0.0 normal score (1.0 lognormal)
- 50 simulations

Relative to set up 1, the use of a central conditioning data point instead of a low value conditioning data point smooths the conditional variance around the conditioning data point as anticipated. Overall variability also appears reduced slightly in the variograms.

Figure 19: Conditional variance map and experimental variograms for set up 2 showing reduced variance from non-extreme conditioning values

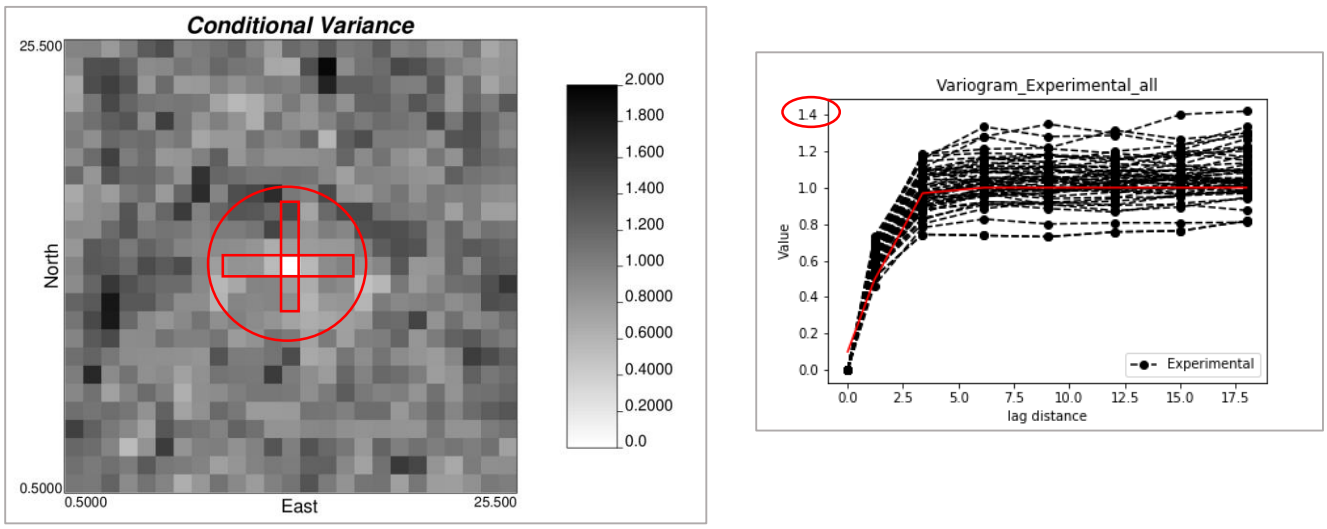


Hypothesis 2: Variogram range should be correlated with variability. A short variogram range should result in lower variance (i.e. lower variogram sill) as by definition, conditioning data variance at any given point likely to be lower (fewer widely spaced values expected in the covariance matrix).

<u>Set Up 3</u>

- <u>Variogram Range and search radius of 4</u>
- Conditioning data point 0.0 normal score (1.0 lognormal)
- 50 simulations

Figure 20: Conditional variance map and experimental variograms for set up 3 showing reduced variance from lower search radius and variogram range



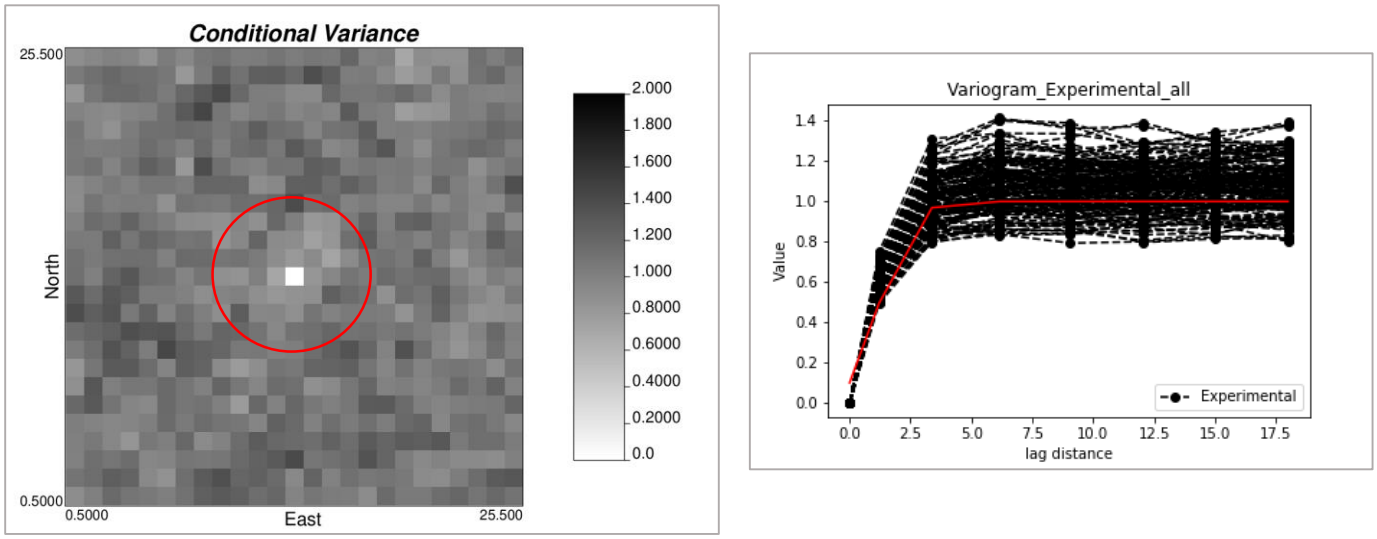
Relative to set up 2, the use of a shorter variogram range reduces the variance in each realization as shown in the experimental variograms that cluster more evenly around the modelled variogram. Conditional variance is also smooth over a shorter range given the lower variogram range.

Hypothesis 3: increasing number of simulations should smooth conditional variance map

Set Up 4

- Variogram Range and search radius of 4
- Conditioning data point 0.0 normal score (1.0 lognormal)
- 150 simulations

Figure 21: Conditional variance map and experimental variograms for set up 4

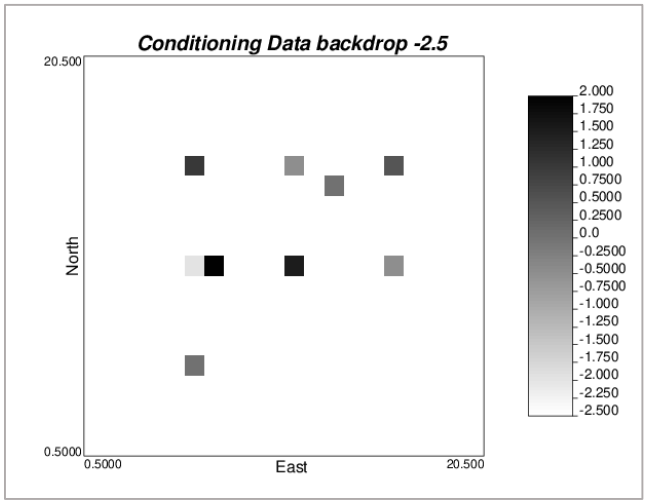


Relative to set up 3, the use of a greater number of simulations significantly smooths the conditional variance map.

3.4. Comparison of Random Function Models

A blank 20 x 20 array was initialized. Nine conditioning data points were assigned. The conditioning data is shown below.

Figure 22: Conditioning data for random function model comparison



The SIA simulation algorithm was then run over the conditioning data for four scenarios:

A) Pure Diffusive Gaussian Model
B) Pure Diffusive Gamma Model (Shape of 2)
C) Gaussian Model with Destructuration Coefficient of 0.0001
D) Gamma Model with Destructuration Coefficient of 0.0001 (Shape of 2)

In each case, 50 simulations were completed producing 50 realizations of the gamma or Gaussian score data and 50 realizations of the back transformed raw data. A simple spherical variogram model was assumed with range of 5 units and 0.1 nugget (total sill is 1.0). The results for the four cases are shown below in figure 23 to 29.

Figure 23: Simulation realizations from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

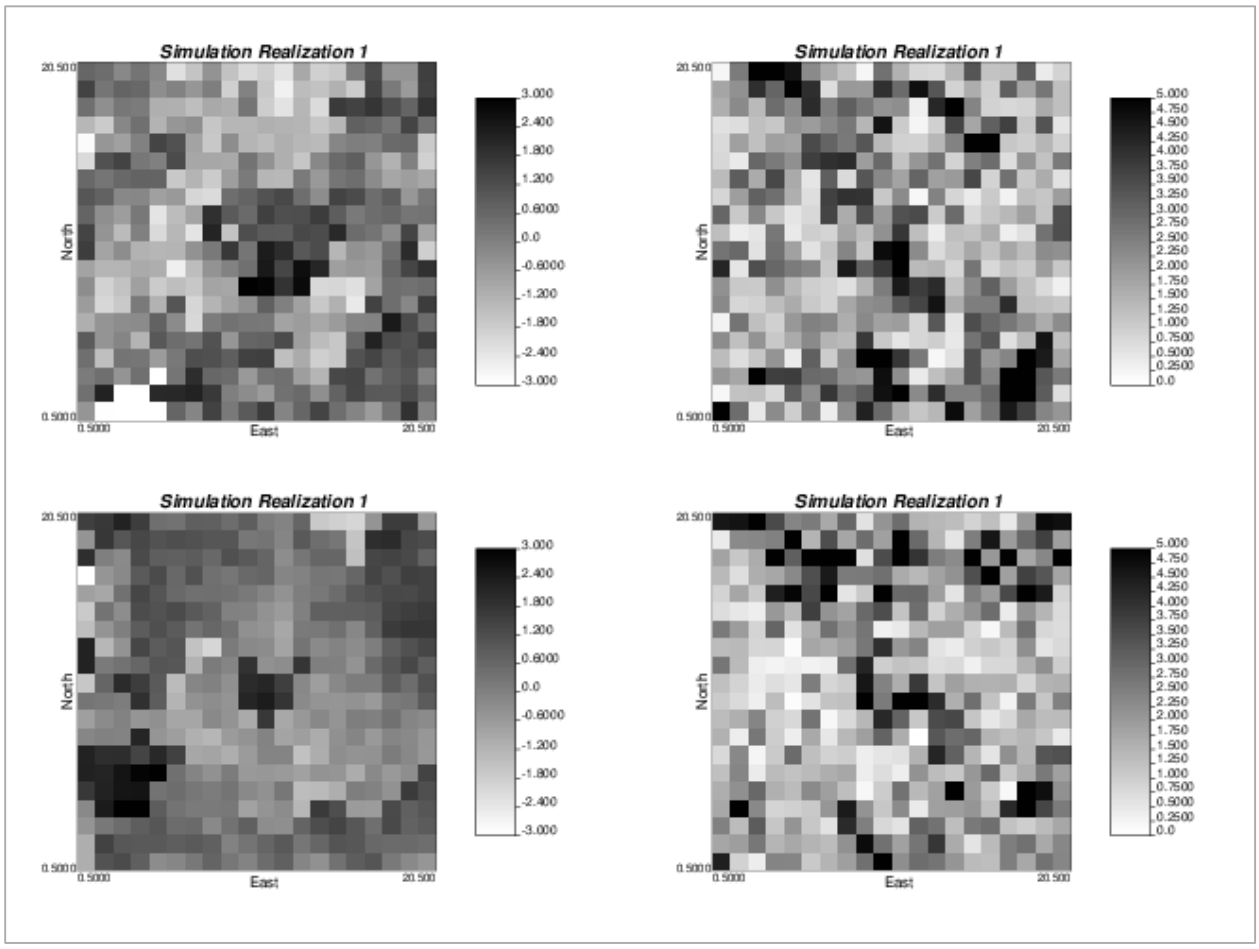


Figure 24: Simulation realization average (E-type) from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

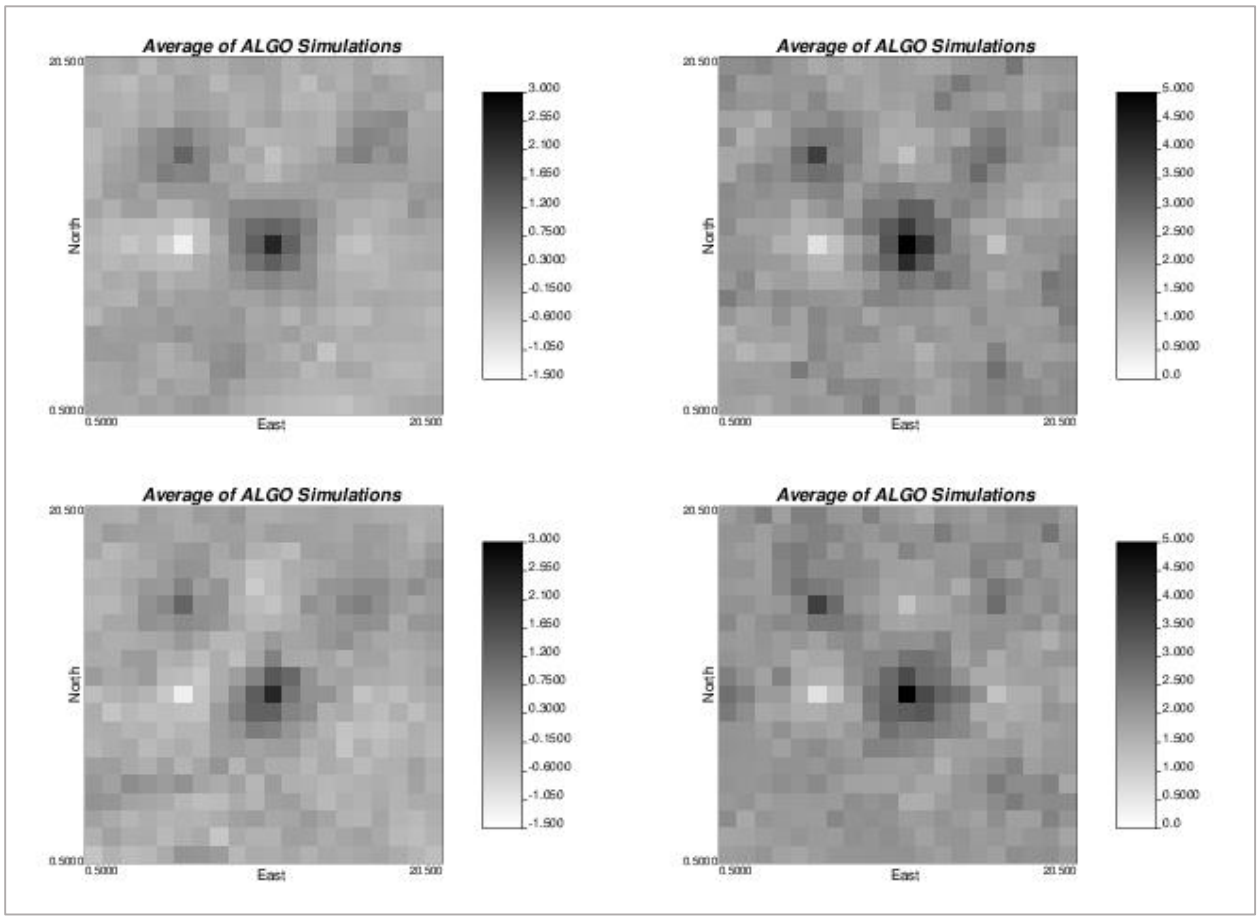


Figure 25: Simulation realization histograms from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

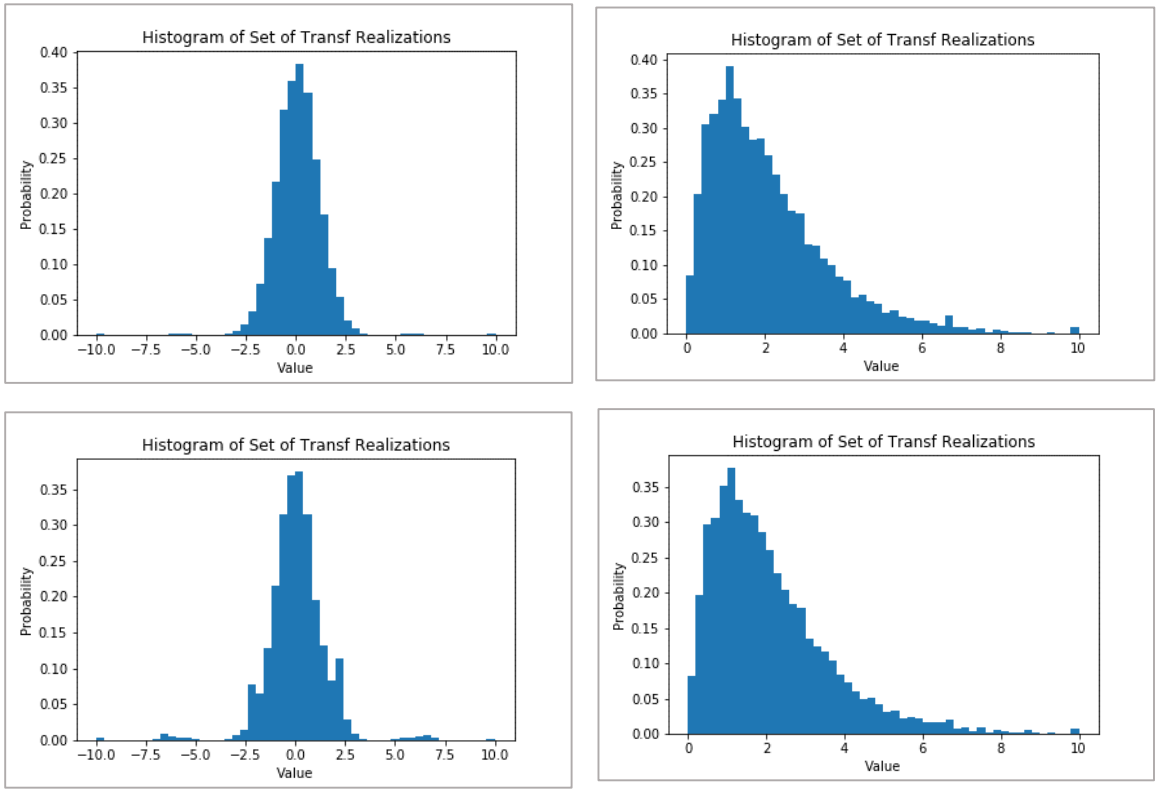


Figure 26: Conditional variance from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

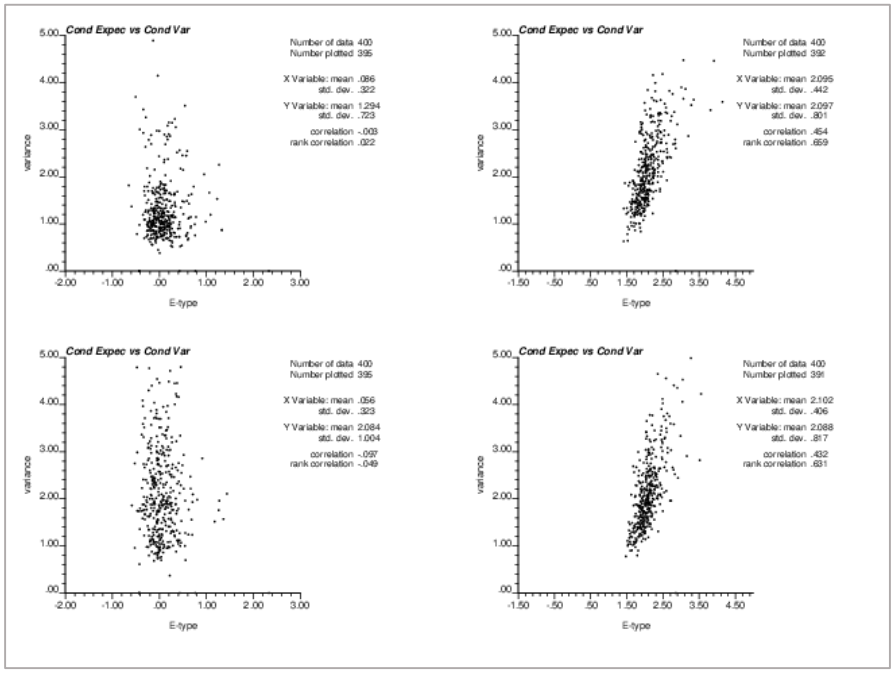


Figure 27: Back transformed average (E-type) of 50 simulations from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

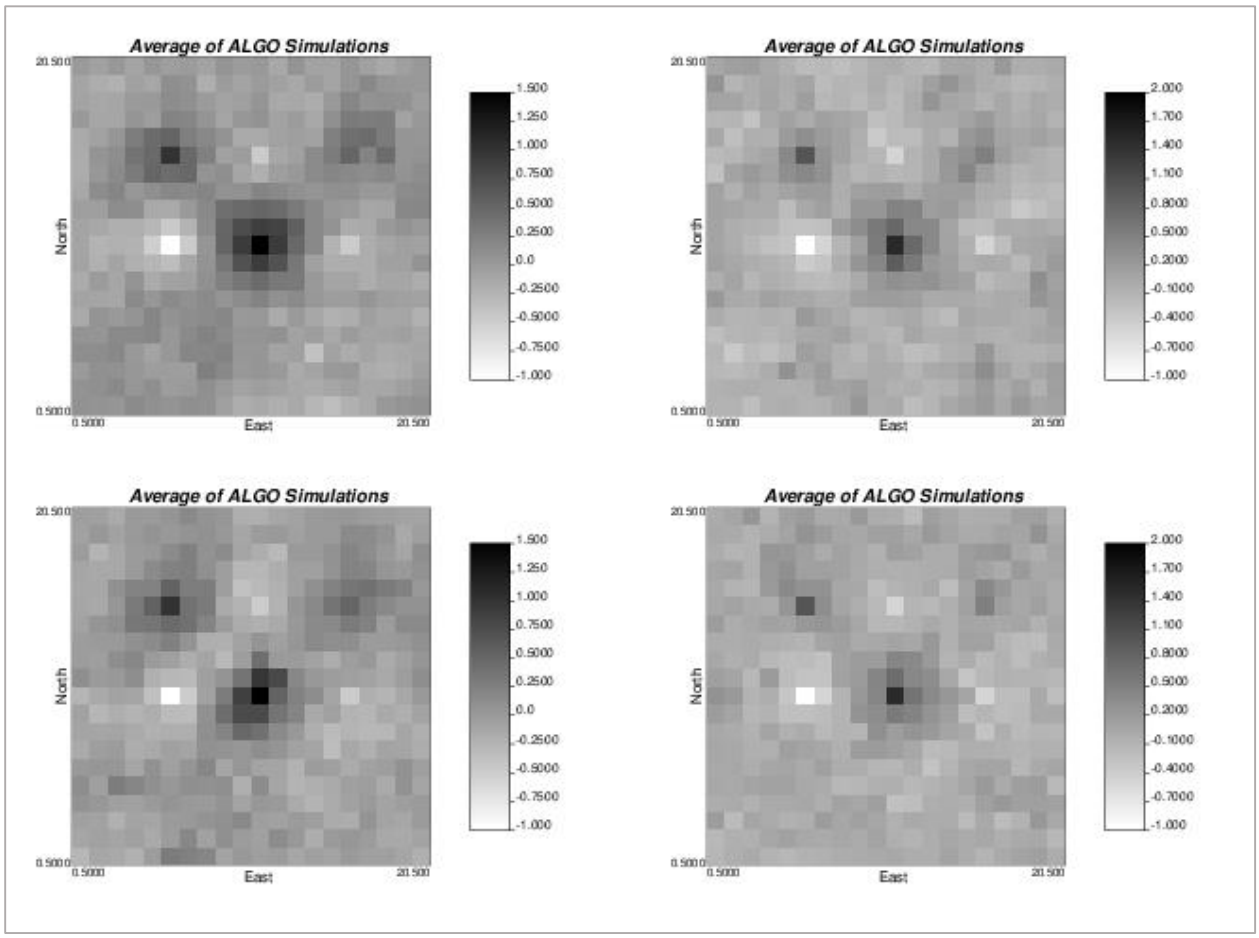


Figure 28: Back transformed conditional variance from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

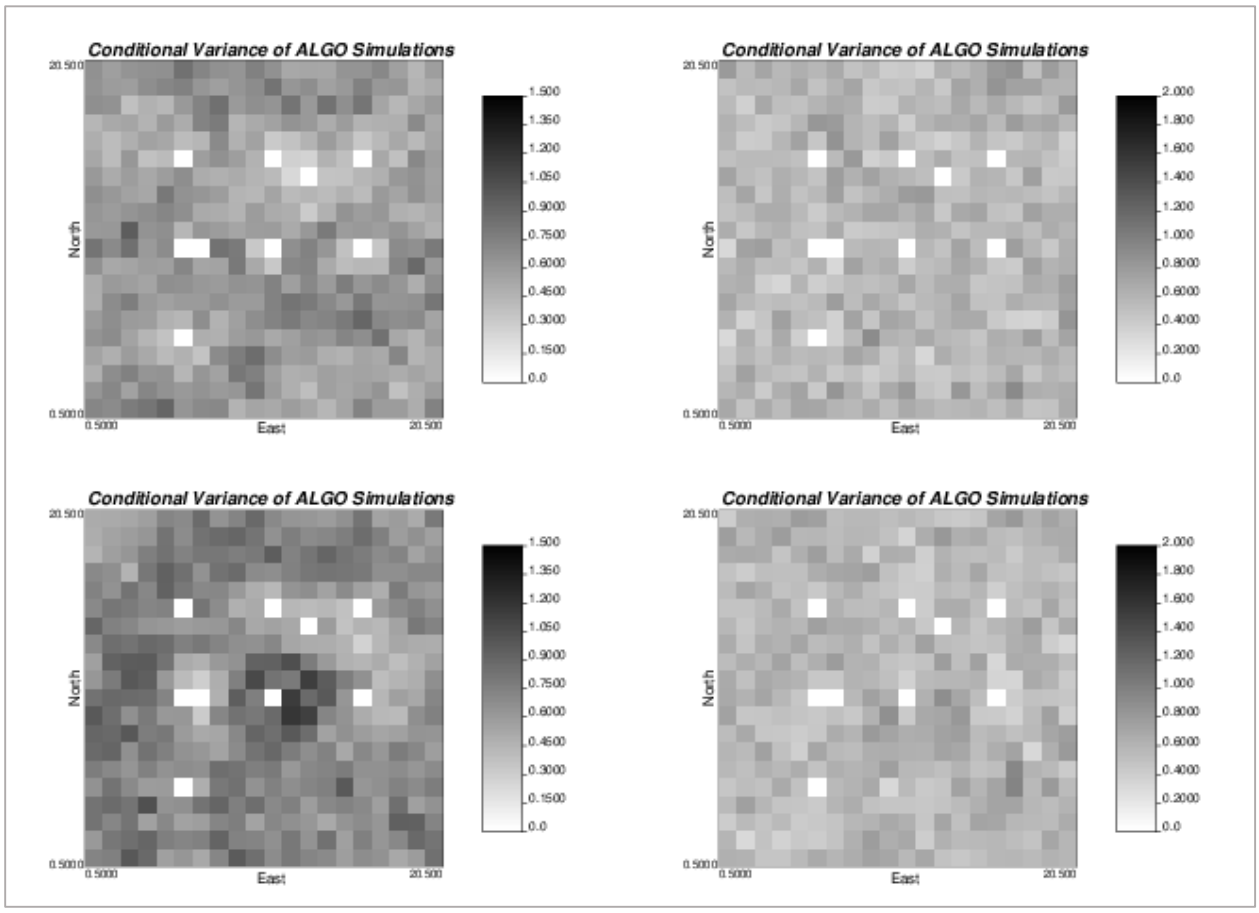
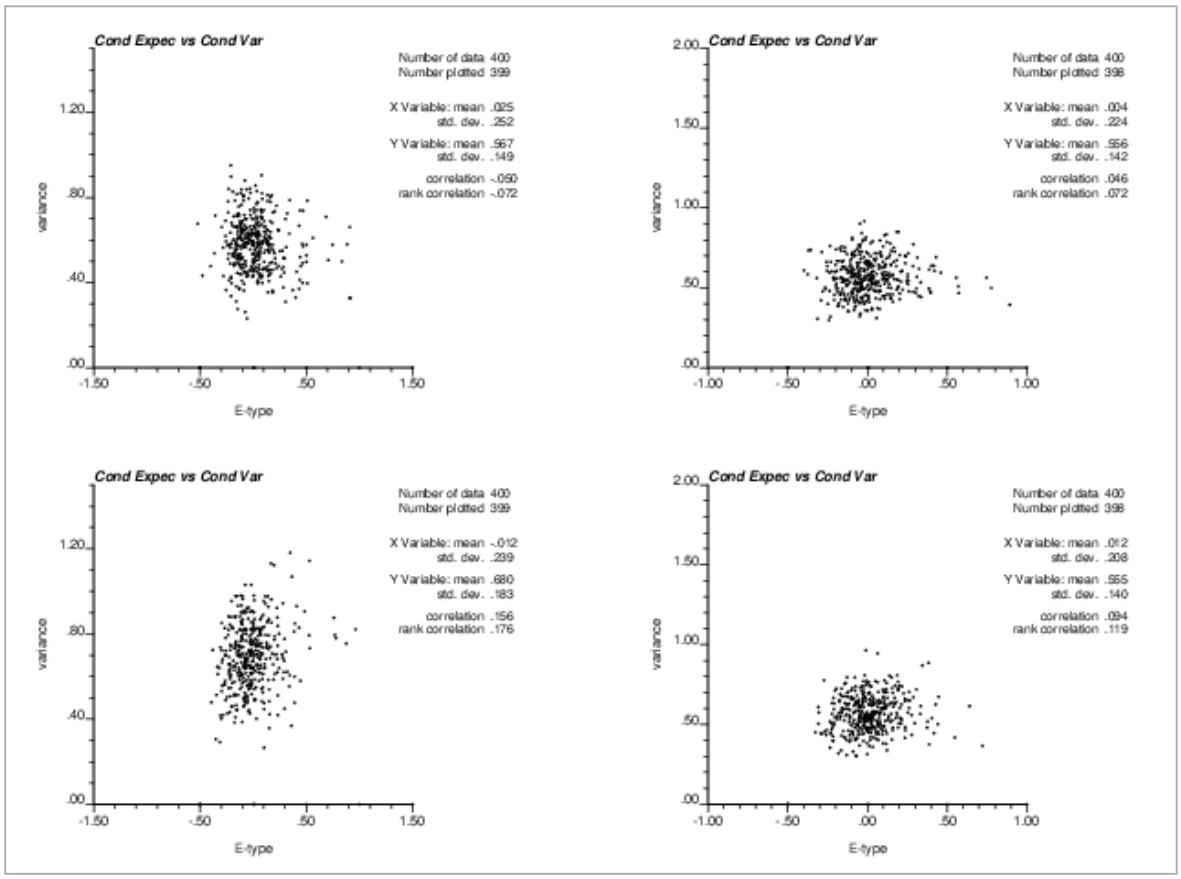


Figure 29: Back transformed conditional variance vs. average (E-Type) from four random function model assumptions; top left is Gaussian diffusive, top right is gamma diffusive, bottom left is Gaussian non diffusive and bottom right is gamma non diffusive.

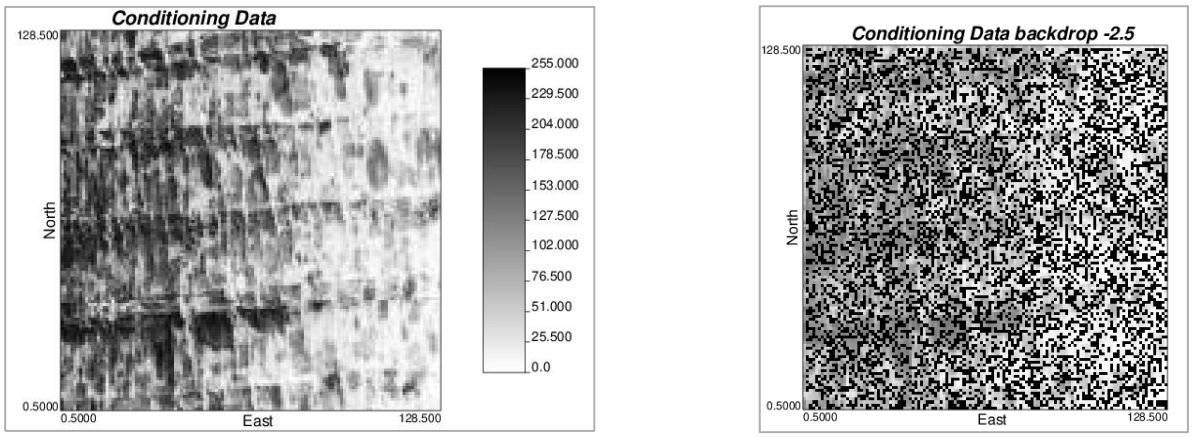


The Gamma model with shape two has a CDF with a lower slope than pure Gaussian, so in general has slightly more variability in simulation. Additionally, conditioning data (in particular extreme conditioning data) bends the local CCDF curve outward creating a more random (variable) simulation draw, vs the Gaussian curve which not only bends outward to accommodate extreme conditioning data but also recenters itself based on the conditioning data. The result is higher conditional variance at higher values for Gamma models as shown in scatterplot of E-Type vs conditional variance. For similar reasons described above, in situations with extreme conditioning data, the local gamma CCDF curve becomes quite variable (i.e., low slope) which reduces the impact of tightening the corners of the local CCDF to account for clustering (relative to a Gaussian local CCDF that translates horizontally to account for extreme conditioning data).

3.5. Illustrative Analysis of a Sampled Data Set

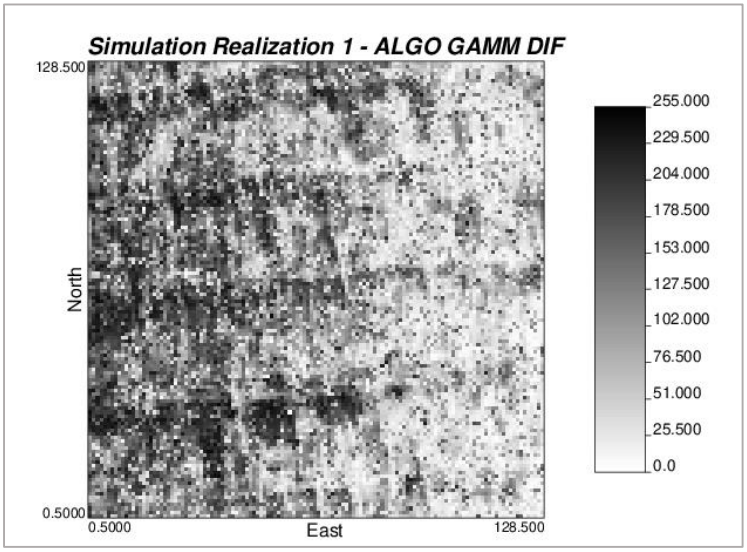
A raw 128 x 128 grey scale image was selected and randomly sampled as shown below in figure 31.

Figure 30: Original Grey Scale Data Set and Randomly Sampled Data Set



A single simulation realization was run using an assumed spherical model with range of 5 and nugget of 0.1. The simulation was run using a gamma model and a destructuration coefficient of 0.00001. The search radius was set to 4 and the minimum points was set to 1.

Figure 31: Single Simulation Realization of Unsampled Values Using SIA Algorithm



4. Conclusions

The SIA algorithm produces intuitive results that deliver expected behavior in both histogram and variogram as well as conditional variance. The algorithm produces distinct results for Gaussian and gamma models and clearly shows the impact of destructuration through clustering of values and sharp boundaries. These initial results suggest that SIA may provide an effective tool to capture a greater range of random function models in simulation and measurement of uncertainty.

5. Acknowledgments

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