

# Simulated Annealing Post Processing for Multiple Point Statistical Reproduction

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## Abstract

*Conventional geostatistical simulation techniques such as sequential indicator simulation (SIS) and truncated Gaussian only account for two point correlations through the variogram. Moreover, realizations from such categorical variable simulation techniques often have systematic biases in the proportions of the categories. The restriction to two point statistics and bias in proportions significantly affect response variables calculated from simulated realizations. Simulated annealing can be used to change a specified starting image to match a set of desired statistics. Using simulated annealing with multiple point statistics to post process simulated realizations can capture realistic geologic features while removing bias in the results.*

*We present an annealing post-processing program and demonstrate how it works. The required multiple point statistics are taken from a training image, which must be deemed representative. The results are shown to visually match the initial features on SIS realizations while simultaneously reproducing the high-order character taken from the training image. The results of a transfer function are shown to be unbiased.*

## Introduction

Stochastic simulation is increasingly used to predict uncertainty in physical models. Typical stochastic methods use two-point statistics such as the variogram to produce the simulated realizations. This process does not always capture all of the relevant spatial structures and arrangements, causing the physical parameters to differ from actual conditions. Recently there has been interest in using multiple-point statistics to improve model characterization. This method could enhance the response characteristics of the models to better match reality.

To account for as many spatial relations as possible, both two-point and multiple-point statistics can be integrated to produce realizations. The method proposed here is to produce an initial realization honouring the two-point statistics, then post-process the realization to reproduce the desired multiple-point characteristics. Sequential indicator simulation (SIS) is the two-point technique chosen for this purpose. Once realizations have been generated with SIS, simulated annealing is the post process selected to honour the multiple-point statistics.

Simulated annealing could be used to generate the images directly; however, there are a number of advantages to working in post-processing mode. First, the statistical fluctuations generated as part of SIS are preserved in the resulting models giving a more realistic measure of uncertainty. Second, the use of a multiple-grid search and long range variogram structure in SIS makes it easier to reproduce long-range features in the final simulated realizations. Finally, the CPU time is very manageable and the features coming from the training image are easily appreciated.

## Sequential Indicator Simulation

Sequential indicator simulation is a geostatistical technique that can be used to characterize variability for models based on categorical variables such as facies types [1,3,5]. The kriged probability of facies  $k$  at location  $\mathbf{u} \in \mathbf{A}$  can be expressed by the equation:

$$[i(\mathbf{u}; k)]_{SK}^* = \sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}; k) \cdot i(\mathbf{u}_{\alpha}; k) + \left[ 1 - \sum_{\alpha=1}^n \lambda_{\alpha}(\mathbf{u}; k) \right] F(k)$$

where  $n$  is the number of data and  $\lambda_{\alpha}(\mathbf{u}; k)$  are the kriging weights, which can be found by solving the SK system:

$$\sum_{\beta=1}^n \lambda_{\beta}(\mathbf{u}; k) \cdot C_I(\mathbf{u}_{\beta} - \mathbf{u}_{\alpha}; k) = C_I(\mathbf{u} - \mathbf{u}_{\alpha}; k) \quad \alpha = 1, \dots, n$$

Once the kriging probabilities are determined, Monte Carlo simulation is performed using the local distribution of uncertainty. The facies corresponding to the random number is assigned to location  $\mathbf{u}$ . Note that the indicator covariance functions  $C_I$  must be inferred for each facies type before the kriging is possible.

SIS reproduces two point statistics based on the covariance function. Since indicator kriging can produce negative probabilities and probabilities that do not sum to 1, the single point statistics are not always reproduced by the realizations. This issue may cause a systematic bias over many realizations and can lead to facies types being over- or under- represented [5].

## Multiple Point Simulated Annealing

Simulated annealing is a method for changing an initial image by *perturbing*<sup>1</sup> it based on some objective function that is used to minimize image's mismatch from the desired characteristics [1]. The starting image can be randomly generated or produced by some stochastic method such as SIS. The objective function could be the difference in the realization variogram from a model variogram, the tonnes above a cutoff, the single point variance, or any other feature that can be quantified and expressed as a function. Usually the objective function is calculated from a *training image*<sup>2</sup> or *control pattern* to ensure that there is at least one realization in which all the desired features are reproduced.

This process of perturbing realizations is analogous to the heating and subsequent cooling of solid metal. Annealing is the process of hot metal cooling and forming new arrangements in its crystalline structure. At higher temperatures the points have more freedom to move to less desirable arrangements. Lower temperatures allow for a crystalline structure at a state of lower energy while giving less freedom in the layout. The objective function is akin to the energy state of the cooling metal. The objective function is allowed to fluctuate up and down slightly at the beginning of the simulation to escape local minima and reach an ultimate optimized value.

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<sup>1</sup> Changing one point at a time.

<sup>2</sup> A realization of facies usually produced from outcrop mapping, zones with large amounts of conditioning data, or from programs that simulate first principles of geologic processes. A training image or control pattern is assumed to be fully representative of the area to be simulated [1].

If a perturbation lowers the objective function it is always accepted and the objective function is adjusted to reflect the change. However, if a perturbation increases the objective function it may be accepted with the probability

$$P_{accept} = e^{\frac{O_{old} - O_{new}}{t}}$$

where  $O_{old}$  is the old objective function,  $O_{new}$  is the new objective function, and  $t$  is the *temperature* of the annealing process. It is analogous to the temperature of solid metal as it is being cooled.

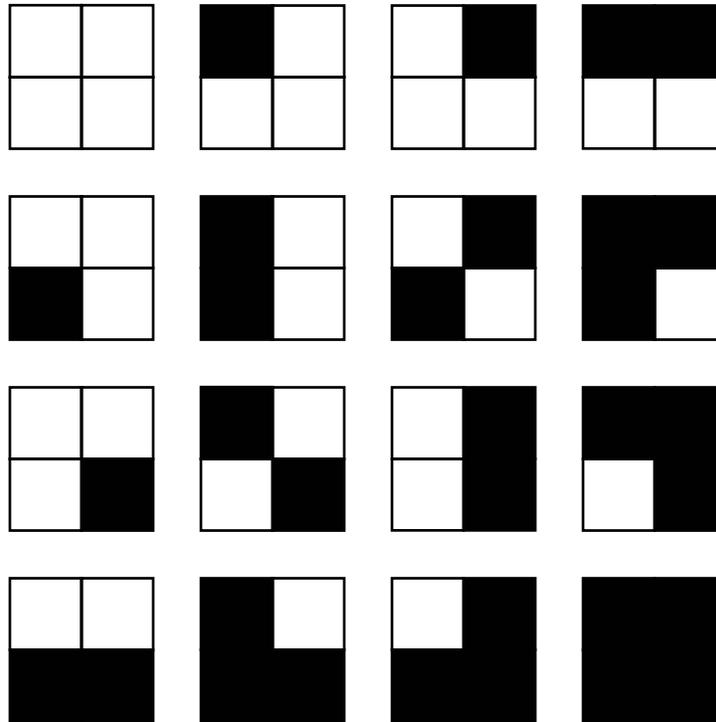
The temperature is typically set high at the start of simulation to allow more undesirable perturbations. As the temperature is lowered fewer increases will be accepted. Permitting some small increases in the objective function allows the simulation to “escape” from local minima to reach lower values and therefore more closely represent the training image. The initial temperature and the rate at which it is decreased is called the *annealing schedule*. This schedule is described by these parameters:

- $t_0$         The initial temperature, which usually ranges from 0.1 for a random initial image or  $10^{-5}$  for post processing.
- $\lambda$         A reduction factor for the temperature,  $0 < \lambda < 1$ . Usually set to 0.1.
- $K_{max}$       The maximum number of perturbations allowed at any single temperature; once  $K_{max}$  perturbations have been performed  $t$  is multiplied by  $\lambda$ . This is typically on the order of 25-100 times the number of grid nodes.
- $K_{accept}$     The maximum number of perturbations to accept at any single temperature; if  $K_{accept}$  perturbations are accepted  $t$  is multiplied by  $\lambda$ . Usually 5-10 times the number of grid nodes.
- $S$          A stopping number. If  $K_{max}$  is reached  $S$  times the simulation is stopped. Typically this is 2 or 3.
- $\Delta O$       The target objective function. It is set very low (i.e.  $10^{-21}$ ) but is not reached before the simulation stops.

Simulated annealing is not constrained to representing only one or two types of functions; multipoint statistics can be combined with two point and single point statistics to make the simulation truly representative of all the required properties of the training image. Multiple point statistics are useful because they can capture many significant and complex features of an image without being very complex in and of themselves. One type of multiple point statistic is the arrangement of points in a square; for four points and two facies types this is shown in figure 1. This kind of statistic has  $K^N$  classes, where  $K$  is the number of facies types and  $N$  is the number of points used for characterization. The points need not be arranged in a square; any pattern could be used to better characterize the geology of the particular case being considered.

It is apparent that for large numbers of facies and/or points this statistic can quickly have many classes. If the distribution among these classes is to be inferred from a training image then there should preferably be at least a hundred points in the training image for every class to ensure even the rarest combinations of facies are properly represented. For greater numbers of facies types this could lead to excessively large training images. Smaller control patterns might be acceptable,

but may not fully characterize all possible facies arrangements; this must be considered for each case based on the geology present.



**Figure 1:** A four-point arrangement for multiple point statistics with two facies types, represented by black and white. This arrangement has  $2^4 = 16$  classes. [1]

### Methodology for Post Processing

Proportions of the different facies as well as variograms for the  $K$  different facies types are needed to perform SIS. These can be found by user iteration or an automatic variogram fit program, but the quality of the variograms will reflect on the SIS output. At least one variogram per facies type is needed. Cross-variograms can be calculated; however, with a large number of facies this would greatly increase the time and effort to be put into the simulation, not to mention the effort in the inference of variograms.

Once the two point statistics have been inferred, many realizations of the  $n$  points can be generated using `sisim` [2]. Statistics for these realizations, such as the proportion of each facies type, can be calculated and compared to the training image.

To correct the single point histogram for the SIS realizations, the program `trans` [2,4] may be used. This forces the facies distributions to match the training image and will correct a systematic bias in the simulations. Some banding and artifacting may be introduced by this.

Once SIS realizations are generated, they can be taken as initial images and perturbed using simulated annealing to generate post processed realizations. To preserve the long range characteristics of the SIS, a low starting temperature should be used for the annealing. A high temperature would force too many undesirable perturbations to be accepted and cause the SIS

realization to be completely rearranged by too many perturbations; this gives the same results as starting the simulated annealing with a random image.

The simulated annealing process follows a random path around the initial image while ensuring every point has an opportunity to be perturbed in each pass. If conditioning data is being used for simulated annealing, a spiral path starting at the data and moving away should be used; for large simulations this significantly increases the process time. By performing SIS first and then post processing, the conditioning data is taken into account without having to develop this spiral path.

### Program: AFS (Annealing Facies Simulation)

The program `afs` [1] follows standard GSLIB conventions. For this program one source code file and one include file are required: `afs.for` and `afs.inc`. The include file contains most of the parameter and variable definitions. This allows the easy modification of the program for use of larger and more complex simulations. The parameters required for the program are:

```

Line  START OF PARAMETERS:
  1      100                                \Number of simulations
  2      200  100  1  5                     \nx, ny, nz, nr (input classes)
  3      1006512                             \Random number seed
  4      ppanneal.out                       \Output File for realization(s)
  5      ppanneal.sta                       \Output File for statistics
  6      ppanneal.dbg                       \Output File for Debugging
  7      ppanneal.tmp                       \Output File for Debugging
  8      3  1000  100                       \Debug lev, Reporting, Max pert

  9      3                                  \starting image option
 10     image.out                          \ starting image file
 11     nocond.dat                         \Conditioning data file
 12     1  2  3  4                         \ ixl, iyl, izl, ivrl
 13     2  1                               \perturbation option and increm
 14     1.0e-21                            \ target objective function
 15     0.000001  0.1  25  5  3           \ SA Schedule:t0,lam,ka,k,e

 16     train.dat                          \Training Image File
 17     200  100  1                         \nx, ny, nz

 18     8  10                              \TWO POINT HIST: ndir, cwt
 19     0.0  0.0  0.0  1.0  1.0          \ angl,ang2,ang3,anis1,anis2:

 20     1  0                               \HIGH ORDER HISTOGRAM: ncube,nir
 21     5                                  \ number of points
 22     0  0  0                            \ point i : ix, iy, iz
 23     1  0  0                            \ point i : ix, iy, iz
 24     2  0  0                            \ point i : ix, iy, iz
 25     3  0  0                            \ point i : ix, iy, iz
 26     4  0  0                            \ point i : ix, iy, iz

```

**Line 1** specifies the number of simulations to be performed. The dimensions of the area to be simulated and the number of facies are on **Line 2**. **Line 3** contains the random number seed. **Line 4** contains the output file the program will write to. **Lines 5** through **7** are the debugging and statistics files that will be created. **Line 8** is the level for the debugging; 0 is no debugging, 10 is the maximum level.

**Line 9** is the option for the starting image: 1 uses a randomly generated image honouring the univariate statistics, 2 uses a single starting image for all realizations, 3 uses each realization from the image file once. **Line 10** contains the name of the image file to be used. If conditioning data is to be used, the conditioning file is outlined on **Line 11** and **Line 12**. **Line 13** is the option for perturbation: 1 uses an automatic annealing schedule; 2 uses the user-defined parameters contained on **Line 15**. **Line 14** has the target objective function.

The training image file is specified on **Line 16** and **Line 17**. On **Line 18** and **Line 19** are the parameters for a histogram of two point relations. `afs` uses a limited number of these relations to ensure the training image's essence is retained. The parameter `ndir` is the number of two-point relations that will be used; `cwt` is a weighting for how important the two point histogram will be considered in the objective function. The information on **Line 19** is the definition of the search ellipsoid for the two point statistics.

The definition of the multiple point statistics is on **Lines 20** through the end of the file. The parameter `ncube` is the number of lags to look in each direction for the multiple point histogram; 1 means a single lag or 4 points in 2D, 8 points in 3D; 2 means two lags which is 9 points in 2D and 27 in 3D; and so on. The `nir` parameter is the number of different shapes to use other than a square/cube: **Line 21** is the number of points to use for one of these shapes and **Lines 21 to 26** are the lags for each point. For this paper `nir` is 0 so only a square/cube multiple point statistic will be used.

### Example

Figure 2 shows a training image and two SIS realizations before and after transforming and annealing. The training image is 200 by 100 points and has 5 facies classes [1]:

1. A background grey facies
2. Light blue ellipsoids
3. Dark blue short horizontal bands that occur only within the ellipsoids
4. A red facies that always and only appears on top of the ellipsoids
5. Green diagonal banding

100 realizations were simulated then post processed using `afs`. A four point square statistic was used, giving  $5^4 = 625$  different classes. Eight two point lags were used in the program. This configuration took 66:54 to perform 100 realizations on a 1.8GHz Pentium 4 with 512MB of RAM for an average of 40.14s per realization. For comparison the 100 SIS realizations took 6:08 for an average of 3.68s per realization. The realizations were also post process-transformed separately to fix the single point histogram and provide a better basis for comparison.

The SIS was performed using these variograms for each facies type:

$$\text{Rock code 1 (Grey):} \quad \gamma(h) = 0.067 + 0.078 \begin{matrix} Sph(h) \\ h \text{ max}=50.1 \\ h \text{ min}=7.97 \\ ang=90 \end{matrix} + 0.085 \begin{matrix} Sph(h) \\ h \text{ max}=50.2 \\ h \text{ min}=45.7 \\ ang=90 \end{matrix}$$

$$\text{Rock code 2 (Light blue):} \quad \gamma(h) = 0.047 + 0.055 \begin{matrix} Sph(h) \\ h \text{ max}=51.3 \\ h \text{ min}=7.23 \\ ang=90 \end{matrix} + 0.061 \begin{matrix} Sph(h) \\ h \text{ max}=52.7 \\ h \text{ min}=77.9 \\ ang=90 \end{matrix}$$

Rock code 3 (Dark blue):  $\gamma(h) = 0.019 + 0.013 \underset{\substack{h \text{ max}=19.5 \\ h \text{ min}=0.216 \\ \text{ang}=90}}{\text{Exp}}(h) + 0.012 \underset{\substack{h \text{ max}=24.1 \\ h \text{ min}=48.1 \\ \text{ang}=90}}{\text{Exp}}(h)$

Rock code 4 (Red):  $\gamma(h) = 0.009 + 0.005 \underset{\substack{h \text{ max}=23.7 \\ h \text{ min}=0.018 \\ \text{ang}=90}}{\text{Sph}}(h) + 0.006 \underset{\substack{h \text{ max}=23.7 \\ h \text{ min}=0.220 \\ \text{ang}=90}}{\text{Exp}}(h)$

Rock code 5 (Green):  $\gamma(h) = 0.055 \underset{\substack{h \text{ max}=35.2 \\ h \text{ min}=0.226 \\ \text{ang}=135}}{\text{Sph}}(h) + 0.022 \underset{\substack{h \text{ max}=35.2 \\ h \text{ min}=0.453 \\ \text{ang}=135}}{\text{Sph}}(h)$

Looking at figure 2 it can be seen that while the SIS captured the long range essence of each facies type, the relations between them and the short range features were not reproduced. The histograms in figure 3 show that SIS did not properly reproduce the histogram of single point statistics from the training image. In particular facies 5 (green) was under-represented systematically among all realizations. Figure 3 shows the histograms taken over all 100 realizations, not just those pictured in figure 2.

The transformed SIS images match the single point histogram almost exactly, even closer than the annealed-post processed realizations. However, there is some banding and artifacts in the resulting image inherent to the transformation.

To better investigate the practicality of post processing, each facies type was assigned a grade and then every realization was block averaged to test the overall response variability of the methods. The grades assigned were:

- Grey / Rock Code 1: 0 – Host rock
- Light blue / Rock code 2: 2 – Low grade mineralized bodies
- Dark blue / Rock code 3: 5 – Enhanced mineralized zones
- Red / Rock code 4: 10 – Extra enhanced mineralized
- Green / Rock code 5: 20 – Heavily mineralized veins

Every realization for each process was block averaged and all realizations were considered for the analysis. The block averages were taken for a 5 by 5 square area, resulting in 40 squares by 20 squares over the entire area. Grade maps of the training image and two realizations for each process are shown in figure 4. The realizations shown are the same two used in figure 2. Histograms for the block averages over all realizations are shown in figure 5. It should be noticed that the SIS histogram has too low of an average grade due to a shortage of facies 5; the transformed realizations match the average grade the closest out of any process but do not match the distribution as well as the post process annealing. The transform also leads to an excess of very high grade blocks.

Grade-tonnage curves calculated across all realizations for each process are shown in figure 6. In reference to the training image curve, the SIS realizations systematically take too little material as ore and consequently end up with too low of a grade. This is mainly due to the under-representation of facies 5 (green), which has the highest grade.

Once the SIS images have been transformed to match the single point histogram of the training image there is not longer a bias in the amount of ore squares present. However, he transformed

realizations do not match the reference values for ore and grade because the spatial distribution of the high and low grade material is not correct. At low cutoff grades the wide dispersion of lower grade ore squares forces too much material to be considered ore at too low of a grade. At higher cutoff grades the bunching of the highest grade squares causes too little material to be taken as ore at too high of a grade.

Post processing by simulated annealing of all realizations matches the reference grade-tonnage curve very closely at all cutoffs. This is because the single point histogram from the training image is matched closely and the spatial characteristics are honoured.

Figure 6 shows the histograms from each process for average grade and proportion of ore for each realization using a cutoff grade of 3.0 per unit square. The cutoff grade is higher than that for the lowest grade ore (facies 2, light blue). Calculated from the training image, the reference proportion of ore is 0.403 and the reference grade is 4.700. Because significant amounts of ore may be contained in the waste blocks, the SIS realizations have too low of a grade at 4.214 and take too little material as ore at a proportion of 0.236 because of the single point bias. When the bias is corrected by `trans` there is the correct amount of high grade points; however, the distribution over the area is not correct so not enough material is considered ore (0.341) and the grade is too high (4.843). This is because of the grouping of high grade values too closely together. Post processing by annealing has an average ore grade of 4.663 while taking 0.399 of the material as ore. This is the closest to the reference values.

## Conclusions

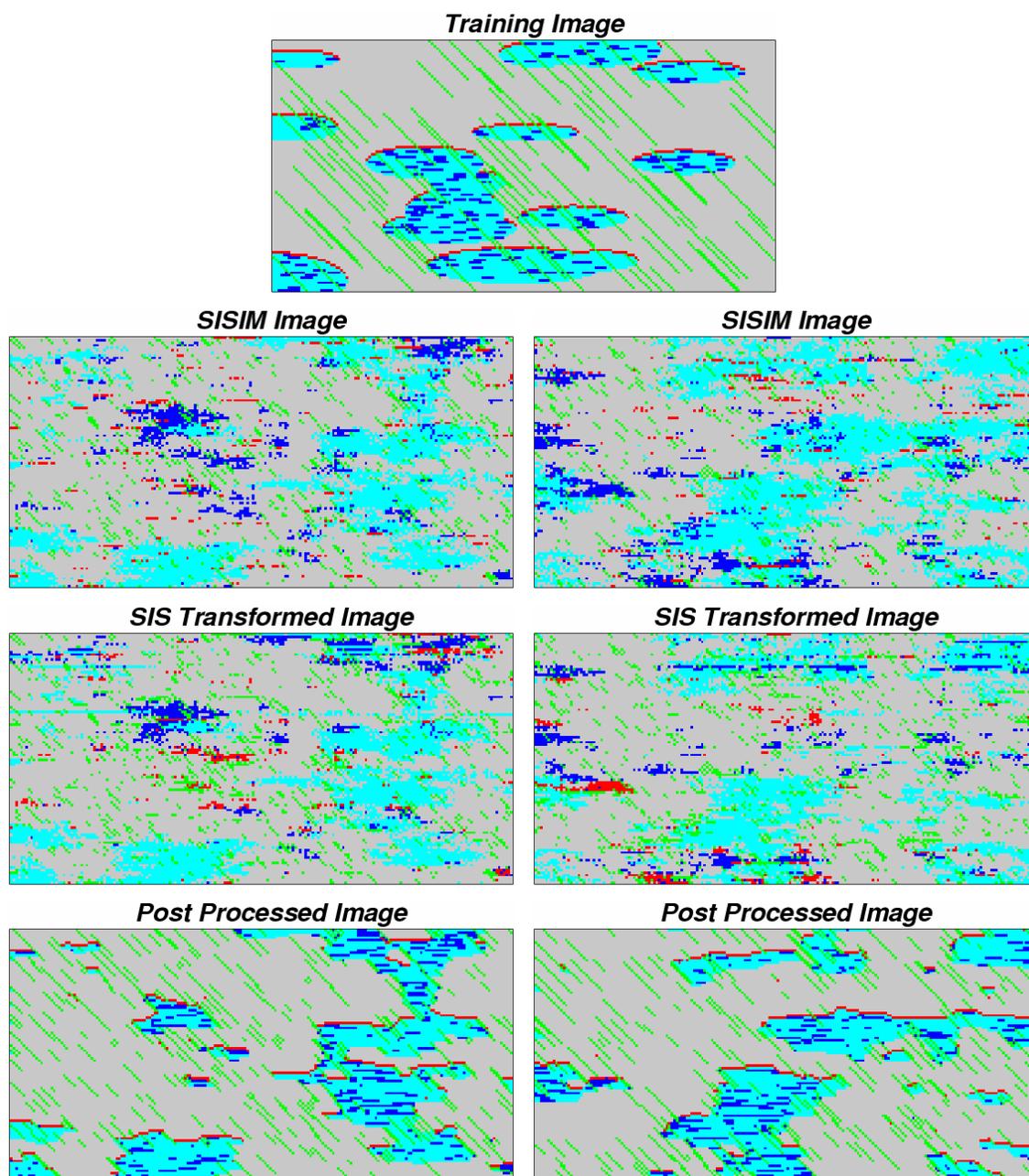
Simulated annealing is a powerful post processing tool. The processing time is significantly more than SIS, but it is not prohibitive and the response results are much closer to the reference. Simulated annealing could also be used to post process the results of any other simulation technique to develop more robust realizations.

The assumption of stationarity means that a representative training image is important for this technique to be effective. The range of responses for each realization also seems to be too confined to being close to that of the training image. Adding variability in the statistics from realization to realization or making a much larger training image than the area being simulated to improve the distribution of facies arrangements could potentially fix this issue.

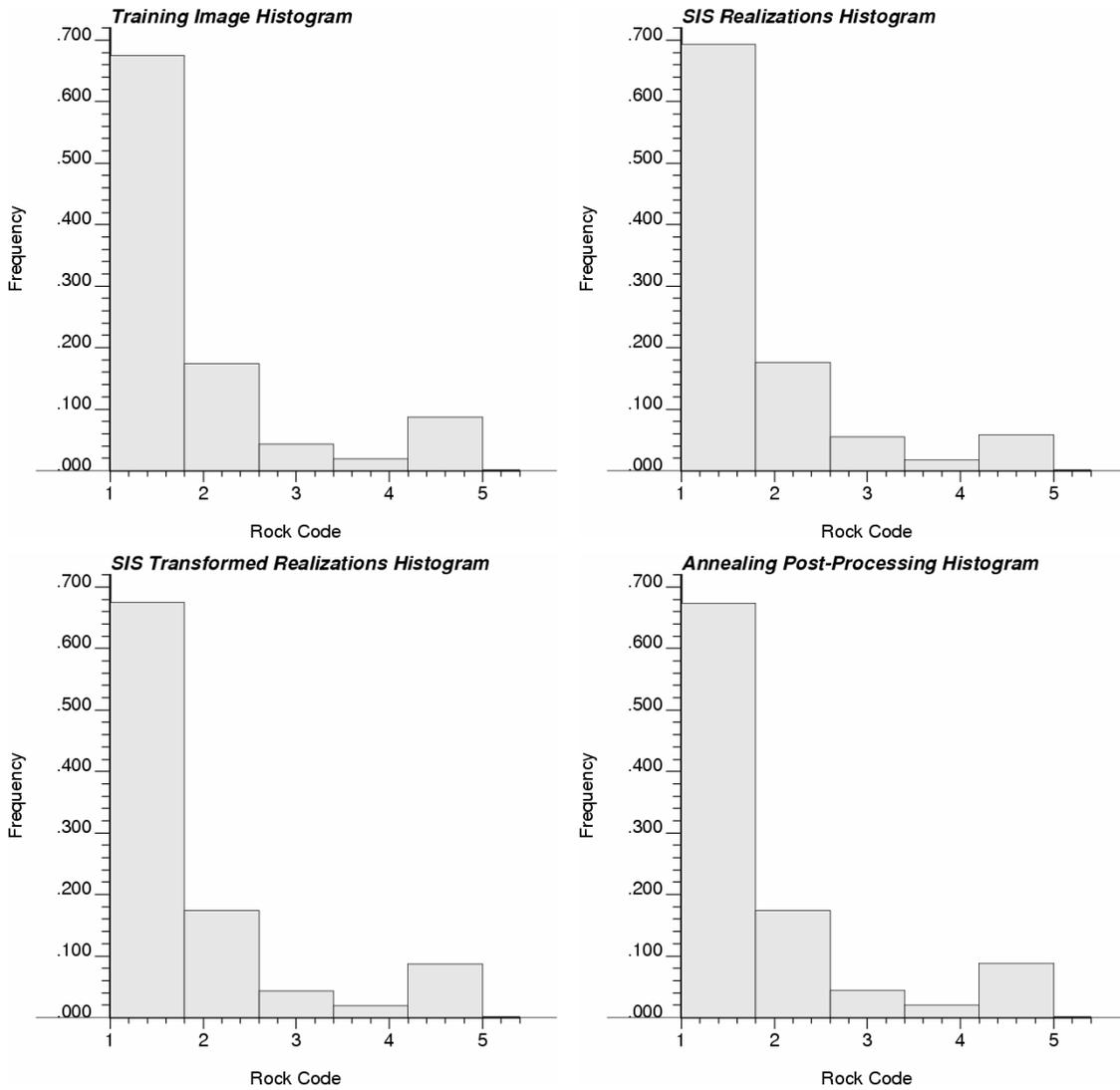
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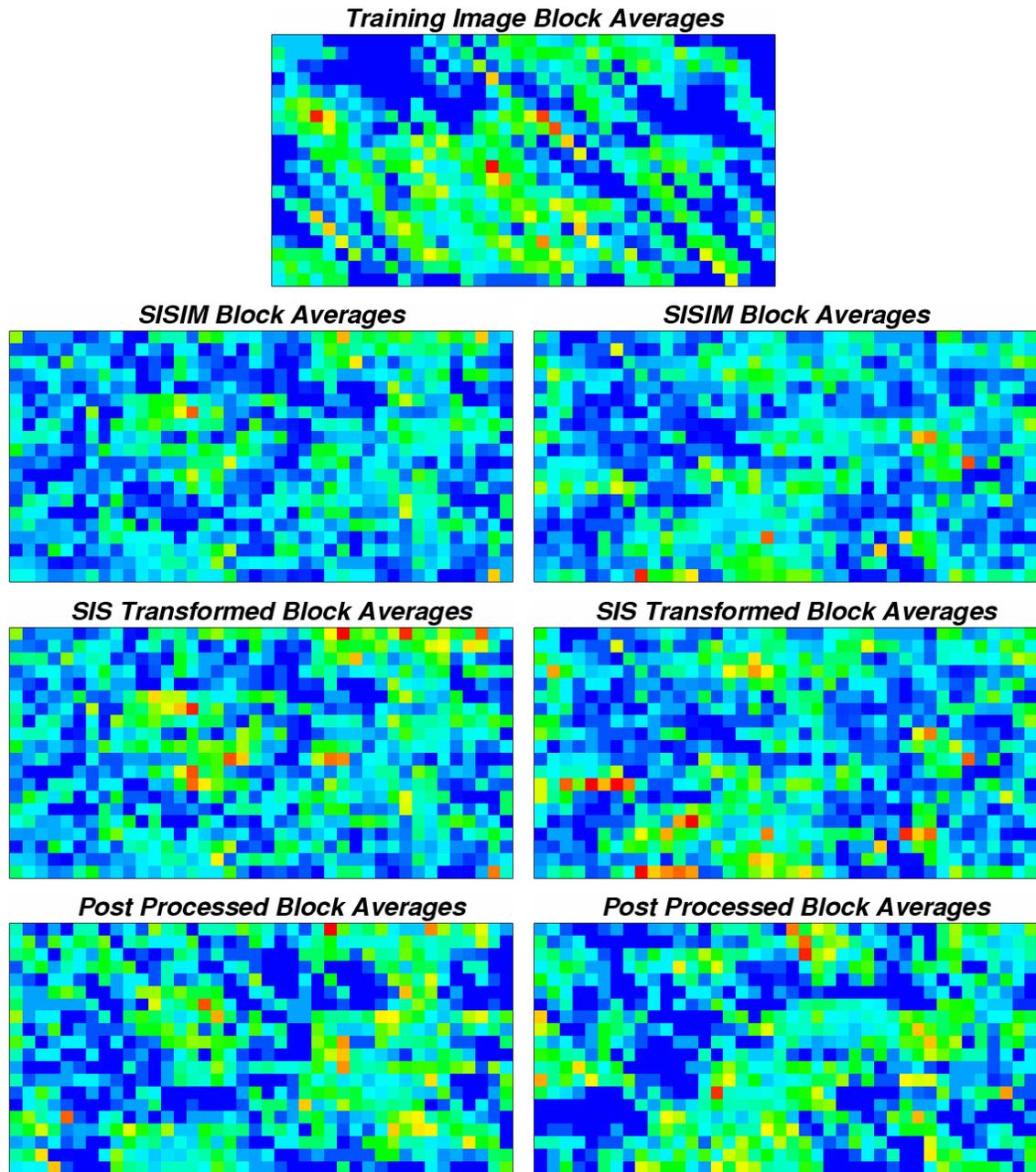
6. J.M. Ortiz. Selected aspects of multiple-point statistics. In *Centre for Computational Geostatistics*, volume 5, Edmonton, AB, 2003.
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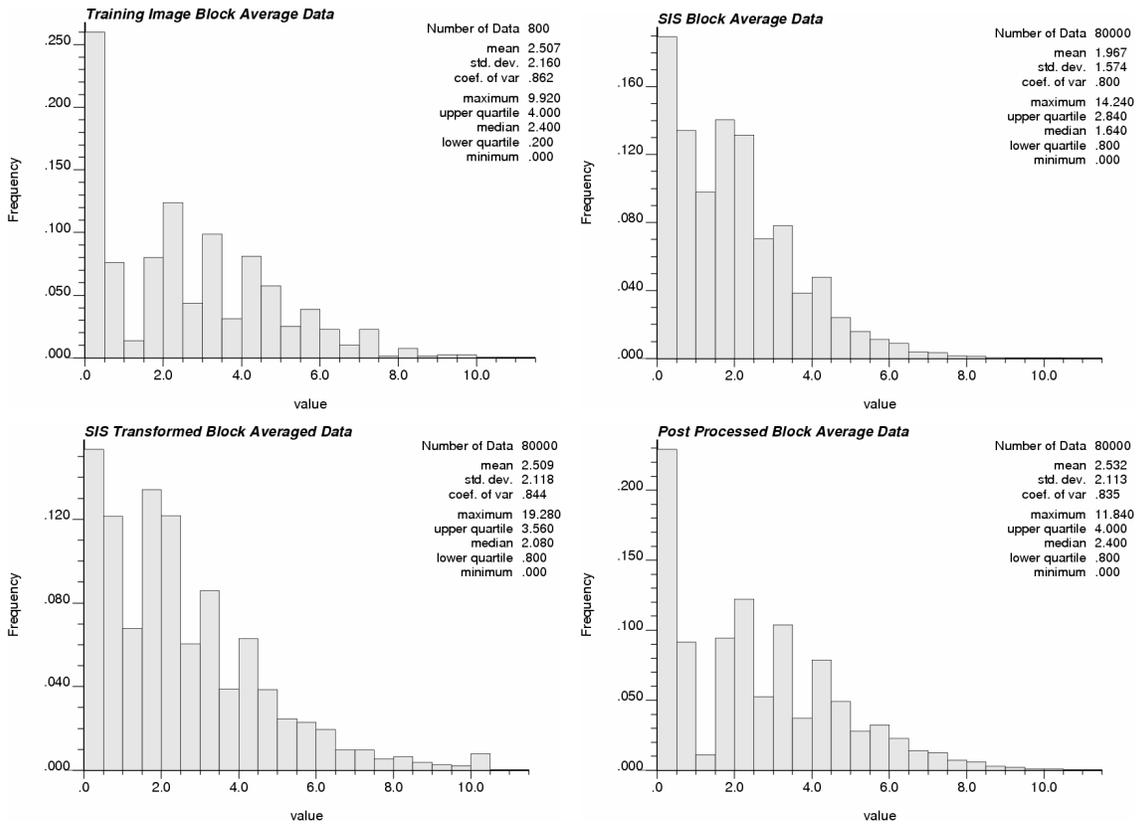
**Figure 2:** Top: the training image used to generate statistics for simulation 1. Lower six images: two realizations from `sisim` before and after post processing. The top images are SIS realizations; the middle are the same realizations transformed to fix the single point histogram; the bottom images are post processed with multiple point simulated annealing.



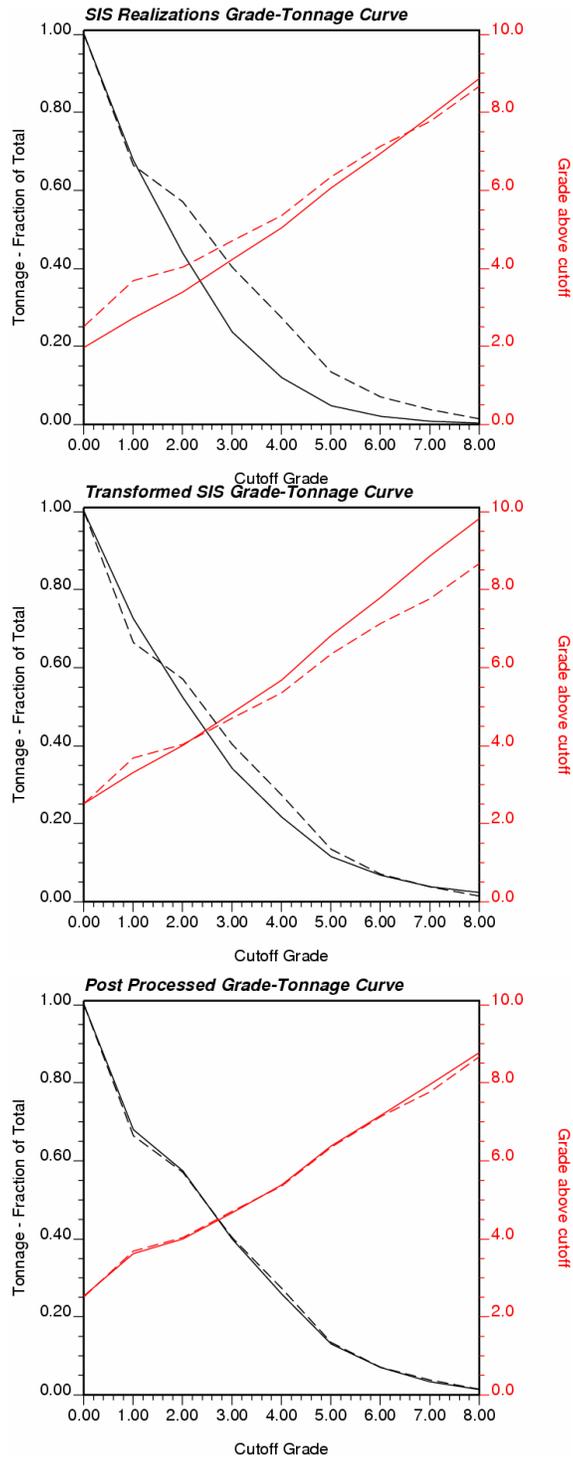
**Figure 3:** Single point distributions of the 5 facies classes in all different cases from figure 2. The training image is at the upper left, all SIS realizations the upper right, all of the transformed SIS realizations the lower left and all annealing post processed realizations the lower right. Notice how the SIS realizations have a slightly skewed distribution, particularly for facies 5.



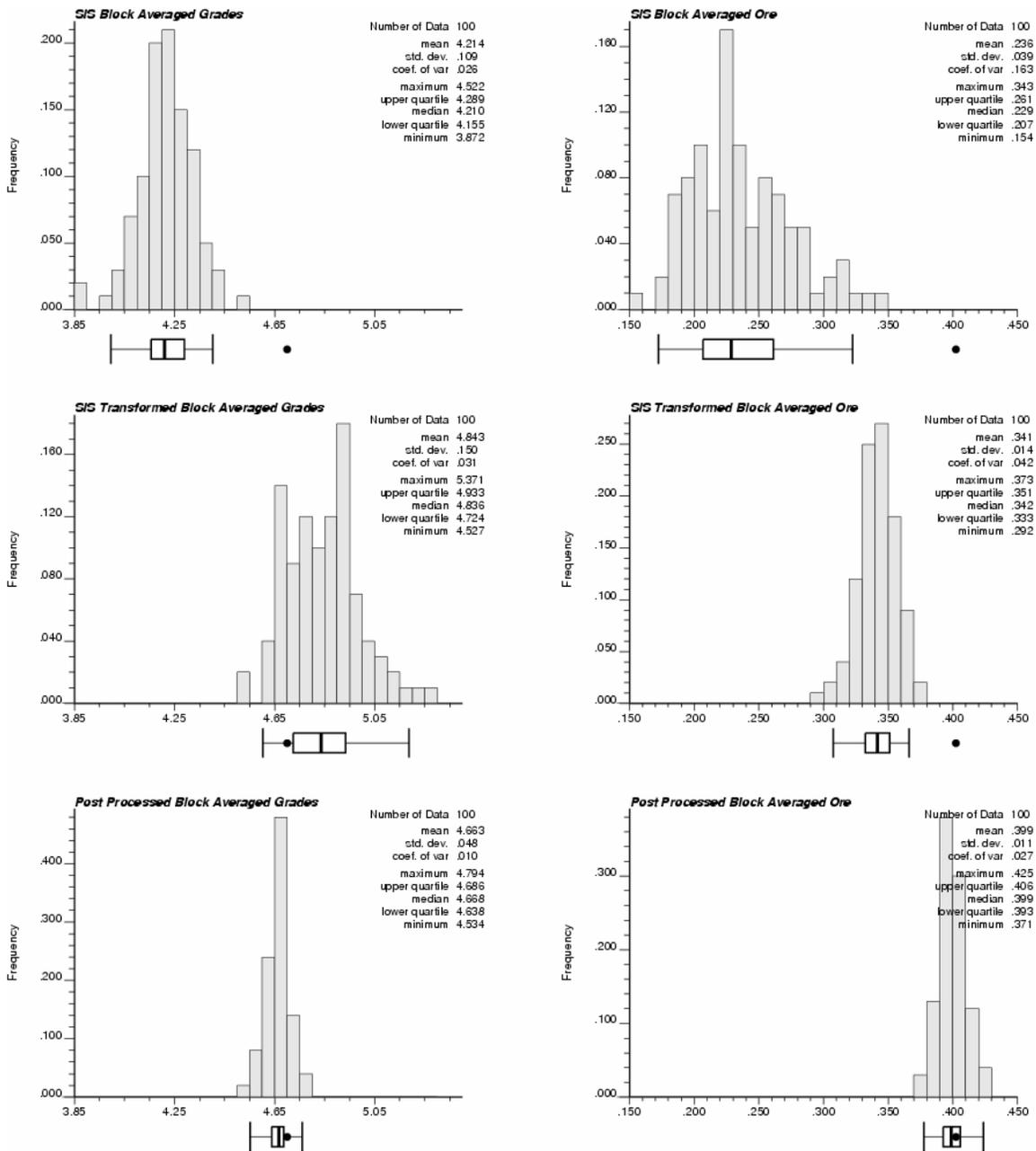
**Figure 4:** Grade block average values for the training image (top) and the same realizations of all processes shown in Figure 2. The blocks are 5 squares by 5 squares. The highest grades (greater than 10 per unit square) are red; the lowest grades (approaching zero) are blue.



**Figure 5:** Histograms for the block averaged grades among all realizations. Upper left: training image histogram. Upper right: SIS output. Lower left: SIS transformed output. Lower right: SIS realizations after being post processed by simulated annealing.



**Figure 6:** Grade-tonnage curves for each process. Top: SIS. Middle: transformed SIS. Bottom: annealing post processed. The dotted lines are the grade-tonnage curves for the training image. In black is the proportion of material taken as ore; in red is the average grade of ore. The grade is taken per unit square.



**Figure 7:** Histograms of all realizations showing average ore grade (left) and proportion of material considered ore (right) using a cutoff grade of 3.0 per unit square. The SIS realizations are at the top; the corrected-histogram SIS realizations in the middle; and the realizations post processed by simulated annealing at the bottom. Reference values inferred from the training image are shown as dots under each scale.