

ASSESSING DIRECT AND CONVENTIONAL BLOCK-SUPPORT CO-SIMULATION FOR IMPROVED MULTIVARIATE TAILINGS MODELING

by

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ORIGINALITY STATEMENT

I, Zhuldyz Koyanbayeva, hereby declare that this submission is my own work and to the best of my knowledge it contains no materials previously published or written by another person, or substantial proportions of material which have been accepted for the award of any other degree or diploma at Nazarbayev University or any other educational institution, except where due acknowledgement is made in the thesis.

Any contribution made to the research by others, with whom I have worked at NU or elsewhere is explicitly acknowledged in the thesis.

I also declare that the intellectual content of this thesis is the product of my own work, except to the extent that assistance from others in the project's design and conception or in style, presentation and linguistic expression is acknowledged.

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ABSTRACT

This thesis compares two multivariate block-support co-simulation workflows applied to mine tailings, both implemented using the BLOCKSGCOSIM algorithm in MATLAB. The case study focuses on the Haveri Au-Cu tailings storage facility in Finland, where copper (Cu), silver (Ag), iron (Fe), sulfur (S), and bulk density are modeled jointly to evaluate reprocessing potential and environmental risk. The primary deposit was mined mainly for copper and gold.

Because grades are ratio variables and therefore non-additive, they cannot be directly averaged across space when density varies. To address this, each grade is transformed into a density-weighted variable prior to simulation. These transformed variables are simulated in the Gaussian domain, and block grades are later reconstructed using simulated density. This ensures that all results remain consistent under block aggregation.

Two workflows are examined. In the conventional approach, co-simulation is performed on a fine point-support grid, and results are averaged to block support using an external BLKAVG step. In the direct approach, simulation is carried out directly at block support, with internal discretization used to approximate block averages during the simulation itself. Both workflows use the same dataset, variogram models, and block geometry, so differences in results reflect only how support is handled.

The comparison focuses on three aspects: (i) reproduction of block-scale statistics, including means, variances, and quantiles; (ii) preservation of multivariate relationships through correlation structures and cross-plots; and (iii) spatial behavior of central tendency and uncertainty, assessed using E-type maps and dispersion measures. Computational performance is evaluated through CPU time and output size.

Results show that both workflows reproduce block-scale statistics and multivariate relationships with similar accuracy. However, the direct block-support approach requires substantially less computation time and storage. This reduction occurs because internal discretization eliminates the need to simulate and store fine-scale nodes. The findings indicate that direct block-support co-simulation provides a more efficient workflow without measurable loss of statistical or spatial consistency, making it suitable for large-scale multivariate tailings modeling.

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1. INTRODUCTION

1.1 Background

Multivariate modeling of mine tailings must reproduce three features simultaneously: spatial continuity, cross-element relationships, and variability at block support. In practice, these requirements are difficult to satisfy because tailings datasets are typically heterogeneous, strongly correlated, and sampled at inconsistent supports. As a result, block-support simulation is required to obtain models that remain consistent with decision-making scales.

Sequential Gaussian co-simulation (SGCOSIM) is widely used for this purpose. However, its standard implementation operates at point support. Block-scale values are obtained only after averaging simulated point values using a predefined discretization. This workflow can reproduce block-scale variability, but it becomes computationally expensive when the grid is large or when many realizations are required.

To reduce this computational burden, direct block-support SGCOSIM introduces discretization inside the simulation algorithm. Instead of storing all point values, the method simulates internal nodes within each block and averages them immediately. This removes the external averaging step and reduces both memory usage and runtime.

Despite these advantages, there is little empirical evidence showing how the two workflows compare under realistic tailings conditions. In particular, their ability to reproduce multivariate structure and block-scale variability has not been tested on the same dataset using identical parameters. This gap motivates a controlled comparison.

1.2 Problem statement

Both conventional and direct block-support SGCOSIM workflows are available in practice, but their relative performance is not clearly established. The conventional workflow - point-support simulation followed by block averaging - can become computationally prohibitive when multiple variables and fine grids are used. Direct block-support simulation reduces computational burden by integrating discretization and averaging directly into the simulation code, but its statistical performance relative to the conventional method remains insufficiently explored. Tailings modeling requires accurate reproduction of histograms, variances, cross-correlations, and spatial continuity at the block scale. These statistical and spatial criteria are

treated as essential requirements rather than quantities that can be freely traded for computational speed. Computational performance is therefore evaluated only after assessing whether each workflow preserves the main geostatistical characteristics of the data. The central problem is to determine whether the faster direct block-support approach can provide a comparable block-scale model while substantially reducing runtime and storage requirements.

1.3 Objectives

The main aim of this thesis is to compare direct and conventional block-support sequential Gaussian co-simulation workflows and determine how each one reproduces multivariate behavior in the Haveri Au-Cu tailings dataset at block support. The dataset used in this study was not collected as part of this thesis; it is an existing Haveri tailings dataset obtained from previous sampling and made available for research purposes. Therefore, the study treats the data as secondary data and explicitly considers its limitations, including heterotopic sampling, unequal analytical coverage among variables, and dependence on the original sampling design. The comparison focuses not only on statistical reproduction, but also on the computational effort required by each workflow.

This aim is developed through five specific objectives.

First, to establish a consistent multivariate simulation framework for the Haveri tailings dataset, including density-based transformation, normal-score transformation, variogram modeling, and block-support definition.

Second, to implement the conventional workflow in which co-simulation is performed at $1\text{ m} \times 1\text{ m} \times 1\text{ m}$ point support and the results are subsequently averaged to $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ block support.

Third, to implement the direct block-support workflow in which co-simulation is performed directly on $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ reporting blocks using internal discretization within BLOCKSGCOSIM.

Fourth, to compare the two workflows in terms of block-scale statistical reproduction, including means, variances, histograms, quantiles, spatial continuity, and inter-variable correlations.

Fifth, to evaluate the computational performance of both workflows using runtime and output-size requirements, and to determine whether the direct workflow provides comparable geostatistical results with lower computational cost.

Taken together, these objectives are designed to answer one central question: whether direct block-support co-simulation can produce block models of similar quality while reducing the computational burden associated with the conventional workflow.

1.4 Hypothesis

It is hypothesized that the direct block-support SGCOSIM approach will require substantially less computational time than the conventional workflow because discretization and block averaging are handled internally during simulation. By removing the need for point-support simulation followed by a separate block-averaging step, the direct method is expected to generate block-scale realizations more efficiently while still reproducing the key statistical and spatial features of the Haveri tailings data.

The conventional approach can reflect slightly finer patterns because it starts at point support, but the much longer runtime outweighs this advantage. Therefore, it is anticipated that the direct block-support implementation will offer a more practical balance between accuracy and efficiency for multivariate block-scale modeling of Cu, Ag, Fe, and S in the Haveri tailings.

1.5 Significance to the industry

Accurate block-scale modeling is essential for modern tailings management, as it supports evaluations related to reprocessing potential, environmental risk assessment, and long-term closure planning. Multivariate simulation is critical because the geochemical behavior of tailings is influenced by the combined spatial distribution of several elements rather than by individual variables considered in isolation. To make reliable decisions, mining practitioners often require many realizations for uncertainty analysis, which places significant computational demands on conventional modeling workflows.

The traditional point-support co-simulation followed by external block averaging has been widely used in industry, but this approach can become slow and inefficient, especially for large datasets or fine discretization schemes. Direct block-support co-simulation offers a more streamlined workflow by integrating discretization and internal block averaging into the

simulation process, potentially reducing computation time while preserving key geostatistical features.

This question is particularly relevant for the mining industry of Kazakhstan, where large copper, polymetallic and uranium operations have generated extensive legacy tailings storage facilities. Many of these deposits are simultaneously long-term environmental liabilities (due to acid generation, metal leaching and dam stability issues) and potential secondary resources in the context of critical-metal supply and circular-economy strategies. In such cases, decisions depend on block-scale estimates of both tonnage and multi-element composition, as well as their uncertainty.

In practice, many tailings facilities in Kazakhstan are characterized by heterogeneous material, uneven sampling density, and long operational histories, which complicate spatial modeling at block support. Under these conditions, datasets are often heterotopic, and variables such as Fe and S show strong spatial coupling related to sulfide mineralization. This makes multivariate approaches necessary, as independent modeling would not preserve these relationships. At the same time, large model sizes and repeated scenario evaluations increase computational demand, which limits the use of conventional workflows.

By comparing conventional and direct block-support co-simulation on a real tailings dataset, this thesis provides a practical way to construct multivariate block models and evaluate their uncertainty at the scale of interest. The results show how similar models can be obtained with different computational effort. This makes the approach directly applicable to Kazakhstan's tailings facilities, where both modeling reliability and computational efficiency are required for reprocessing studies and environmental assessments.

1.6 Scope of work

This thesis is limited to a comparative assessment of two multivariate block-support co-simulation workflows implemented with BLOCKSGCOSIM in MATLAB. The comparison is based on one case study: the Haveri tailings storage facility.

The work includes exploratory data analysis, density-based transformation of non-additive variables, normal-score transformation, variogram and cross-variogram modeling, and the generation of multiple realizations under both workflows. The conventional workflow uses a fine $1\text{ m} \times 1\text{ m} \times 1\text{ m}$ simulation grid followed by external block averaging. The direct

workflow simulates directly on $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ reporting blocks using internal discretization. In both cases, outputs are evaluated at the same final support.

The analysis focuses on four variables: Cu, Ag, Fe, and S, together with bulk density as a co-simulated variable required for grade reconstruction. Model comparison is based on histogram reproduction, summary statistics, spatial continuity, cross-correlations, E-type patterns, uncertainty measures, and computational performance.

Several boundaries are set deliberately. First, the study does not compare BLOCKSGCOSIM with other simulation families such as indicator simulation, plurigaussian methods, or non-Gaussian machine-learning workflows. Second, it does not test multiple block sizes or alternative discretization schemes beyond those needed for the conventional and direct comparison. Third, the work evaluates statistical and computational behavior of the workflows, not the economic feasibility of tailings reprocessing itself. Finally, conclusions are drawn for this dataset and this simulation framework; broader generalization would require testing on additional deposits and sampling configurations.

In this sense, the thesis does not attempt to solve all block-modeling problems in tailings. Its scope is narrower and more specific: to determine how two support-handling strategies behave when applied to the same multivariate tailings dataset under controlled conditions.

2. LITERATURE REVIEW

2.1 Tailings management

Tailings management has moved from a simple idea of “storing waste safely” to a broader concept that connects waste reduction, secondary resource use, and long-term environmental protection. Recent work on green mining suggests that tailings should be viewed as both environmental liabilities and potential resources. In this view, reprocessing, repurposing, and rehabilitation are planned as part of the overall mine design, rather than handled only at the end of the operation (Cheng et al., 2016; Herrington, 2021). This perspective argues that future tailings management must support decarbonization and the security of raw-material supply, while also addressing legacy contamination, the structural stability of storage facilities, and expectations from local communities and regulators.

Another group of studies focuses on how tailings systems should be designed from the outset to achieve better environmental, social, and economic outcomes, rather than being treated solely as containment structures. These design frameworks suggest that geotechnical stability, water management, closure plans, and options for future re-mining or repurposing should be combined into a single life-of-mine strategy (Edraki et al., 2014). At the same time, reviews of recycling, reuse, and rehabilitation indicate that tailings can be used as construction materials or soil amendments or converted into revegetated land. However, they also note that these options often fail or remain limited in practice because tailings chemistry is poorly understood and their spatial variability is high, making performance difficult to predict (Lottermoser, 2011). Overall, these contributions describe tailings management as a multi-objective problem in which physical stability, environmental performance, and future resource potential must be considered together.

On the operational side, more research now examines how to reprocess tailings and under what conditions such projects are technically and economically feasible. A recent state-of-practice review of tailings reprocessing describes existing and emerging unit operations used to recover metals from many types of tailings. It identifies important gaps, including limited experience in scaling up processes, uncertain recoveries when feed properties vary, and poor use of geometallurgical information in project evaluations (Holley et al., 2024). Techno-economic studies on the recovery of critical raw materials from large national tailings inventories show that producing vanadium or rare-earth oxides can be profitable in some cases. However, the

results are susceptible to changes in metal prices, financial assumptions, and process design (Araya et al., 2020). These findings indicate that tailings management decisions cannot be based solely on average grades; they must also account for spatial variability and the relationships among several elements that influence processing performance.

Environmental assessment studies add another important dimension and support a more quantitative approach to tailings management. Prospective life-cycle assessments of sulfidic copper tailings reprocessing show that, depending on the chosen flowsheet and energy mix, reprocessing can reduce greenhouse gas emissions per ton of tailings treated. However, these benefits depend on efficient use of co-products and careful control of energy and reagent consumption (Adrianto and Pfister, 2022). At the same time, the literature suggests that conventional tailings disposal continues to pose long-term risks, such as acid mine drainage (AMD) and dam failures, and argues that better tailings management should integrate prevention, risk reduction, and valorization within a single framework.

Into this broader policy and technology context, geostatistical modelling has become an important tool for tailings management. Three-dimensional modelling of a tailings storage facility using universal sequential Gaussian simulation shows that detailed spatial models of grades, porosity, and bulk density can be used to estimate both remaining resource potential and the distribution of environmentally critical elements in a highly heterogeneous deposit (Blannin et al., 2023). This work highlights slurry deposition methods, changes in processing over time, and weathering processes that create strong spatial trends and anisotropies. Therefore, using simple interpolation methods or assuming too much stationarity can lead to inaccurate representations of economic tonnages and areas with higher environmental risk.

A related methodological step forward is the explicit treatment of multielement, compositional geochemical data using transformations and multivariate geostatistics. A recent framework for assessing resource potential in tailings combines compositional data analysis, isometric log-ratio transformation, and sequential Gaussian simulation with minimum/maximum autocorrelation factors (MAF). This approach allows the joint modelling of valuable and hazardous elements and provides probabilistic estimates of remaining resources in legacy tailings (Karacan et al., 2023).

Concrete case studies show how such geostatistical models inform tailings management and valorization choices. For the Haveri gold (Au) and copper (Cu) tailings in Finland, re-use of

historical drill-core data together with three-dimensional block modelling of cobalt (Co), Cu, and Au made it possible to estimate remaining metal resources and to compare their economic potential with that of current mining operations (Parviainen et al., 2020).

Despite these advances, several gaps remain that are directly relevant to multivariate block-support simulation for tailings. Most existing geostatistical applications to tailings use kriging or sequential Gaussian simulation at point support or in relatively small blocks and often focus on a single variable. Such a gap supports the motivation of the present thesis, which aims to assess direct and conventional BLOCKSGCOSIM block-support co-simulation for improved multivariate tailings modelling as a basis for more informed and resilient tailings management.

2.2 Geostatistical modeling

Geostatistical modeling has become important to understanding the spatial structure of tailings deposits, both for resource evaluation and for assessing environmental risks. Compared with traditional interpolation or simple volume-average calculations, recent studies show that geostatistical approaches can capture spatial heterogeneity, account for non-stationary trends, and provide uncertainty measures essential for decision-making on reprocessing and remediation in tailings storage facilities.

One example is the study, which highlights the three-dimensional modeling of the Davidschacht tailings deposit in Germany, where universal sequential Gaussian simulation was used to estimate both valuable metals (Zn, Pb, Cu, In) and toxic elements (As, Cd) within the tailings volume (Blannin et al., 2023). The study demonstrates that tailings exhibit strong vertical and lateral gradients due to slurry deposition processes, changes in plant operations, and post-depositional weathering, thereby violating simple stationarity assumptions. Universal kriging-based simulation, rather than ordinary kriging or inverse-distance methods, was therefore selected to account for these trends. The results show that, even with relatively sparse deep drilling and denser shallow sampling, robust tonnage estimates and confidence intervals can be obtained, and that a limited number of drillholes may be sufficient for practical resource assessment when the geostatistical model is specified correctly (Blannin et al., 2023).

Another example of geostatistical modeling in tailings characterization focuses on the specific challenges posed by compositional multielement geochemical data. At the Katherine Mine tailings in the USA, a methodology was developed that combines compositional data analysis

with geostatistical simulation to assess resource potential and environmental hazards jointly (Karacan et al., 2023). After clustering geochemical parts and applying isometric log-ratio and MAF transformations, sequential Gaussian simulation was used to model both valuable metals (Au, Ag, Cu, Zn, Pb) and environmentally concerning elements (Hg, As). The study shows that ignoring the compositional structure can lead to unrealistic predictions and biased uncertainty estimates, while the proposed workflow yields tonnage distributions and 5-95% uncertainty ranges for each element. It further demonstrates how realizations can be combined with geometric information on the tailings body and downstream channels to estimate the amount of material, including hazardous elements, that has been eroded and transported out of the facility (Karacan et al., 2023).

Geostatistical modeling is also being used directly to support revalorization studies at the case-study level. For the Haveri Au-Cu tailings in southwest Finland, an extensive historical database of 1201 tailings samples from 165 drill cores was used to build a three-dimensional block model for Co, Cu, and Au (Parviainen et al., 2020). The work reconstructs the base surface of the tailings deposit from drillholes that reach the underlying geology, interpolates this surface to approximate the former topography, and then estimates remaining resources using block modeling. Grades and tonnages of Au, Co, and Cu are compared with current production levels, and a simple feasibility analysis is performed (Parviainen et al., 2020).

More recently, geostatistical research has started to explore methods specifically adapted to tailings geometries and grade continuity. In another study on the Haveri tailings, ordinary kriging was compared with transitive kriging for modeling gold, cobalt, copper, and iron grades (Soto et al., 2022). The authors argue that traditional geostatistical methods may not perform optimally in narrow deposits with weak spatial continuity and complex internal structure and propose transitive geostatistics as an alternative that exploits the fully delimited domain of a tailings dam. This work shows that choices in the interpolation framework can significantly affect block-grade distributions in tailings and suggests that alternative kriging variants may be better suited than standard approaches for specific metals and deposit geometries (Soto et al., 2022).

When viewed together, these four studies show a clear evolution in the use of geostatistical modeling for tailings. Early efforts concentrated on obtaining reasonable block models and tonnage estimates using kriging or simple interpolators, as in the historical database-driven revalorization of Haveri (Parviainen et al., 2020). Subsequent work introduced more advanced

techniques such as universal sequential Gaussian simulation, which addresses non-stationarity and provides uncertainty quantification at the Davidschacht tailings (Blannin et al., 2023). Methodological developments have then extended this approach to compositional data, incorporating transformations and multivariate simulation to jointly model economic and hazardous elements and derive probabilistic resource and risk measures, as illustrated at the Katherine Mine site (Karacan et al., 2023). Finally, transitive kriging has been tested as a specialized tool for narrow-tailings deposits, with evidence that it can reduce smoothing and improve predictions for certain critical metals (Soto et al., 2022).

At the same time, these studies also clarify important gaps directly relevant to this thesis. First, geostatistical applications to tailings have focused mainly on estimation or univariate simulation, even when many elements are modeled in parallel. Cross-correlations between variables are usually handled indirectly (for example, by decorrelating transformed components) rather than explicitly preserved through multivariate simulation or co-simulation at the block level. Second, most work has been carried out at point or small-block support and then aggregated, rather than directly modeling variables at final block support, accounting for changes of support and smoothing effects in multivariate settings. Third, while universal SGSIM, compositional SGSIM, and transitive kriging improve on basic kriging in different ways, there has been little systematic comparison of alternative multivariate simulation frameworks for tailings deposits, especially in terms of their ability to reproduce joint distributions and correlations that control metallurgical behavior and environmental risk.

2.3 Non-additivity and block-support considerations

A fundamental requirement for most geostatistical estimation and simulation techniques is that the variables being modeled are additive over space, meaning that values can be summed over blocks and larger supports in a physically meaningful way. Grades, recoveries, and other geometallurgical responses are often defined as ratios or proportions and thus are not additive in their usual form. Carrasco (2008) formalized this distinction, showing that while extensive quantities such as metal mass or ore tonnage are additive, intensive quantities like metallurgical recovery or grade are not, and that naïve averaging of non-additive variables across blocks results in biased resource and performance predictions.

This distinction becomes critical when moving from sample support to block support. Drillhole samples describe grades over short intervals, whereas resource evaluation and tonnage

calculation are performed at block scale. In this study, tonnage is calculated for $5 \times 5 \times 1$ m blocks, not for individual samples. Because of this change of support, grades and density must be represented at the same scale. Block-support simulation is used for that purpose: it generates values directly at the support where tonnage and metal quantities are evaluated. If point-support values are transferred to blocks without proper upscaling, local variability is overemphasized and the resulting grade–tonnage relationship becomes inconsistent (Rossi and Deutsch, 2014; Emery and Séguet, 2020).

For this reason, block-scale grades should be derived from additive quantities rather than obtained by direct averaging of grade values. A grade represents a concentration and is therefore meaningful only in relation to the mass or volume of material to which it applies. When density varies spatially, equal-volume samples or discretization nodes do not necessarily represent equal masses of material. Consequently, direct arithmetic averaging of grades may violate mass balance and distort the relationship between grade, tonnage, and contained metal. A more consistent approach is to model additive variables, such as density-weighted grade or metal accumulation, and then recover grade as a ratio after aggregation to the target block support.

In geometallurgical contexts, the non-additivity problem is particularly acute for recovery functions, which are typically defined as the ratio between recovered metal and feed metal. Carrasco (2008) showed that directly interpolating or simulating recovery at the block scale leads to inconsistencies when aggregating over larger volumes, because the arithmetic mean of ratios does not equal the ratio of the summed metal quantities. This result motivated the shift toward modeling additive “service variables”, such as metal accumulation and ore tonnage, and reconstructing non-additive responses only after spatial prediction.

Subsequent work operationalized this principle by re-expressing non-additive variables as additive form. Adeli et al. (2021), for example, treated metallurgical recovery as a derived quantity defined as the sum of two additive components: the mass of metal in the concentrate and the mass of metal in the feed. Both quantities were modeled by cokriging, and recovery was then obtained as their ratio. This approach directly addresses non-additivity while preserving multivariate relationships and allowing preferential sampling effects to be incorporated. It also provides a useful analogy for block-support grade modeling, where additive variables must be simulated first and ratios recovered afterward.

Similar concerns appear in geometallurgy-oriented mine scheduling. Campos et al. (2022) emphasized that recovery and other plant performance indicators are inherently non-additive and are usually calibrated at small support levels, such as sample or test-work scale. In contrast, mine planning decisions are made at block or panel support levels. They showed that applying regression-based recovery models directly at block support without accounting for support and non-additivity can distort both the spatial distribution of predicted performance and the resulting production schedule, leading to suboptimal economic outcomes. Their work reinforces the need to use additive, volume-consistent variables when transferring geometallurgical information from drillhole to mine-planning scales.

The additivity issue also arises for grades when they are treated purely as concentration ratios (mass of element per mass of rock) without explicit reference to the underlying masses. Emery and Séguret (2020), in their geostatistical treatment of geometallurgy, stress that, regardless of the chosen geostatistical algorithm, the variables under study must be additive at the support of interest, and that non-additive responses should be handled through appropriate transformations to additive quantities (e.g., metal content and tonnage) prior to spatial modeling. Rossi and Deutsch (2014) described this idea through the concept of “service variables” or accumulations, in which grade is multiplied by thickness to obtain metal content, an additive quantity that can be estimated or simulated together with thickness. Block grades are then recovered by dividing accumulated metal by accumulated thickness. They also noted that compositing can be weighted by specific gravity, further acknowledging that density is a key bridge between intensive variables (grade) and extensive quantities (metal mass).

Deraisme et al. (2014) provided a multivariate block-simulation case study where non-additivity was handled explicitly within a discrete Gaussian model framework. In a lateritic nickel deposit, they distinguished between additive estimation variables—metal accumulations and ore tonnage—and the non-additive selection variable, the SMU nickel grade defined as the ratio of accumulation to tonnage. Their workflow used direct block simulations to generate multivariate realizations of the additive variables at SMU support and then derived grades and recoverable resources through post-processing. This example shows clearly why block-support simulation is needed for tonnage calculation: tonnage and metal content are additive at block support, whereas grade is meaningful only after those additive quantities have been combined.

In tailings deposits, the issue is further amplified by spatial variability in density. Blocks with the same volume can contain different amounts of material, depending on density. As a result,

direct averaging of grades across space can lead to incorrect estimates of both tonnage and metal content. Working with additive quantities during simulation and reconstructing grades afterward avoids this inconsistency.

In this study, this principle is implemented through a density-based transformation prior to simulation. Each grade variable is converted into an additive form by multiplying it by density, producing a variable proportional to metal content. Co-simulation is then performed on these transformed variables together with density in the Gaussian domain. After simulation, block-scale grades are recovered by dividing the simulated additive quantities by the corresponding block density. This ensures that both grade and tonnage are defined at the same support and remain physically consistent throughout the modeling workflow.

2.4 Multivariate geostatistics

Multivariate geostatistics extends the univariate framework by modelling two or more spatial variables together and explicitly preserving their cross-correlation in space. Instead of analyzing only direct variograms or covariances for a single attribute, multivariate approaches jointly model auto- and cross-variograms (or covariances) for all variables of interest (Matheron, 1963; Goovaerts, 1997; Wackernagel, 2003). The key idea is that grades, geochemical indicators, or geometallurgical parameters rarely vary independently; ignoring their spatial co-dependence can bias both resource estimates and environmental risk evaluations.

The formal basis of most multivariate algorithms is the linear model of coregionalization (LMC), which expresses the direct and cross-variograms of several variables as linear combinations of a standard set of basic structures (Chilès and Delfiner, 2012; Wackernagel, 2003). In practice, this requires a joint modelling step in which nested variogram structures and their sill matrices are adjusted to remain positive semi-definite and to reproduce both individual continuity and cross-continuity. This model then underpins conventional cokriging and Gaussian-based co-simulation, allowing the simultaneous interpolation or simulation of all variables while reproducing the original correlation structure at the scale of interest (Goovaerts, 1997; Journel and Huijbregts, 1978).

For compositional or strongly correlated geochemical data, multivariate geostatistics often requires the use of transformation strategies. Log-ratio transformations provide a way to honor

the constant-sum constraint of compositional data and avoid spurious correlations (Aitchison, 1986; Pawlowsky-Glahn and Olea, 2004). More advanced frameworks apply several transformations in sequence, for example, log-ratios followed by minimum/maximum autocorrelation factors (MAF) to decorrelate variables prior to simulation, with inverse transformations applied at the end to return to the original units (Park, 2014). These methods have been used to generate realizations of multi-element geochemical fields that reproduce both marginal distributions and cross-correlations, providing a richer description of joint uncertainty than separate univariate models.

Recent developments focus on multivariate simulation at the block level, which is particularly relevant for mine planning and tailings management. Direct block-support algorithms aim to simulate several correlated variables at the block scale without first simulating on a very fine grid and then averaging, thus reducing memory requirements and improving computational efficiency (Boucher and Dimitrakopoulos, 2009). In these approaches, MAF or similar factorization techniques are used to orthogonalize the multivariate Gaussian model; independent factors are simulated at point or block scale and then recombined to recover the original variables at block support (Boucher and Dimitrakopoulos, 2012; Chilès and Delfiner, 2012). Such methods can preserve cross-correlation and change-of-support effects in a single framework, which is essential when project-level decisions depend on block-scale joint distributions of metals and environmental indicators. In the context of tailings deposits, multivariate geostatistics is therefore not only a technical extension of univariate modelling, but a necessary tool for representing how multiple elements co-occur and co-vary in space.

2.5 Conventional and direct block support simulations

Change of support is a central issue in geostatistical modeling for mining because data are typically available at quasi-point support (e.g., drillhole composites). At the same time, decisions are made at the selective mining unit (SMU) or block support. Classical recoverable resource workflows, therefore, require a way to propagate small-scale variability and uncertainty to the block scale in a statistically consistent way (Rossi and Deutsch, 2014; Bassani and Costa, 2022). Within this context, stochastic simulation, in particular sequential Gaussian simulation, has become a standard tool for generating multiple realizations that can be post-processed into grade-tonnage curves and risk measures at block support (Journel and Kyriakidis, 2004; Ortiz, 2020).

The conventional practice for obtaining block-support realizations is to simulate at point support on a fine grid that discretizes the domain and then average the simulated point values within each block. Emery and Ortiz (2011) explicitly describe this approach. Each block is discretized into a finite set of nodes, sequential Gaussian simulation is performed at those nodes, and block values are computed as arithmetic averages of the simulated point-support grades. This strategy is simple, compatible with existing point-support algorithms, and requires no explicit change-of-support model beyond the numerical discretization. However, both Emery and Ortiz (2011) and Rossi and Deutsch (2014) emphasize that the computational burden escalates rapidly when large deposits and fine discretizations are used, because millions of blocks translate into tens or hundreds of millions of simulated points that must be visited, stored, and then aggregated. Memory demands become especially problematic for algorithms that keep all simulated nodes in memory, such as LU-based Gaussian simulation, and the number of neighborhood searches grows with the number of conditioning points rather than the number of blocks (Emery and Ortiz, 2011).

These computational limitations motivated the development of direct block-support simulation algorithms, in which block values are simulated without storing the complete set of internal point-support realizations. The early theoretical basis can be traced to the change-of-support work of Matheron (1976) and subsequent developments in discrete Gaussian models, in which block variables are treated as regularized transforms of an underlying Gaussian field. Building on this foundation, Marcotte (1994) and later Emery (2009) proposed algorithms for direct block simulation that combine explicit change-of-support relationships with conditional simulation schemes. Emery (2009) presented computer programs that implement such models for both simple and ordinary kriging conditioning and showed how they can also incorporate the information effect arising from differences between planning-scale and production-scale information densities. These contributions formalised direct block-support simulation as a practical alternative rather than a purely theoretical construct.

In the multivariate context, Boucher and Dimitrakopoulos (2009, 2012) developed the dbmafsim framework for joint direct block simulation of correlated variables. Their approach uses minimum/maximum autocorrelation factors (MAF) to decorrelate the original variables into orthogonal “service variables,” which are then simulated directly at block support using a grouped sequential Gaussian simulation algorithm (Boucher and Dimitrakopoulos, 2009). Because simulation proceeds block by block and only block-support results are stored, the

method avoids the large memory footprint associated with storing point-support realizations. The application at the Yandi iron ore deposit, involving five correlated elements, demonstrated that direct block-support simulation via dbmafsim can reproduce direct and cross-variograms at block support while substantially reducing the number of modeled variograms and the size of output files, making the method attractive for routine multivariate resource modeling (Boucher and Dimitrakopoulos, 2012).

Emery and Ortiz (2011) extended direct block-support simulation explicitly to conditional co-simulation of cross-correlated variables and implemented their algorithms in the BLOCKSGCOSIM program. They proposed two strategies: a block-support sequential Gaussian co-simulation and a spectral block-support co-simulation based on the discrete Gaussian model. In the sequential algorithm, each block is discretized into a set of nodes. At each simulation step, a Gaussian vector at those nodes is drawn with mean equal to the co-kriging predictions and covariance equal to the co-kriging error covariance matrix. Only the block averages are retained for conditioning subsequent blocks. Hence, the method reduces both memory requirements and the number of searches by working with block-support data rather than an ever-growing set of point-support simulated values (Emery and Ortiz, 2011). The spectral algorithm, in turn, incorporates an explicit discrete Gaussian change-of-support model into a spectral simulation framework, further tightening the link between point- and block-support covariance structures.

Recent case studies have demonstrated the practical impact of direct block-support co-simulation in complex, multi-element deposits. Hosseini et al. (2017) applied the block-support sequential Gaussian co-simulation of Emery and Ortiz (2011) to the Sungun porphyry Cu-Mo deposit. They explicitly contrasted the “usual” point-support simulation plus block averaging with a direct block-support implementation. They highlighted that the latter avoids storing point-support values, leading to substantial gains in CPU time and memory while still reproducing multivariate statistics and delivering block-scale realizations suitable for recoverable resource estimation. In a related study at the Mehdiabad Zn-Pb-Ag deposit, Hosseini et al. used block-support SGCOSIM to forecast grade-tonnage curves and their uncertainty directly at SMU support, again emphasising the ability of direct block-support co-simulation to handle multi-element cut-off criteria and local uncertainty in a computationally efficient manner. Deraisme et al. (2014) adopted direct multivariate block simulations within a discrete Gaussian model framework for a lateritic nickel deposit, where roughly 1.5 million

SMUs had to be simulated. Their work showed that direct block simulations at SMU support, coupled with appropriate post-processing and scenario reduction, can address support effects, information effects, and non-additivity in a multivariate setting without resorting to point-support simulation followed by re-blocking.

Taken together, these contributions delineate a clear evolution from conventional point-support simulation with subsequent block averaging toward direct block-support (co-)simulation methods that explicitly address the change of support and computational efficiency. Conventional workflows remain widely used due to their conceptual simplicity and integration with standard software. However, they become increasingly costly in terms of CPU time and memory as the number of blocks, discretization density, and number of simulated variables increase. Direct block-support approaches - whether based on MAF-decorrelated service variables (Boucher and Dimitrakopoulos, 2012), discrete Gaussian change-of-support models (Emery, 2009; Deraisme et al., 2014), or block-support SGCOSIM (Emery and Ortiz, 2011; Hosseini et al., 2017) - offer clear numerical advantages and more explicit control over support effects.

Although the literature on block-support simulation has advanced significantly, several gaps remain that are directly related to the objectives and hypotheses of this thesis. First, most studies either apply only the conventional point-support simulation with block averaging or only a direct block-support method; very few works apply both workflows to the same multivariate dataset using the same variogram models and the same co-simulation engine, and then compare them in a strict, quantitative way. In particular, systematic comparisons that report computational time, memory usage, and the quality of block-scale multivariate reproduction are rare (Emery and Ortiz, 2011; Boucher and Dimitrakopoulos, 2012). Second, existing applications are mainly focused on hard-rock ore deposits such as porphyry copper, iron ore, or lateritic nickel. At the same time, multi-element tailings systems, where density variations, non-additivity, and environmental drivers are important, are largely unexplored. Third, there is limited analysis of how specific implementation choices in block-support SGCOSIM, such as block discretization strategies and the internal handling of support, affect both numerical performance and the fidelity of the resulting block models. This thesis addresses these gaps by comparing conventional point-support SGCOSIM with block averaging and direct block-support SGCOSIM on a single multivariate tailings dataset, with explicit attention to computational efficiency and block-scale multivariate behaviour.

3. METHODOLOGY

3.1 Overall research design

This thesis adopts a quantitative, simulation-based research design built around a single, well-defined case study: a multivariate tailings storage facility in Haveri. The work is structured as a controlled numerical comparison of two geostatistical workflows for multivariate block-support modeling:

- a conventional workflow, in which sequential Gaussian co-simulation is run at point support and the results are subsequently averaged to block support, and
- a direct block-support workflow, in which block values are simulated directly using an internal block discretization.

Both workflows use the same MATLAB executable (BLOCKSGCOSIM), but with different settings for block discretization and post-processing. In the conventional case, the discretization is set to $1 \times 1 \times 1$ (effectively simulating at point support), and block-support values are obtained afterwards using a separate averaging program (BLKAVG). In the direct block-support case, a non-trivial discretization (e.g., $5 \times 5 \times 1$) is defined for each block, and BLOCKSGCOSIM performs the internal averaging, without storing all node-scale values.

For each workflow, several realizations are generated and evaluated using a coherent set of criteria. These include reproducing marginal statistics at block support, multivariate relationships between variables, spatial continuity, spatial patterns of uncertainty, and computational performance (CPU time and, as far as possible, memory usage). Because the only procedural differences between the workflows are how block support is handled within BLOCKSGCOSIM and how averaging is carried out (internal versus external), the design isolates the impact of “conventional” versus “direct” block-support co-simulation on the final block models.

A key conceptual element of the design is the explicit treatment of non-additivity. Since grades are ratio-type variables and cannot be added directly when density varies, the thesis employs density-based transformations to convert grades into additive variables prior to co-simulation. Both workflows operate on these additive variables in the Gaussian domain and subsequently reconstruct block grades from simulated accumulations and density.

The overall logic can be summarized in five main stages: (i) data preparation and density-based transformation of variables; (ii) normal-score transformation and variogram modeling using standalone executables (nscore.exe, gamv.exe, vargfit.exe); (iii) conventional point-support SGCOSIM with subsequent block averaging via BLKAVG; (iv) direct block-support SGCOSIM with internal block averaging; and (v) post-processing and comparative analysis in ISATIS.

3.2 Dataset, variables, and model grid

The case study dataset consists of multivariate drillhole samples collected from a tailings storage facility at Haveri. The dataset was not collected specifically for this thesis. It represents secondary data from previous investigation of the Haveri tailings storage facility and was used here as the basis for a controlled methodological comparison. As a result, the analysis is constrained by the assumptions and limitations of the original data collection, including the original drillhole layout, fixed sample support, variable analytical coverage, and heterotopic sampling pattern. These limitations are important because they influence variogram modeling, correlation analysis, and the reliability of co-simulation for sparsely sampled variables such as sulfur. The variables considered in this thesis include copper (Cu), silver (Ag), iron (Fe), sulfur (S), and bulk density. These variables are relevant both for assessing potential metal recovery and for understanding geochemical behavior, particularly in relation to acid mine drainage.

Samples are available at approximately constant vertical support (fixed-length intervals along boreholes). However, spatial coverage and analytical completeness differ between variables, leading to heterotopic sampling and motivating the use of multivariate co-simulation.

A three-dimensional block model is defined to cover the volume of interest within the Haveri tailings storage facility. The target reporting block size is $5\text{ m} \times 5\text{ m} \times 1\text{ m}$, representing the support on which model outputs are interpreted and compared in this thesis. In the conventional workflow, an additional fine simulation grid with $1\text{ m} \times 1\text{ m} \times 1\text{ m}$ cells is defined; this grid serves as support for sequential Gaussian co-simulation and is later aggregated into $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ reporting blocks. For the direct block-support workflow, the simulation is performed on the $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ reporting blocks, with an internal discretization of $5 \times 5 \times 1$ nodes per block. In both workflows, the same reporting block model ($5\text{ m} \times 5\text{ m} \times 1\text{ m}$) is used for comparison; the difference lies in whether the simulation is run first at $1\text{ m} \times 1\text{ m} \times 1\text{ m}$ and then averaged or run directly at $5\text{ m} \times 5\text{ m} \times 1\text{ m}$ with explicit internal discretization.

3.3 Density-based transformation and treatment of non-additivity

Grades expressed as concentrations (e.g., percent or ppm) are non-additive and cannot be summed up or averaged directly across samples when density varies. To make the variables compatible with linear geostatistics and block aggregation, the thesis uses a density-based transformation that converts grades into additive quantities.

For each drillhole sample with grade Z (for Cu, Ag, Fe, or S) and density ρ , an additive variable Z^* is defined as:

$$Z^* = Z \times \rho , \quad (1)$$

Interpreted as a density-weighted grade (or metal content per unit volume, depending on the support definition). These transformed variables $\{Cu^*, Ag^*, Fe^*, S^*\}$ are used together with density (ρ) in the co-simulation. All co-simulation in BLOCKSGCOSIM is performed on this set of additive variables in the Gaussian domain. At block support, correct average grades are recovered by dividing the simulated additive variables by the simulated density:

$$Z_{block} = \frac{Z_{block}^*}{\rho_{block}}. \quad (2)$$

Bulk density is derived from the original data using a mass-balance approach: compositional information (percentages and ppm) is converted to mass fractions, associated with assumed mineral or elemental densities, and combined to estimate a bulk density for each sample. The resulting densities are then checked to ensure that they lie within plausible ranges for tailings material (for example, around $1\text{-}2 \text{ g}\cdot\text{cm}^{-3}$) and are subsequently treated as a separate variable in the co-simulation.

3.4 Conventional block-support co-simulation

The conventional block-support co-simulation workflow follows the usual two-step strategy:

- 1) simulate at a fine $1 \text{ m} \times 1 \text{ m} \times 1 \text{ m}$ support, and
- 2) average these small cells to the target $5 \text{ m} \times 5 \text{ m} \times 1 \text{ m}$ blocks.

This workflow is executed using a sequence of standalone executables and the BLOCKSGCOSIM engine:

1. Normal-score transformation (nscore.exe)

The original additive variables (Cu*, Ag*, Fe*, S*, ρ) are transformed to normal scores with nscore.exe. The transformation tables are stored for later back-transformation.

2. Variogram analysis (gamv.exe and vargfit.exe)

Experimental variograms are computed for each normal-score variable using gamv.exe. Theoretical models are fitted with vargfit.exe by adjusting the parameters in the corresponding parameter file until an acceptable fit is obtained.

3. Fine simulation grid (creategrid.exe, 1×1×1 m cells)

A fine simulation grid is generated with creategrid.exe. In the conventional workflow, this grid has a cell size of 1 m × 1 m × 1 m (for example:

- first node coordinates: 460450.00, 844950.00, −9.25.
- number of nodes: 450 (x), 250 (y), 20 (z).
- spacing: 1.0 m in x, 1.0 m in y, 1.0 m in z).

Each of these 1×1×1 cells are treated as a simulation node.

4. Point-support co-simulation (BLOCKSGCOSIM with discretization 1:1:1)

The MATLAB routine blocksgcosim.m (BLOCKSGCOSIM) is then used to perform sequential Gaussian co-simulation on the fine grid. For the conventional workflow, the block discretization is set to 1:1:1, meaning that each 1×1×1 cell is represented by a single node. BLOCKSGCOSIM produces realizations of the Gaussian variables at 1×1×1 m support for all variables.

5. Block averaging to 5×5×1 m

The fine-scale realizations are then aggregated to the target reporting support using blkavg.exe. The reporting block model is defined with a block size of 5 m × 5 m × 1 m, and each reporting block is associated with the underlying 5 × 5 × 1 = 25 small 1×1×1 cells. blkavg.exe averages the simulated values within each group of 25 cells and assigns a single value per 5×5×1 block for each variable and each realization.

6. Export for post-processing

The resulting $5 \times 5 \times 1$ m block-support realizations for $\{\text{Cu}^*, \text{Ag}^*, \text{Fe}^*, \text{S}^*, \rho\}$ are exported to formats compatible with ISATIS, where they are later back-transformed and converted to grades.

In this conventional workflow, the reporting block size is $5 \times 5 \times 1$ m. However, the simulation itself is performed at $1 \times 1 \times 1$ m, and block-support values are obtained only after an explicit averaging step using `blkavg.exe`.

3.5 Direct block-support co-simulation

The direct block-support co-simulation workflow uses the same dataset, variogram models, and variables as the conventional one. However, BLOCKSGCOSIM is configured to simulate directly at the $5 \times 5 \times 1$ m block support, using an internal discretization.

The steps are as follows:

1. Normal-score transformation and variogram modeling

The same normal-score transformations (`nscore.exe`) and variogram models (`gamv.exe` and `vargfit.exe`) used in the conventional workflow are adopted here.

2. Reporting block model ($5 \times 5 \times 1$ m) with internal discretization 5:5:1

The simulation grid now coincides with the reporting block model. Each block has dimensions $5 \text{ m} \times 5 \text{ m} \times 1 \text{ m}$ and is internally discretized into $5 \times 5 \times 1$ nodes. BLOCKSGCOSIM uses these internal nodes to approximate the block average.

3. Direct block-support co-simulation (BLOCKSGCOSIM with discretization 5:5:1)

BLOCKSGCOSIM is run again via `blocksgcosim.m`, but in this case the block size is $5 \times 5 \times 1$ m and the discretization is 5:5:1. For each block along a random simulation path:

- BLOCKSGCOSIM builds the co-simulation system using the normal-score data and previously simulated blocks,
- simulates Gaussian values at the $5 \times 5 \times 1$ internal nodes of that block, and
- averages these node values internally to produce a single Gaussian value per variable at block support.

Only the block averages are stored and used as conditioning values for subsequent blocks; the internal node values are not saved.

4. No external blkavg step

In contrast to the conventional workflow, there is no call to blkavg.exe in the direct approach because block-support averaging is already performed inside BLOCKSGCOSIM through the 5:5:1 discretization. The output from this workflow consists directly of $5 \times 5 \times 1$ m block-support Gaussian realizations for all variables.

5. Export for post-processing

These block-support realizations for $\{Cu^*, Ag^*, Fe^*, S^*, \rho\}$ are exported for back-transformation and grade recovery in ISATIS, using the same post-processing steps as in the conventional workflow.

In this direct workflow, both the simulation support and the reporting support are $5 \times 5 \times 1$ m. The main difference from the conventional approach is that internal discretization and averaging are performed immediately within BLOCKSGCOSIM rather than via a separate external averaging step.

3.6 Advantages and limitations of the methodology

The adopted methodology has several advantages in relation to the objectives of this thesis. First, it provides a controlled and internally consistent comparison: both workflows use the same dataset, reporting block model ($5 \text{ m} \times 5 \text{ m} \times 1 \text{ m}$), set of variables, normal-score transformations, and variogram models, and the same simulation engine (BLOCKSGCOSIM). The only procedural difference is the treatment of support (a $1 \times 1 \times 1$ m simulation with BLKAVG versus a direct $5 \times 5 \times 1$ m simulation with 5:5:1 discretization), isolating the impact of support handling. Second, the explicit density-based treatment of non-additivity ensures that mass balance is maintained and that both workflows operate on additive variables, with grades reconstructed consistently. Third, the use of standalone executables for all core steps, combined with a familiar post-processing environment in ISATIS, makes the workflow reproducible and close to realistic industrial practice.

At the same time, several limitations must be acknowledged. The analysis is restricted to a single tailings storage facility, so conclusions about the relative performance of the workflows

may not transfer directly to other deposit types or sampling configurations. The framework is entirely Gaussian, relying on normal-score transformation and sequential Gaussian co-simulation; alternative non-Gaussian or indicator-based approaches are not examined. Density is treated as a standard co-simulated variable, and possible systematic errors in its estimation are not modeled explicitly, even though they would affect recovered grades. Finally, computational performance is evaluated for a specific hardware configuration and a set of grid and discretization choices, so absolute run times are not general, even though the relative differences between conventional and direct block-support co-simulation remain informative.

4. RESULTS

4.1 Case Study

The case study uses heterotopic multi-element sampling to examine the Haveri tailings storage. Ten elements - Ag, As, Au, Co, Cu, Fe, Ni, Pb, S, and Zn - that were measured on tailings samples are included in the dataset. Ag, As, Au, Co, Ni, Pb, and Zn are mostly reported in parts per million (ppm), whilst Cu, Fe, and S are in percent (%). Notably, sulfur is sampled less frequently than the base-metal suite (Figure 1). This likely reflects the original analytical program, in which economically relevant metals were analyzed more consistently, while sulfur was measured only for a smaller subset of samples related to sulfide mineralization and acid-generation assessment. This unequal analytical coverage creates a heterotopic dataset and is treated as a limitation in the co-simulation workflow.

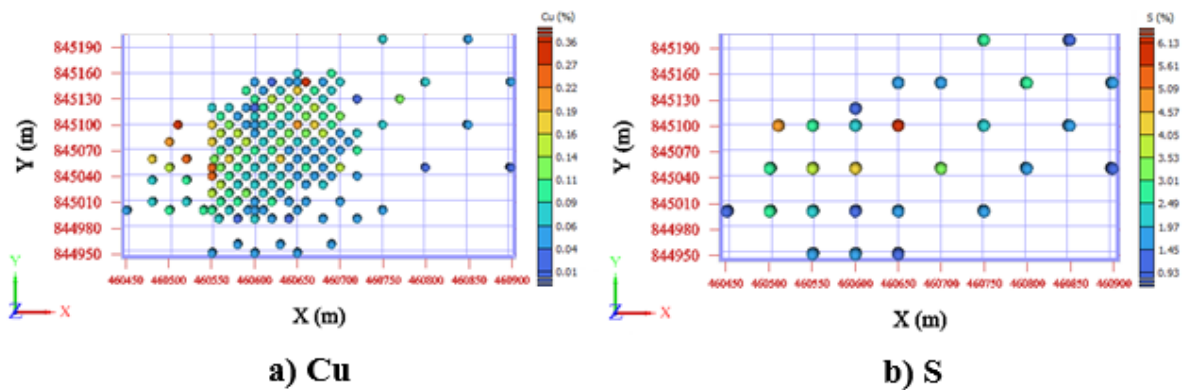


Figure 1. Spatial distribution of boreholes for a) Cu and b) S

4.2 Exploratory Data Analysis

Exploratory data analysis was performed in ISATIS using the original sample data before normal-score transformation and co-simulation. The correlation matrix in Table 1 was calculated from available paired observations for each variable pair, meaning that each coefficient was based only on samples where both variables were measured. This approach is appropriate for the heterotopic structure of the dataset, where not all elements were assayed in every sample. Scatter plots were also generated in ISATIS for the strongest Cu-related relationships to visually assess whether the statistical correlations were supported by recognizable bivariate trends.

The results show that Cu, Ag, Fe, and S form the most relevant group for further modeling. The correlation matrix indicates moderate positive relationships between Cu and Ag ($\rho \approx 0.68$), Cu and S ($\rho \approx 0.60$), and Cu and Fe ($\rho \approx 0.48$). These values suggest that the variables are related, but not strongly enough to be treated as redundant.

The same relationships are visible in the scatter plots (Figure 2). The Cu-Ag pair forms the clearest trend, with a relatively compact cluster and a consistent increase of Ag with Cu. In contrast, the Cu-Fe relationship is more dispersed. At higher Cu values, Fe shows a wider spread, which suggests that Fe is influenced by additional factors beyond Cu alone.

The Cu-S relationship is weaker and less structured. At low Cu values, S varies considerably, and the data cloud becomes more scattered. However, higher Cu values are generally not associated with low S, which indicates a partial coupling between these elements. This is consistent with the presence of sulfide minerals, although the relationship is not strictly proportional.

Overall, the variables show moderate correlation combined with noticeable scatter. This combination is important: the relationships are strong enough to justify joint modeling, but not strong enough to be captured by simple regression. A co-simulation approach is therefore required to preserve both correlation and variability.

Table 1. Correlation matrix for values in the dataset

	Ag (ppm)	As (ppm)	Au (ppm)	Co (ppm)	Fe (%)	Ni (ppm)	Pb (ppm)	S (%)	Zn (ppm)	Cu (%)
Ag (ppm)	1									
As (ppm)	0.03	1								
Au (ppm)	0.4	0.03	1							
Co (ppm)	0.07	0.53	-0.06	1						
Fe (%)	0.44	0.10	0.48	0.34	1					
Ni (ppm)	0.31	0.04	0.21	0.02	0.33	1				
Pb (ppm)	-0.03	0.00	-0.06	0.08	0.13	0.02	1			
S (%)	0.30	0.08	0.21	0.65	0.85	0.59	0.11	1		
Zn (ppm)	0.14	-0.21	-0.11	0.22	0.28	0.59	0.07	0.45	1	
Cu (%)	0.68	0.22	0.36	0.37	0.48	0.09	0.14	0.60	0.25	1

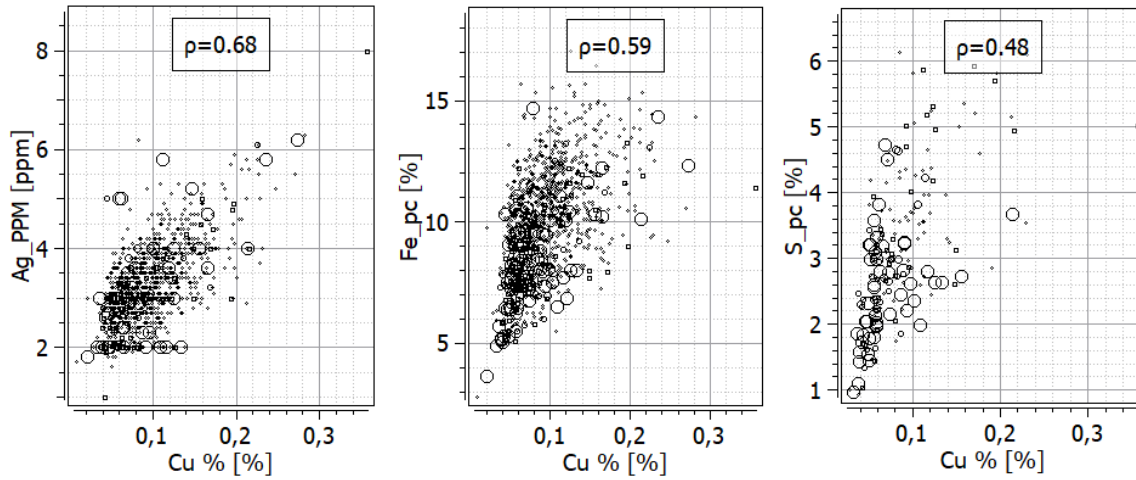


Figure 2. Correlation plots for Cu–Ag, Cu–Fe, and Cu–S

4.3 Variogram analysis

Prior to variogram modelling, all additive variables (Cu^* , Ag^* , Fe^* , S^* , and ρ) were transformed to normal scores using *nscore.exe*, converting each empirical cumulative distribution function to a standard normal distribution (mean = 0, variance = 1) through a quantile-based mapping that preserves rank order. The transformation tables were retained for back-transformation of simulated values to the original grade units after co-simulation. Variogram modelling was performed on the normal-score variables, as the spatial correlation structure must be characterized in Gaussian space to satisfy the assumptions of sequential Gaussian co-simulation.

Experimental direct and cross-variograms were computed for all variable pairs using *gamv.exe*, and theoretical models were fitted using *vargfit.exe*. The resulting linear model of coregionalization (LMC) describes the joint spatial continuity of Ag^* , Cu^* , Fe^* , and S^* through a nugget component and two nested spherical structures, capturing both short-range and long-range spatial correlation. The fitted LMC is expressed in equation (3). All sill matrices were verified to be positive semi-definite, ensuring that the model is admissible for multivariate co-simulation. Direct variograms for each normal-score variable are shown in Figure 3, where the fitted models are superimposed on the experimental values.

$$\begin{aligned}
\gamma \begin{pmatrix} \gamma_{Ag} & \gamma_{Ag/Cu} & \gamma_{Ag/Fe} & \gamma_{Ag/S} \\ \gamma_{Cu/Ag} & \gamma_{Cu} & \gamma_{Cu/Fe} & \gamma_{Cu/S} \\ \gamma_{Fe/Ag} & \gamma_{Fe/Cu} & \gamma_{Fe} & \gamma_{Fe/S} \\ \gamma_{S/Ag} & \gamma_{S/Cu} & \gamma_{S/Fe} & \gamma_S \end{pmatrix} &= \begin{pmatrix} 0.31 & 0.07 & -0.05 & -0.19 \\ 0.07 & 0.24 & -0.02 & -0.10 \\ -0.05 & -0.02 & 0.19 & 0.11 \\ -0.19 & -0.10 & 0.11 & 0.17 \end{pmatrix} \text{nugget} + \\
\begin{pmatrix} 0.47 & 0.30 & 0.35 & 0.18 \\ 0.30 & 0.26 & 0.22 & 0.25 \\ 0.35 & 0.22 & 0.44 & 0.22 \\ 0.18 & 0.25 & 0.22 & 0.39 \end{pmatrix} \text{sph}(9.32m, 7.7m, 400m) + \\
\begin{pmatrix} 0.22 & 0.25 & 0.20 & 0.35 \\ 0.25 & 0.50 & 0.38 & 0.54 \\ 0.20 & 0.38 & 0.29 & 0.43 \\ 0.35 & 0.54 & 0.43 & 0.66 \end{pmatrix} \text{sph}(132.66m, 142.24m, 5m)
\end{aligned} \tag{3}$$

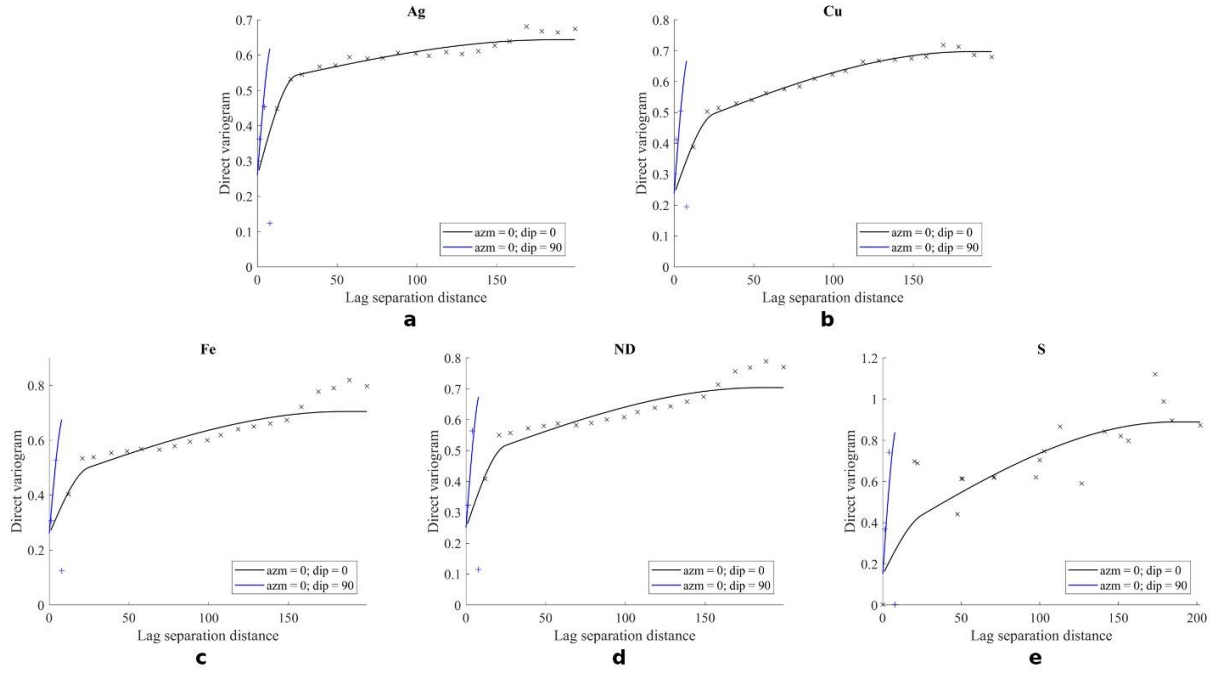


Figure 3. Direct variograms: a – Ag*, b – Cu*, c – Fe*, d - normalized density (ND), e – S*.

4.4 Simulation Results

Following co-simulation in BLOCKSGCOSIM, the Gaussian realizations of the additive variables (Cu*, Ag*, Fe*, S*) were back-transformed to normal-score space and subsequently converted to grade units through post-processing in ISATIS. Block grades were recovered by dividing each simulated additive variable by the corresponding simulated bulk density, as described in Section 3.3, ensuring mass-consistent grade reconstruction at the $5 \times 5 \times 1$ m reporting support.

To summarize spatial patterns across all 100 realizations, E-type maps were computed for each variable under both workflows. Figure 4 presents the E-type maps for Cu, Ag, Fe, and S, respectively, with the direct block co-simulation result shown on the left and the conventional point co-simulation result on the right.

In general, the spatial patterns observed in the E-type maps are largely consistent across the two workflows for all four variables. Both methods produce a similar overall grade distribution within the tailings footprint, although the block-support results show slightly reduced local variability. Specifically, elevated Cu and Ag values are concentrated in similar areas, and the spatial trends of Fe and S show comparable shapes and magnitudes, with slightly smoother transitions in the block-support results.

This visual agreement suggests that the two workflows converge to similar representations of the average grade field at block support, with minor differences in local variability. The block-support results are, however, slightly smoother than the point-support ones. This is most visible in the continuity of grade zones, where local fluctuations are less pronounced in the direct workflow. The difference is subtle but consistent and reflects the use of internal discretization during simulation.

The first realizations for each variable are presented in Figure 5. Unlike the E-types, individual realizations capture local variability and reflect the stochastic nature of the simulation. The first realizations from both workflows display similar spatial structures, though local differences between individual realizations are expected and do not indicate systematic divergence between the methods, while a slight reduction of small-scale variability is visible in the block-support results. These differences arise primarily from the stochastic nature of the simulation, but a slight reduction of small-scale variability is visible in the block-support realizations. This reflects the averaging effect introduced by internal discretization during simulation rather than methodological bias.

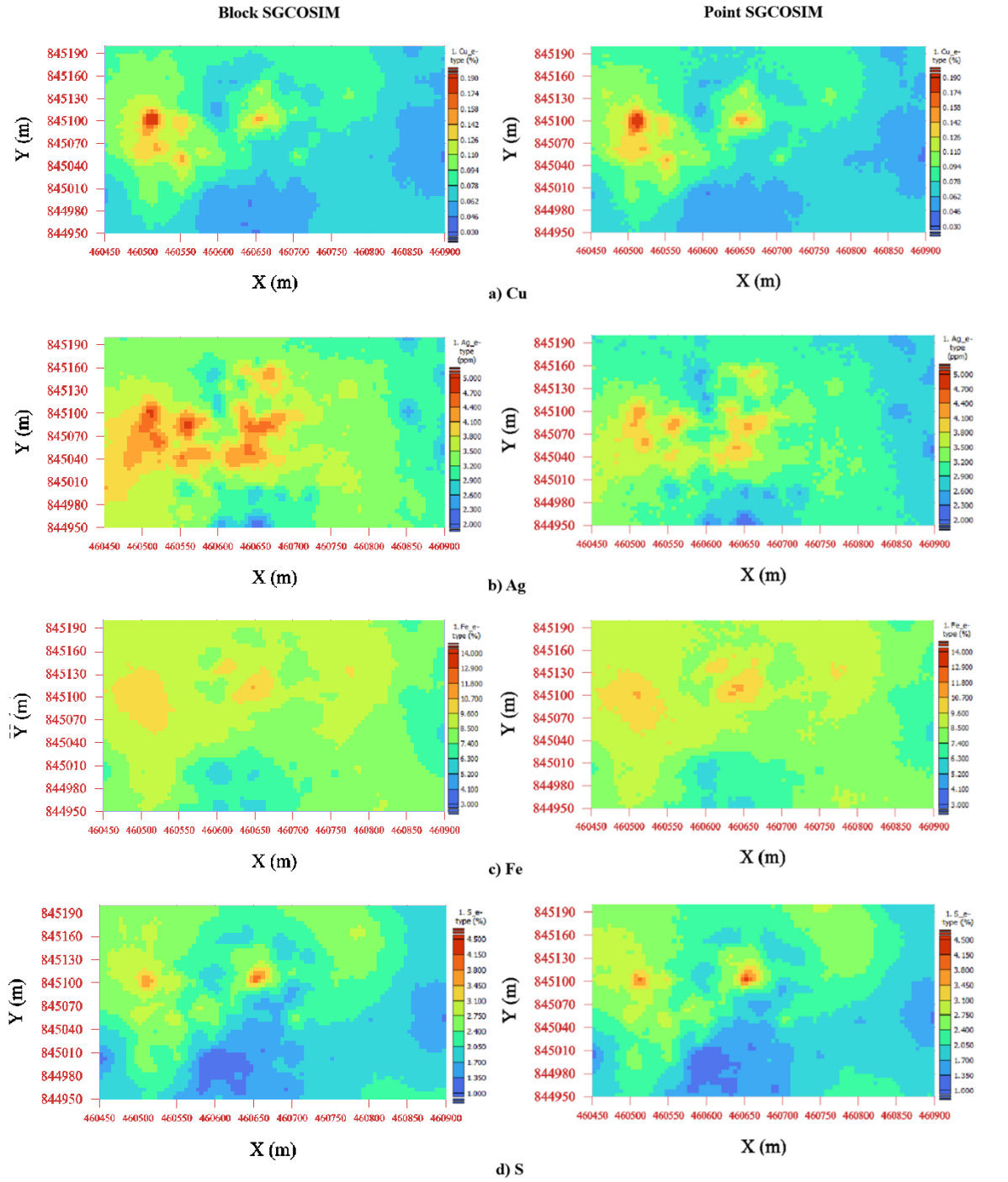


Figure 4. E-type maps for Block SGCOSIM (left) and Point SGCOSIM (right): a) Cu (%), b) Ag (ppm), c) Fe (%), d) S (%).

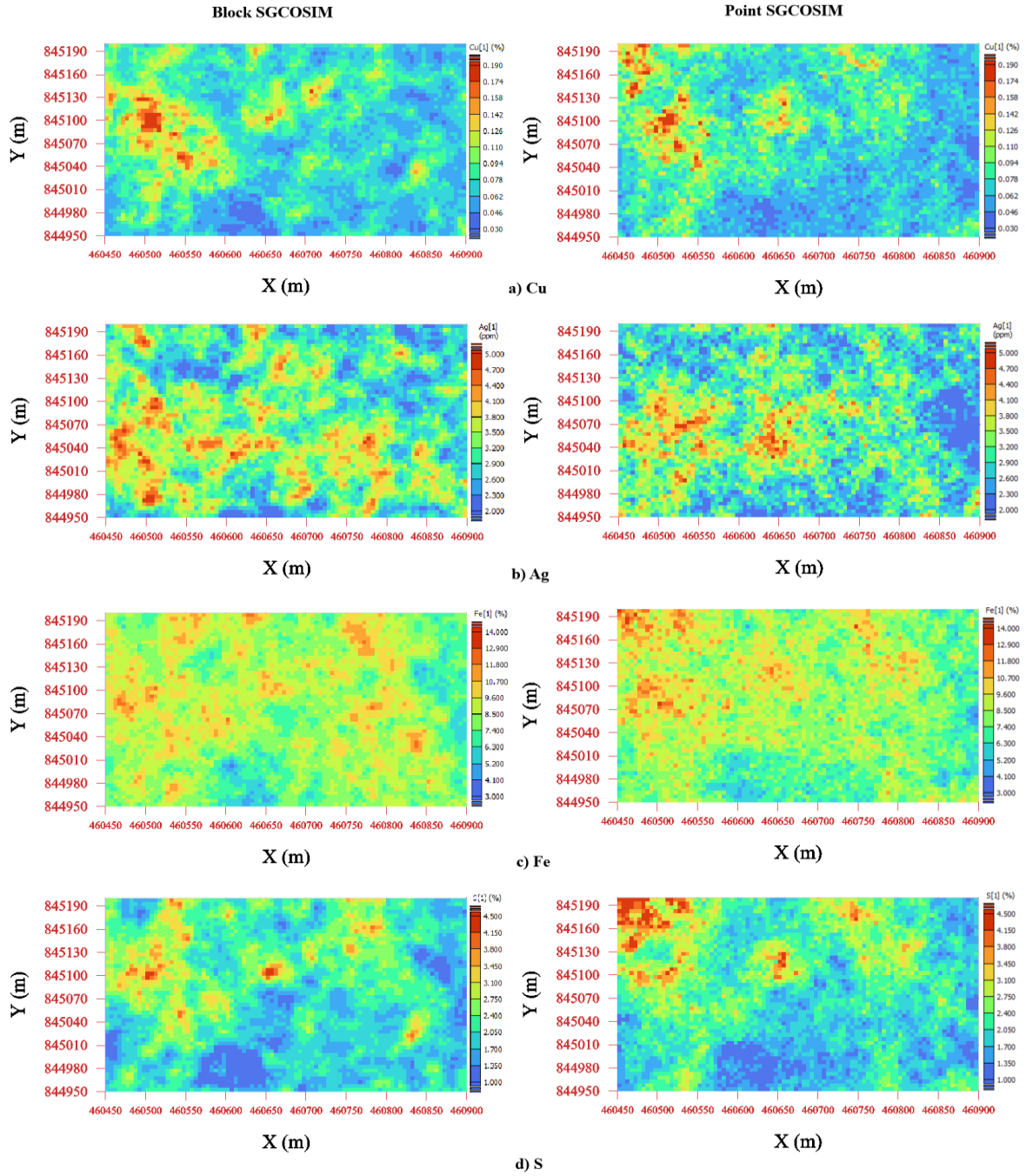


Figure 5. First realizations of Block SGCOSIM (left) and Point SGCOSIM (right): a) Cu (%), b) Ag (ppm), c) Fe (%), d) S (%).

4.5 Geostatistical Validation

Geostatistical validation was carried out to evaluate how the two workflows reproduce the statistical and spatial characteristics of the dataset at block support. The assessment includes histogram reproduction, summary statistics, inter-variable relationships, and variogram behavior.

The comparison of marginal distributions is shown in Figure 6, which presents histograms of the original data alongside the first realization from both workflows. For all variables, the simulated distributions follow the overall shape of the original data, with Cu and Ag remaining positively skewed and Fe and S showing more compact distributions. At the same time, both workflows produce visibly narrower histograms than the original dataset, with less pronounced tails, indicating a reduction in variability at block support. This effect is consistent across all variables and appears similar for both block and point co-simulation.

The same pattern is reflected in the summary statistics reported in Table 2, where mean values remain close to the original data for all variables. For example, the mean Cu grade changes from 0.0838 in the original dataset to 0.086 for Block SGCOSIM and 0.0855 for Point SGCOSIM, while similar agreement is observed for Ag, Fe, and S. In contrast, standard deviations are consistently reduced in both workflows relative to the original data. For Cu, the standard deviation decreases from 0.0427 to 0.025 (block) and 0.0270 (point), and comparable reductions are observed for the remaining variables. Minimum and maximum values are also less extreme after simulation, further confirming the reduction in dispersion caused by block-support averaging. The reduction is slightly stronger in the block-support results than in the point-support ones, which indicates that internal discretization introduces a marginally higher degree of smoothing.

Inter-variable relationships were evaluated using both scatter plots and correlation coefficients. The scatter plots in Figure 7 (Block SGCOSIM) and Figure 8 (Point SGCOSIM) show that the general positive relationships between Cu-Ag, Cu-Fe, and Cu-S are preserved in both workflows. The Cu-Ag relationship remains visible but becomes more diffuse, while the Cu-Fe and Cu-S relationships appear more compact, particularly at higher values. The overall structure of the point clouds is similar between the two workflows, with no systematic differences in trend direction or distribution shape, although the block-support results appear slightly more compact due to reduced local variability.

These observations are supported by the correlation coefficients reported in Table 3. The Cu-Ag correlation decreases from 0.68 in the original data to 0.45 (block) and 0.46 (point), while Cu-Fe increases from 0.59 to 0.75 (block) and 0.77 (point), and Cu-S increases from 0.48 to 0.82 and 0.84. The values obtained from the two workflows are nearly identical for all variable pairs, indicating that both approaches reproduce inter-variable relationships in a similar way.

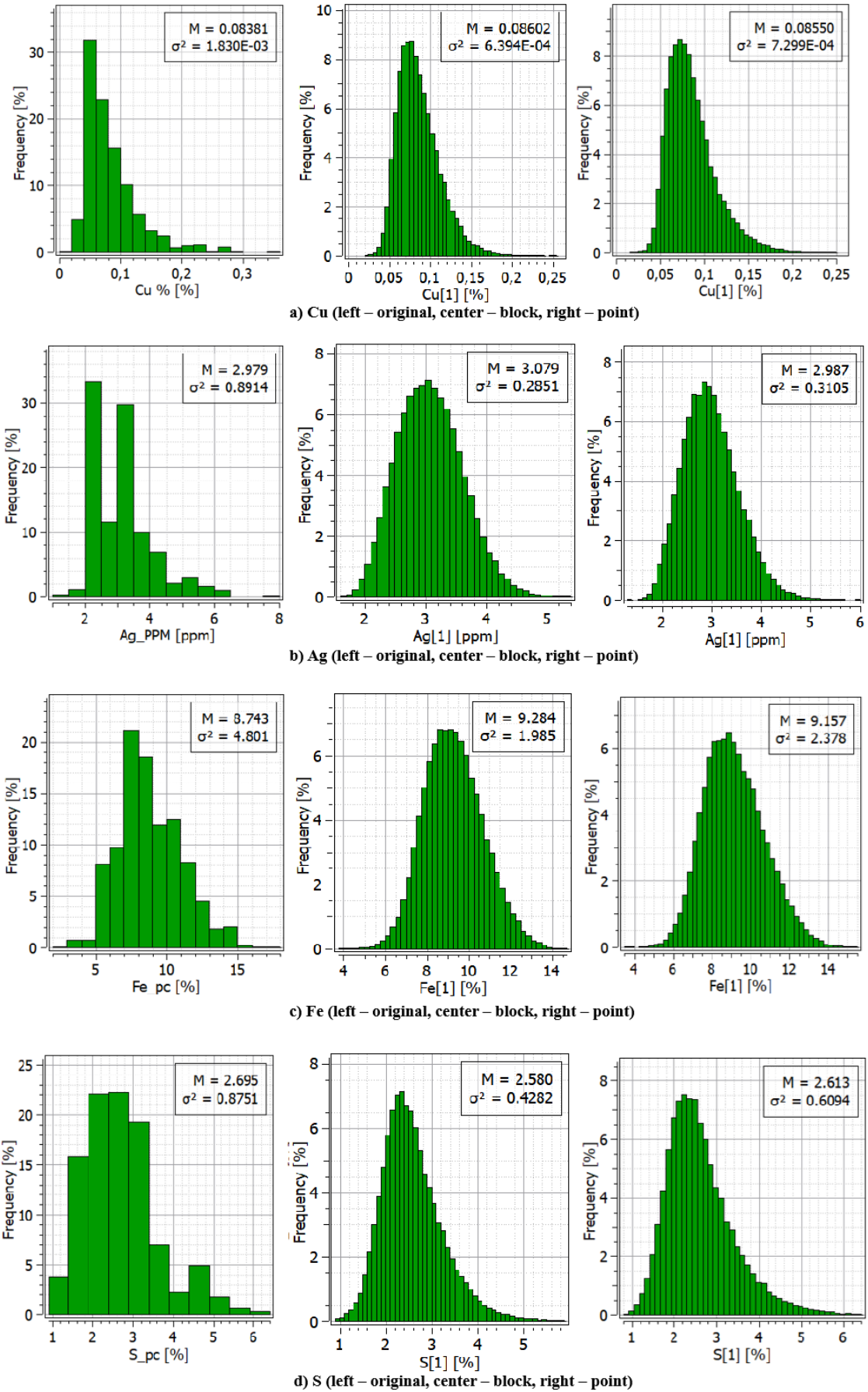


Figure 6. Comparison of histograms for original values and first realizations after block and point co-simulation

Table 2. Comparison of statistical parameters of original values and values after block and point co-simulations.

Statistical Parameter	Element	Original	Block Co-simulation: Realization 1	Point Co-simulation: Realization 1
Mean	Cu	0.0838	0.086	0.0855
	Ag	2.979	3.079	2.987
	Fe	8.743	9.284	9.157
	S	2.695	2.580	2.613
Standard Deviation	Cu	0.0427	0.025	0.0270
	Ag	0.9442	0.534	0.5573
	Fe	2.191	1.409	1.542
	S	0.9364	0.654	0.7806
Min Value	Cu	0.01	0.022	0.018
	Ag	1	1.978	1.349
	Fe	2.79	3.827	3.572
	S	0.93	0.919	0.893
Max Value	Cu	0.36	0.251	0.246
	Ag	8	5.361	5.975
	Fe	17.01	14.604	15.468
	S	6.13	5.838	6.373

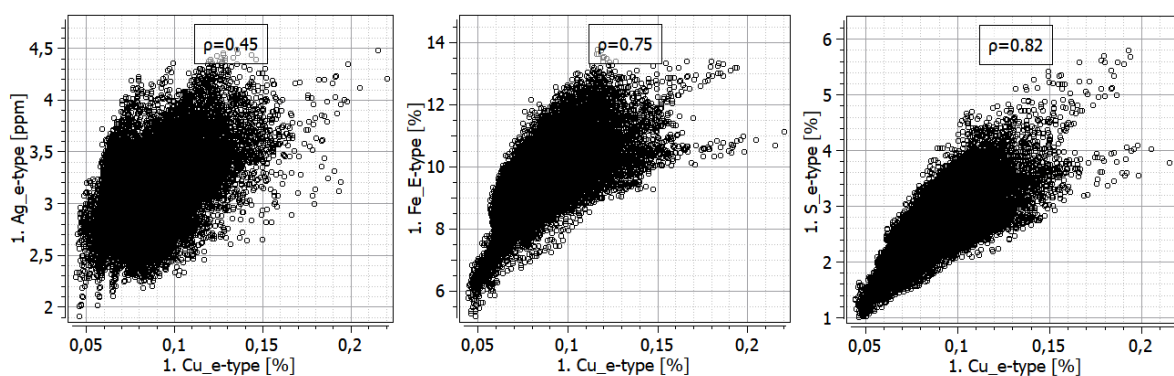


Figure 7. Correlation plots after block SGCOSIM (top left - Cu-Ag, top right - Cu-S, bottom center - Cu-Fe)

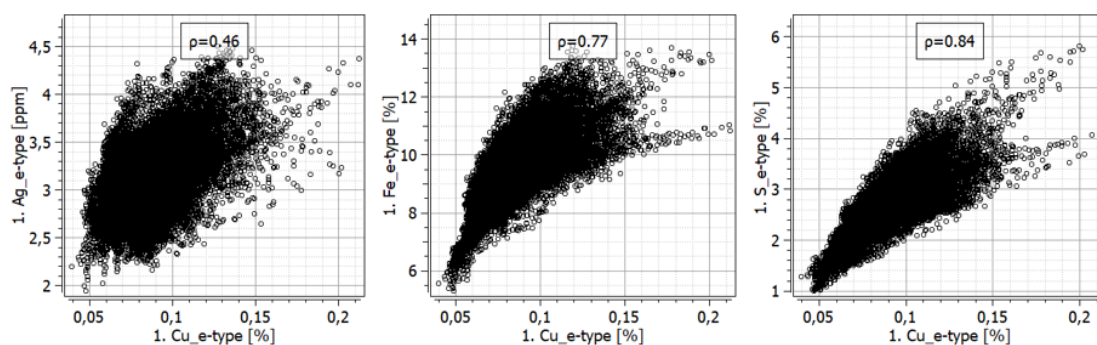


Figure 8. Correlation plots after point SGCOSIM (top left - Cu-Ag, top right - Cu-Fe, bottom center - Cu-S)

Table 3. Comparison of correlation factors of original dataset and after Block and Point Sequential Gaussian Co-Simulations

	Original	Block SGCOSIM	Point SGCOSIM
$\rho(\text{Cu-Ag})$	0.68	0.45	0.46
$\rho(\text{Cu-Fe})$	0.59	0.75	0.77
$\rho(\text{Cu-S})$	0.48	0.82	0.84

Variogram reproduction was assessed by comparing the average experimental variograms from multiple realizations with the theoretical block-support model. As shown in Figure 9, the mean experimental variograms for Cu, Ag, Fe, and S follow the theoretical model closely over the full range of lag distances. Individual realizations form a relatively narrow band around the mean, with slightly greater dispersion for Fe and S at larger lags. The overall agreement between experimental and theoretical variograms is similar for both workflows.

Overall, the validation results show that both workflows reproduce the main distributional, relational, and spatial characteristics of the dataset at block support. Differences between the two sets of results are small and consistent across all validation measures.

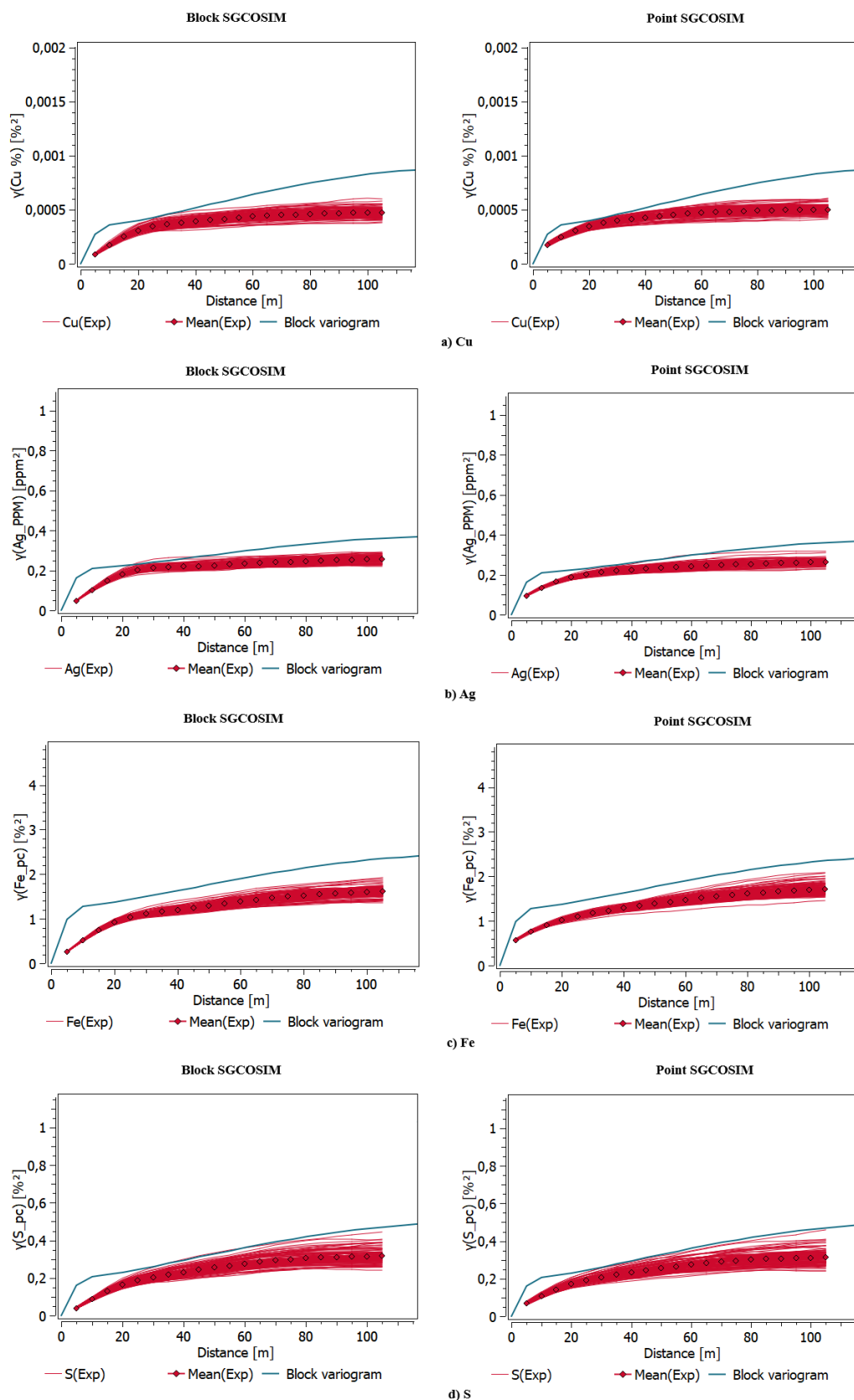


Figure 9. Variogram reproduction for Block SGCOSIM (left) and Point SGCOSIM (right) for a) Cu, b) Ag, c) Fe, and d) S. Red lines - individual realization variograms; diamonds - mean of realizations; solid blue line – theoretical block variogram model.

5. DISCUSSION

5.1 Main comparative outcome of the two workflows

The central result of this study is that the two workflows converge to very similar block-scale models, with minor differences in local variability. In the conventional workflow, values are first simulated on a fine $1 \times 1 \times 1$ m grid and only then averaged to the $5 \times 5 \times 1$ m reporting support. In the direct workflow, the same reporting support is handled inside BLOCKSGCOSIM through internal discretization. Despite this procedural difference, the output remains closely aligned across all main checks, although small differences in variability can be observed.

This agreement is already visible in the E-type maps shown in Figure 4, where Cu, Ag, Fe, and S display the same broad spatial patterns under both workflows, with slightly smoother transitions in the direct block-support results. High-value zones occur in the same areas, low-value domains remain in the same parts of the tailings body, and no systematic shift appears from one method to the other, although small-scale variability is slightly reduced in the direct workflow. The first realizations in Figure 5 lead to the same conclusion. Local differences exist, and they are small and spatially scattered rather than directional or persistent, with slightly lower variability in the direct workflow. That matters because a methodological bias would usually appear as a recurring spatial contrast between the two workflows. Here, that contrast is absent.

The numerical validation supports the same conclusion. As reported in Table 2, mean values for all four variables remain very close between the two approaches, and the differences are minor relative to the magnitude of the variables. The same pattern appears in Table 3, where the correlation coefficients obtained from Block SGCOSIM and Point SGCOSIM are very similar for all tested pairs. Variogram reproduction leads to the same interpretation: in Figure 9, the mean experimental variograms for both workflows follow the theoretical block-support model, and the width of the realization bands is comparable.

Taken together, these results indicate that the choice between direct and conventional support handling does not materially change the large-scale structure of the final block model, although minor differences in variability remain at the $5 \times 5 \times 1$ m scale used in this study. This outcome is consistent with the design of the comparison. Both workflows use the same input dataset,

the same density-based transformation, the same normal-score framework, and the same linear model of coregionalization. Once those components are fixed, the main remaining question is whether internal averaging and external averaging produce different block-scale behavior. In this case, they do not materially differ on a large scale, although minor differences in local variability are present due to the internal discretization in the direct workflow.

For this reason, the two workflows should not be viewed here as competing statistical models. They are better understood as two implementations of the same multivariate modeling logic under a common block-support target. The important difference is therefore not model quality, but how efficiently that similar result is obtained, with the direct workflow producing slightly smoother realizations.

5.2 Support effect, smoothing, and reduction of extreme values

The most consistent statistical change observed in both workflows is the reduction of variability relative to the original sample data. This appears clearly in the histograms shown in Figure 6 and in the standard deviations reported in Table 2. For all four variables, the simulated block models retain the overall distributional shape of the original data, but the distributions become narrower and the tails contract. The same pattern is visible in the minimum and maximum values, which are less extreme after simulation.

This result is expected from geostatistical theory, yet it remains important to state it explicitly. The direct block-support workflow shows a slightly stronger smoothing effect, as internal discretization performs block averaging during simulation rather than after simulation. The input samples represent a smaller support than the final reporting blocks. Once values are represented at $5 \times 5 \times 1$ m support, local extremes are averaged together with neighboring material, and the resulting block distribution becomes less dispersed. In other words, the reduction in spread is not a sign of model failure. It is the direct statistical consequence of the change of support, as established in classical geostatistics and recoverable resource theory (Journel and Huijbregts, 1978; Rossi and Deutsch, 2014).

The magnitude of this reduction is also coherent with the workflow design. For Cu, the standard deviation declines from 0.0427 in the original data to 0.025 in Block SGCOSIM and 0.0270 in Point SGCOSIM. Ag, Fe, and S follow the same pattern, although the degree of contraction varies by variable. This indicates that the block-support effect is not uniform across the dataset

but depends on the original dispersion and spatial continuity of each variable prior to averaging. Cu and Ag, for example, exhibit pronounced positive skewness in the original data; consequently, when modeled at block support, their upper tails are reduced more noticeably.

The direct workflow is, in some cases, slightly smoother than the conventional one, especially for Cu and Ag. The difference is small, but it is consistent with the sequence of operations and reflects the stronger smoothing introduced by internal discretization in the direct workflow. In the direct workflow, the block average is imposed during simulation. In the conventional workflow, the average is imposed afterward, after 25 point-support values have already been generated within each block. The two procedures converge to similar results, but the direct method leaves slightly less room for very local fluctuations to persist in the final block values.

That said, the difference should not be overstated. It affects local variability rather than large-scale spatial patterns. The dominant effect in Table 2 is not the contrast between workflows; it is the contrast between sample support and block support. This is a more useful way to read the results. The block model is smoother because it represents the deposit at block support rather than at sample support. The direct workflow does not create a new smoothing problem; it reproduces the same support-related smoothing already inherent in the conventional approach.

This point is especially relevant in tailings applications. The purpose of the model here is not to recover sample-scale extremes, but to represent the material at the support where decisions are made. Reprocessing options, environmental screening, and uncertainty assessment are all evaluated on blocks or larger domains, not on individual drillhole intervals. In that context, preservation of physically meaningful block-scale variability matters more than persistence of every local extreme present in the raw data.

5.3 Multivariate behavior after transformation and co-simulation

The multivariate results are more complex than the univariate results. On the one hand, both workflows reproduce the same inter-variable structure after simulation. On the other hand, that reproduced structure does not match the original sample-scale correlations exactly. This behavior is most clearly observed in Table 3 and in the correlation plots shown in Figures 7 and 8.

The first important point is that the two workflows behave almost identically. The Cu-Ag correlation changes from 0.68 in the original data to 0.45 and 0.46 in the block and point workflows, respectively (Table 3). Cu-Fe changes from 0.59 to 0.75 and 0.77, and Cu-S from 0.48 to 0.82 and 0.84. These are not minor numerical coincidences. They show that the support-handling strategy itself is not driving correlation changes. Whatever alters the correlations acts before the two workflows diverge, or at least outside the internal-versus-external averaging step.

The more difficult question is why correlations change in different directions. Cu-Ag weakens, whereas Cu-Fe and Cu-S strengthen. The results suggest that the answer lies in the full modeling chain rather than in one single operation. First, the variables are transformed to normal-score space, which standardizes their marginal distributions and preserves rank order while altering linear relationships and the influence of extreme values. Second, the multivariate structure is imposed through the fitted LMC in Eq. (1), which represents spatial co-dependence through admissible direct and cross-variogram structures rather than through raw Pearson correlations alone. Third, the final grades are recovered through the density-based back-transformation, so each simulated additive variable is divided by simulated density. Once several variables share the same denominator, some pairwise relationships can tighten while others weaken.

The behavior of Cu-S and Cu-Fe is particularly understandable in this context. Both pairs are linked to sulfide-bearing and Fe-rich mineral assemblages in the tailings. Their stronger correlations after simulation are therefore consistent with a modeling framework that emphasizes common spatial structure and shared block-scale continuity. The Cu-Ag pair behaves differently. Its original relationship is clear in Figure 2, but after simulation the point clouds in Figures 7 and 8 become more diffuse. That suggests part of the Cu-Ag association present in the raw data may occur at a finer scale than the final block support, or may be expressed more strongly in sample-scale grade variability than in block-scale spatial co-structure.

This distinction is important. A multivariate block model is not required to reproduce every sample-scale correlation exactly. Its first task is to reproduce a coherent spatial co-structure at the target support. In this study, both workflows do that in a stable and internally consistent way, as shown by the near-identical correlation coefficients and the similar scatter-plot geometry in Figures 7 and 8. At the same time, the results make clear that preservation of raw

linear correlation is not automatic, even when the same variables are simulated jointly. In multivariate geostatistics, the LMC governs spatial covariance; it does not guarantee exact preservation of all Pearson correlations after transformation and back-transformation (Goovaerts, 1997; Chilès and Delfiner, 2012).

That result strengthens one of the broader motivations of the thesis. In multivariate tailings modeling, it is not enough to simulate variables side by side. The modeling chain must be read as a linked system: additive transformation, Gaussian transformation, coregionalization, simulation, and back-transformation all affect the final relationships between variables. The present results show that this system remains internally stable across both workflows, but they also show where the strongest distortions can appear.

5.4 Computational Performance

Once the statistical and spatial equivalence of the two workflows is established, computational performance becomes the main practical distinction. In this study, the conventional workflow required approximately 6 hours, whereas the direct workflow completed the same number of realizations in approximately 2 hours and 20 minutes (2.33 hours). This corresponds to a reduction of about 61%.

It should be noted that the reported 6-hour runtime for the conventional workflow refers only to the co-simulation stage. To obtain block-support results, an additional BLKAVG step is required to aggregate the $1 \times 1 \times 1$ m realizations into $5 \times 5 \times 1$ m blocks. This external block-averaging step introduces additional computational time, meaning that the total runtime of the conventional workflow is higher than reported for the simulation stage alone.

It should be noted that post-processing in this study refers to the reconstruction of grades from simulated additive variables (grade $\times$ density), which is carried out in ISATIS for both workflows. Consequently, this step does not contribute to the difference in computational performance. The additional computational burden in the conventional workflow arises from the BLKAVG step, which aggregates point-support simulations into block-support values.

The source of this difference lies in how support is handled. The conventional approach simulates the full $1 \times 1 \times 1$ m grid, which contains $450 \times 250 \times 20 = 2,250,000$ nodes, and then averages those values to reporting blocks. Each realization therefore requires both fine-scale simulation and subsequent aggregation. In contrast, the direct workflow operates at block

support from the outset. Internal discretization is used to approximate block averages, but only block-scale values are retained, and no external averaging step is required.

As a result, the computational cost is reduced at two stages: fewer simulation nodes and output values are stored, and the post-simulation averaging step is eliminated. This leads to a shorter overall runtime and a simpler workflow.

The implication is practical rather than theoretical. Since both workflows produce similar block-scale results, the reduction in runtime directly increases the feasibility of running multiple realizations and updating models. This becomes especially relevant for large datasets or workflows that require repeated simulations, where the additional cost of fine-grid simulation and external averaging can accumulate rapidly. The reported runtimes are specific to the computational hardware and simulation settings used in this study.

6. CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

This study sets out to compare two co-simulation workflows applied to the same multivariate tailings dataset under controlled conditions. Both workflows used identical inputs – variables, transformations, variogram model (Eq. 1), and reporting grid – so any differences arise only from how support is handled.

At the level of spatial results, the two approaches lead to nearly the same outcome. The E-type maps (Figure 4) show that Cu, Ag, Fe, and S follow the same spatial patterns, with high and low values occurring in the same zones. Individual realizations differ locally (as expected for stochastic simulation), but these differences do not persist spatially and do not form systematic patterns.

At the level of statistics, both workflows reproduce the main characteristics of the dataset at block support. Mean values remain close to the original data, while standard deviations decrease for all variables. This reduction appears consistently in Table 2 and in the histogram comparison (Figure 6), where distributions become narrower and extreme values are less frequent. The change follows directly from the shift from sample support to $5 \times 5 \times 1$ m blocks, where local variability is averaged out.

Multivariate behavior is reproduced in a consistent way across both workflows. The correlation coefficients after simulation are almost identical between the two approaches, which shows that support handling does not control inter-variable relationships. At the same time, the correlations differ from those observed in the original dataset. For example, Cu-Ag weakens, while Cu-Fe and Cu-S become stronger. This change occurs after transformation, co-simulation, and back-transformation, where variables are reconstructed using simulated density. The result is not a loss of structure, but a shift in how relationships are expressed at block support.

The main difference between the workflows appears in computational performance. The conventional workflow requires approximately six hours for co-simulation alone, with additional time for block averaging using BLKAVG to aggregate the $1 \times 1 \times 1$ m simulations into $5 \times 5 \times 1$ m blocks. In contrast, the direct workflow produces block-support results in

approximately two hours and twenty minutes, without the need for external block averaging. In both workflows, post-processing is subsequently performed in ISATIS to reconstruct grades from the simulated additive variables (grade $\times$ density) through density-based back-transformation. Therefore, the computational advantage of the direct approach arises solely from differences in support handling and the elimination of the BLKAVG step, rather than from any differences in grade reconstruction.

Taken together, the results show that both workflows produce comparable block-scale models, while the direct approach reduces computational effort. The difference is not in the final model, but in how efficiently that model is obtained.

6.2 Recommendations

The comparison presented in this study is based on a single tailings dataset and a specific set of modeling parameters. Extending the analysis to other deposits would help assess the robustness of the observed behavior under different geological and sampling conditions. For example, datasets characterized by stronger anisotropy or more irregular sampling patterns may respond differently to internal discretization.

The role of discretization in the direct workflow also warrants further investigation. In this thesis, a $5 \times 5 \times 1$ scheme was adopted to match the reporting support; however, alternative configurations could be tested. Varying the number of internal nodes may influence variance reproduction and local variability, particularly in zones with strong spatial gradients.

The treatment of density deserves closer examination. In this study, density is co-simulated and used directly in grade reconstruction, linking all variables through a common denominator. Small variations in density can therefore influence multiple variables simultaneously. Testing alternative density models or incorporating uncertainty in density estimation would help evaluate the robustness of reconstructed grades.

Another potential extension concerns the number of realizations. The present study employs 100 realizations, which is sufficient to observe general patterns. However, the reduced runtime of the direct workflow makes it feasible to generate larger ensembles. This would improve the stability of uncertainty measures and enable more detailed analyses of extreme scenarios.

Finally, the workflow may be applied beyond statistical comparison. In tailings studies, block-scale models are commonly used for reprocessing decisions, environmental risk assessments, and uncertainty analyses. Applying both workflows within such decision-making frameworks would demonstrate whether the computational advantages of the direct approach translate into practical benefits when multiple scenarios or thresholds are evaluated.

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