

Article

A Computational Framework for Reproducible Generation of Synthetic Grain-Size Distributions for Granular and Geoscientific Applications

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Abstract

Particle size distribution (PSD), also referred to as grain-size distribution (GSD), is a fundamental characteristic of granular materials, influencing packing density, porosity, permeability, and mechanical behavior across soils, sediments, and industrial powders. Accurate and reproducible representation of PSD is essential for computational modeling, digital twin development (i.e., virtual replicas of physical systems), and machine learning applications in geosciences and engineering. Despite the widespread use of classical distributions (log-normal, Weibull, Gamma), there remains a lack of systematic frameworks for generating synthetic datasets with controlled statistical properties and reproducibility. This paper introduces a unified computational framework for generating virtual PSDs/GSDs with predefined statistical characteristics and a specified number of grain-size fractions. The approach integrates parametric modeling with two histogram-based allocation strategies: the equal-width method, maintaining uniform bin spacing, and the equal-probability method, distributing grains according to quantiles of the target distribution. Both methods ensure statistical representativeness, reproducibility, and scalability across material classes. The framework is demonstrated on representative cases of soils (Weibull), sedimentary and industrial materials (Gamma), and food powders (log-normal), showing its generality and adaptability. The generated datasets can support sensitivity analyses, experimental validation, and integration with discrete element modeling, computational fluid dynamics, or geostatistical simulations.

Keywords: particle size distribution; grain-size modeling; synthetic datasets; statistical modeling; granular materials; geoscientific simulation; reproducible computation



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1. Introduction

Granular materials are ubiquitous in both natural and engineered systems, encompassing soils, sands, sediments, industrial powders, and bulk solids [1–3]. A fundamental aspect of their characterization is the particle size distribution (PSD), also referred to as the grain-size distribution (GSD), which describes the statistical spread of particle diameters within a granular bed [4–7]. Whether naturally occurring or artificially produced, PSD plays a decisive role in determining the structural, physical, and mechanical behavior of granular systems, as it influences key properties such as packing density, porosity, permeability, mechanical stability, and flowability, making it critical for applications in geotechnics, civil engineering, agriculture, pharmaceuticals, and environmental science [8–14]. In materials science and geosciences alike, PSD informs the interpretation of sediment

transport, soil formation, and diagenetic processes, as well as the design of composites, catalysts, and functional materials, where particle morphology directly affects macroscopic performance [6,13,15–17].

The complexity of PSD analysis arises from the diversity of granular materials and the variability in research objectives. Depending on the context, different statistical models may be more appropriate, and the choice of model can significantly impact the interpretation of experimental data and the accuracy of numerical simulations [18–21]. Classical distributions such as log-normal, Weibull, Rosin–Rammler, and gamma are commonly employed in the analysis of both natural sediments and engineered powders [22–24].

The growing reliance on computational modeling and digital twin concepts in geosciences and materials engineering has amplified the need for robust and reproducible input data, including synthetic PSDs [25–28]. With the rise in simulation-based approaches to soil mechanics, sediment transport, and multiphase flow, generating statistically controlled granular systems has become essential. Despite the availability of PSD models, there is no integrated framework that combines statistical flexibility with reproducibility and scalability across different granular systems. This gap limits the comparability of simulation results and hinders the development of standardized benchmarking protocols.

Beyond empirical measurements, the ability to generate synthetic PSD datasets with predefined statistical characteristics has become increasingly important. Virtual distributions enable controlled simulations, sensitivity analyses, and validation of experimental setups without extensive physical sampling [28–31]. They are particularly valuable when material availability is limited, experiments are costly, or reproducibility across laboratories is required. Moreover, synthetic datasets allow systematic exploration of hypothetical or extreme scenarios, facilitating investigations into how variations in PSD affect macroscopic behaviors such as compaction, permeability, or rheological response [32–34]. However, despite these advantages, existing approaches lack a unified, reproducible framework for generating synthetic PSDs across diverse granular systems, i.e., a gap this study aims to fill.

To address these limitations, this study introduces a unified framework for systematic generation of virtual PSDs with predefined statistical properties and a specified number of particle size fractions. The framework integrates parametric modeling constrained to strictly positive domains, reflecting the physical reality that particle diameters cannot be negative, with two complementary histogram binning procedures. The equal-width approach ensures uniform bin spacing across the particle size range, while the equal-probability approach allocates particles according to quantiles of the target distribution. Together, these methods balance resolution control with statistical representativeness, ensuring reproducibility and scalability across different granular systems. This directly addresses the identified gap by providing a standardized, scalable methodology for virtual PSD generation.

It should be emphasized that the proposed method does not introduce a new probabilistic distribution. Rather, it generates a synthetic grain-size distribution by numerically reproducing the analytical form of one selected model from the predefined set of twelve classical GSDs.

The applicability of the framework is demonstrated through case studies using literature data for soils (Weibull distributions) [35,36], industrial granular materials (Gamma distributions) [37], and food powders (log-normal distributions) [38]. These examples highlight how the proposed methodology differs from earlier model-specific or case-dependent approaches by offering a generalizable and integrative perspective. By combining theoretical insights with practical computational tools, the framework bridges the gap between empirical data collection and virtual material simulation. It provides reproducible and application-ready datasets for discrete element modeling (DEM), computational fluid

dynamics (CFD), and geostatistical modeling, paving the way for standardized protocols, virtual replicas of physical systems (i.e., so-called “digital twins”), and open science initiatives in granular and geoscientific research.

2. Review of Mathematical Models for Particle Size Distribution in Granular Systems

The mathematical description of particle size distribution has been the subject of intensive research due to its fundamental role in governing the structural and functional properties of granular materials. Various models have been proposed, ranging from purely empirical equations to probability-based statistical distributions [18–20,22,39–41]. Each model offers distinct advantages in terms of interpretability, computational efficiency, and ability to reproduce experimental data across a wide range of particle sizes. The choice of an appropriate model is therefore not only a methodological consideration but also a determinant of the predictive reliability of granular system simulations.

Among the most applied approaches are empirical models, such as the Rosin–Rammler and Gaudin–Schuhmann distributions, historically used in mining, powder technology, and soil mechanics. These models provide relatively simple closed-form expressions that capture the general shape of PSDs but lack flexibility when applied to highly heterogeneous or multimodal samples [24,42–44].

In contrast, analytical and statistical models derived from probability theory offer greater adaptability. Distributions such as normal, log-normal, Weibull, gamma, and beta are widely used in materials science and geotechnical engineering because they are mathematically well-defined for non-negative values and can accommodate skewness and kurtosis typical of granular data [11,37,38,45]. For example, the log-normal distribution is particularly suitable for naturally fragmented or weathered materials, while the Weibull distribution provides a useful framework for systems governed by fracture and breakage processes.

The selection of a PSD model is context dependent. Factors such as the origin of the material, the measurement technique (e.g., sieve analysis, laser diffraction, or image-based methods), and the intended application strongly influence model suitability. Geotechnical analyses often favor simple parametric models for rapid classification, whereas pharmaceutical applications may require high-resolution statistical modeling to ensure reproducibility and regulatory compliance.

Table 1 summarizes the most frequently applied models for describing PSDs in granular systems. It emphasizes practical aspects, including typical applications, advantages, and limitations, providing guidance for model selection depending on material type, research objectives, and data availability.

In addition to widely applied log-normal, Rosin–Rammler, or Weibull functions, a number of less common empirical and process-based distributions have been used in specialized domains. These include the Fredlund function in geotechnical engineering [46,47], the Gompertz and Johnson families for asymmetric or skewed PSDs [48–51], and process-derived functions such as the Lifshitz–Slyozov–Wagner (LSW) model for Ostwald ripening or the Nukiyama–Tanasawa law in spray atomization research [52–55]. While these models often provide superior fit within their original domains, their broader applicability is constrained by mathematical complexity or domain-specific assumptions. Nevertheless, they highlight the diversity of approaches to PSD modeling, bridging purely statistical fitting with physically grounded process descriptions.

Table 1. Applications, advantages, and limitations of empirical and statistical models for describing particle size distributions in granular systems.

Distribution Model	Typical Applications	Advantages	Limitations
Normal (Gaussian)	basic modeling, unimodal PSDs	simple, intuitive	allows negative diameters, poor fit for skewed PSDs
Rosin–Rammler	mining, comminution, powder technology	simple, widely used, good for crushed materials	limited flexibility for multimodal or skewed PSDs
Gaudin–Schuhmann	soil mechanics, mineral processing	easy to apply, intuitive	oversimplified, cannot represent fine fractions accurately
Log-normal	sediments, soils, natural materials	flexible, suitable for naturally fragmented systems	poor fit for strongly asymmetric or bimodal PSDs
Weibull	fracture mechanics, powders, reliability	versatile, models breakage-dominated processes	parameter estimation sensitive to data quality
Gamma	civil engineering, porous media	flexible, effectively models skewness	requires iterative fitting, rarely used
Beta	normalized fractions, fine powders	highly flexible, models symmetric and asymmetric shapes	requires normalization, limited intuitive interpretation
Fredlund	soil mechanics, gradation curves	captures soil gradation	domain-specific
Gompertz	biological fragmentation	suitable for skewed, bounded distributions	weak physical basis
Jaky	geotechnics, soil PSDs curves	simple, soil-specific	very limited applicability
Johnson (SU, SB, SL, SN)	flexible fitting of skewed PSDs	very versatile, mimics many distributions	complex parameter fitting
Lifshitz–Slyozov–Wagner	Ostwald ripening, metallurgy	process-based, time-dependent description	valid only for diffusion-controlled growth
Nukiyama–Tanasawa	sprays, atomization, combustion	classical spray droplet law	limited to atomization processes
Skaggs	soil physics, hydrology	links PSD with hydraulic properties	soil-specific, limited general use

3. Mathematical Foundations of Particle Size Distribution Generation

This section outlines the mathematical foundations underlying the generation of virtual particle size distributions. A key requirement for constructing synthetic granular systems is the availability of a well-defined cumulative distribution function (CDF), preferably in closed analytical form. The CDF directly relates particle size to its probability of occurrence, enabling reproducible sampling of particle diameters and controlled generation of synthetic granular systems. Table 2 summarizes the availability and form of CDFs across commonly applied PSD models, distinguishing between those with closed-form solutions, empirically defined functions, and models requiring numerical integration.

Table 2. Availability and form of cumulative distribution functions for particle size distribution models.

Distribution Model	CDF Availability
Normal (Gaussian)	closed form (via error function)
Log-normal	closed form (via normal CDF of $\log(x)$)
Weibull	closed form
Rosin–Rammler	closed form (special case of Weibull model)
Gaudin–Schuhmann	closed form (power law)
Gamma	closed form (via incomplete gamma function)
Beta	closed form (via incomplete beta function)
Gompertz	closed form
Johnson (SU, SB, SL, SN)	closed forms (transformations of normal CDF)
Fredlund	defined empirically
Jaky	defined empirically
Skaggs	defined empirically
Lifshitz–Slyozov–Wagner	no closed form—requires numerical integration
Nukiyama–Tanasawa	no closed form—requires numerical integration

Based on the availability of clearly defined, closed-form cumulative distribution functions, only distributions suitable for reproducible numerical generation were selected for further consideration. The selected models, presented in Table 3, include the Normal, Log-normal, Weibull (with Rosin–Rammler as a special case), Gaudin–Schuhmann, Gamma, Beta, Gompertz, and Johnson families (SU, SB, SL, SN). In the following sections, these distributions provide the mathematical foundation for constructing virtual particle size distributions.

Table 3. Cumulative distribution functions of the considered PSD models, together with the interpretation of their parameters.

Distribution Model	CDF	Model Parameter(s)
Normal (Gaussian)	$\frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x-\mu}{\sigma\sqrt{2}} \right) \right]$	μ —mean particle diameter, σ —standard deviation (spread)
Log-normal	$\frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sigma\sqrt{2}} \right) \right], x > 0$	μ —mean of $\ln x$, σ —spread of $\ln x$
Weibull	$1 - \exp \left[- \left(\frac{x}{\lambda} \right)^k \right], x \geq 0$	λ —scale parameter, k —shape parameter
Rosin–Rammler	$1 - \exp \left[- \left(\frac{x}{x_0} \right)^n \right], x \geq 0$	x_0 —characteristic particle size, n —spread parameter
Gaudin–Schuhmann	$\left(\frac{x}{x_{max}} \right)^n$	n —shape parameter
Gamma	$\frac{1}{\Gamma(\alpha)} \int_0^{x/\beta} t^{\alpha-1} e^{-t} dt, x \geq 0$	α —shape parameter, β —scale parameter
Beta	$I_x(\alpha, \beta), x \in [0, 1]$	α, β —shape parameters
Gompertz	$1 - \exp[-b(\exp(cx) - 1)], x \geq 0$	b —scale parameter, c —growth/shape
Johnson SU	$\Phi \left[\gamma + \delta \sinh^{-1} \left(\frac{x-\xi}{\lambda} \right) \right]$	γ, δ —shape parameters, ξ —location, λ —scale parameter

Table 3. Cont.

Distribution Model	CDF	Model Parameter(s)
Johnson SB	$\Phi\left[\gamma + \delta \ln\left(\frac{x-\xi}{\xi+\lambda-x}\right)\right], x \in [\xi, \xi + \lambda]$	γ, δ —shape parameters, ξ —location, λ —scale parameter
Johnson SL	$\Phi[\gamma + \delta \ln(x - \xi)], x > \xi$	γ —shape parameter, ξ —location, δ —scale parameter
Johnson SN	$\Phi\left[\gamma + \delta \frac{x-\xi}{\sqrt{(x-\xi)^2 + \lambda^2}}\right]$	γ, δ —shape parameters, ξ —location, λ —scale parameter

4. Procedures for Generating Virtual Particle Size Distributions

Generating a particle size distribution (PSD) involves creating a histogram that represents the number of particles within defined diameter ranges. Each bin corresponds to a particle size fraction, and the count in each bin reflects the number of particles within that range. For virtual granular systems used in simulations, larger numbers of bins and total particles are typically employed to ensure statistical robustness and high resolution. In contrast, physically assembled granular beds are constrained by material availability and labor, limiting both the range of particle diameters and the total number of particles.

Two procedures are proposed:

- The equal-width method, which ensures uniform bin spacing across the size range;
- The equal-probability method, which partitions the distribution into bins of equal probability mass based on the target CDF.

Each method has its own advantages and limitations, making them suitable for different applications [56,57].

4.1. Equal-Width Bin Method

Objective—to create a histogram where all bins have the same width in terms of particle size (i.e., mm), and the bar heights represent the probability density function (PDF).

Step 1: Define the number of histogram bins and range

Choose the number of bins N (this value determines the histogram resolution and can be chosen according to the application or desired granularity) and determine the particle size range $[d_{min}, d_{max}]$, then compute the bin width:

$$\Delta d = \frac{d_{max} - d_{min}}{N} \quad (1)$$

Step 2: Compute bin boundaries

$$x_i = d_{min} + i \cdot \Delta d, \quad i = 0, \dots, N. \quad (2)$$

Step 3: Generate samples using inverse transform sampling

Generate M uniform random values $u_j \sim U(0, 1)$. To avoid numerical instabilities (i.e., division by zero or undefined quantile values) at the boundaries (i.e., $u = 0$ or $u = 1$), uniform values should be restricted to a safe range such as e.g., $u_j \in (0.0001, 0.9999)$, then map them to particle sizes using the inverse CDF:

The expected number of samples n_i in each bin $[x_{i-1}, x_i]$ is calculated as:

$$x_j = F^{-1}(u_j), \quad (3)$$

where F^{-1} is the quantile function of the target distribution.

Step 4: Assign samples to bins and compute PDF

Count the number of samples n_i in each bin, and compute the PDF for each bin:

$$\text{PDF} = \frac{n_i}{M \cdot \Delta d}. \quad (4)$$

The resulting histogram approximates the probability density function of the target distribution.

4.2. Equal-Probability Bin Method

Objective—to create a histogram where each bin represents the same probability mass, resulting in variable bin widths.

Step 1: Define the number of histogram bins

Let N be the desired number of bins in the histogram.

Step 2: Determine the bins boundaries using the inverse CDF

To partition the probability space uniformly, the bin boundaries $x_0, x_1, \dots, x_N$ are computed using the inverse CDF (quantile function):

$$x_i = F^{-1}\left(\frac{i}{N}\right), \quad i = 0, \dots, N. \quad (5)$$

This ensures each bin represents an equal probability mass of $\frac{1}{N}$, resulting in variable bin widths depending on the distribution shape.

Step 3: Generate samples using inverse transform sampling

Same as in the equal-width method, i.e., using Equation (3).

Step 4: Assign samples to bins and compute PDF

Given a total number of samples M , the expected number of samples n_i in each bin $[x_{i-1}, x_i]$ is calculated as:

$$\text{PDF} = \frac{n_i}{M \cdot (x_i - x_{i-1})}. \quad (6)$$

This directly relates the probability mass within each bin to the expected sample count. The resulting histogram approximates the probability density function of the target distribution.

4.3. Comparison of Methods

The proposed procedures provide a robust and reproducible framework for generating virtual PSDs from any known cumulative distribution function.

In practice, the equal-width method is recommended when comparing PSDs across multiple samples or aligning with experimental sieve data, as it provides a consistent scale and facilitates direct interpretation of particle size ranges.

The equal-probability method, on the other hand, is particularly useful for visualizing quantiles and ensuring that all bins contain data, which is advantageous for analyzing distribution tails or highly skewed particle size distributions.

A detailed comparison of both methods is presented in Table 4.

The choice of binning procedure has practical implications for subsequent modeling and simulation workflows. Equal-width binning provides direct comparability with laboratory sieve analysis, making it suitable for validation studies, calibration of empirical models, and routine PSD characterization. In contrast, equal-probability binning better captures the statistical extremes of a distribution, which may dominate processes such as filtration, transport, or percolation in porous media. It is also particularly useful in machine learning pipelines, where balanced representation of quantiles can improve feature extraction and reduce bias toward dominant particle sizes. In numerical simulations, such as DEM-based modeling of granular flows, the choice of binning strategy directly affects

input dataset resolution and the accuracy of predicted macroscopic behavior. Thus, the selection of a binning method should be aligned with the intended application, whether it emphasizes physical comparability with experimental data or statistical representativeness of distribution tails [56,57].

Table 4. Comparison of two histogram generation methods for synthetic PSDs—equal-width bins vs. equal-probability bins.

	Equal-Width Bins	Equal-Probability Bins
Bin width	constant across the range	variable (narrow in dense regions, wide in tails)
Interpretation	directly comparable heights, standard in PSD analysis	each bin represents the same probability mass
Advantages	intuitive, easy comparison with theoretical PDFs, aligns with sieve analysis	highlights tails, ensures all bins are populated
Disadvantages	sparse bins in tails, may hide rare events	bar heights less intuitive, variable widths complicate interpretation
Computational cost	low computational overhead, only requires linear binning	higher, requires repeated evaluation of the quantile function
Best use	comparing PSDs, matching lab data, computing statistics	visualizing quantiles, emphasizing distribution tails, balanced data for ML workflows

Figure 1 illustrates the comparison of equal-width and equal-probability binning applied to an exemplary synthetic log-normal particle size distribution ($\mu = 0$, $\sigma = 0.5$). The example was generated with $N = 15$ bins and $M = 100,000$ samples.

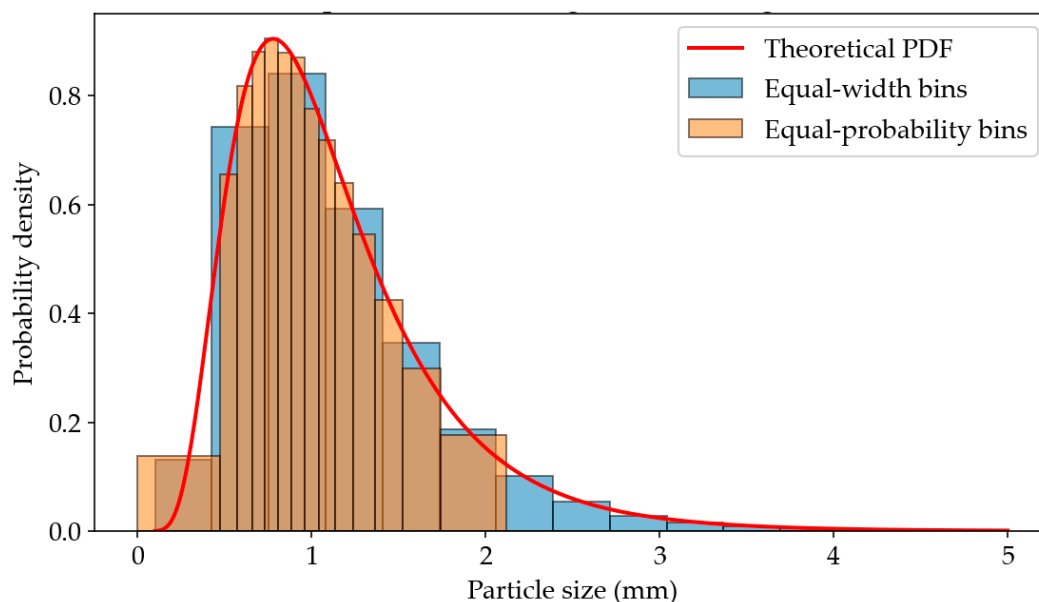


Figure 1. Comparison of particle size distribution histograms generated using the equal-width method (blue) and the equal-probability method (orange) for a log-normal distribution. Parameters: number of bins = 15, total number of samples $M = 100,000$. The theoretical probability density function is shown as a red line.

The equal-width method results in a histogram with constant bin size across the entire diameter range, which allows straightforward interpretation and direct comparability with sieve-based laboratory data. However, this approach produces sparse bins in the tails of the

log-normal distribution, underrepresenting rare but potentially important particle fractions. The equal-probability method, in contrast, partitions the probability space uniformly, producing variable bin widths that ensure balanced representation of both the central peak and the distribution tails. This highlights quantile structure and rare events, though the variable bar heights may be less intuitive. The superimposed theoretical log-normal probability density function demonstrates that both approaches adequately approximate the target distribution, albeit with different emphases.

5. Implementation and Case Studies of Synthetic Particle Size Distributions Generation

To demonstrate the practical applicability of the methodology described in Section 3, several case studies were conducted. Model parameters were sourced from literature for various materials, including soils and powders. These parameters were then used to generate virtual particle size distributions (PSDs) with a predefined number of bins and a fixed total number of particles.

5.1. Computational Environment

The framework was implemented in Python 3.11, utilizing NumPy 2.1.3 for numerical computations and matplotlib 3.10.0 for visualization, all within the Spyder 6.0.7 environment. All statistical analyses were performed using the same setup.

5.2. Generation of Virtual Particle Size Distributions for Soil Analysis Using the Weibull Distribution

The first case study focuses on the Weibull distribution, a widely used model for soils and other granular materials. Model parameters, i.e., scale (λ) and shape (k), were obtained from a literature dataset comprising 27 natural soils from Austria and Nepal, covering cobbles (Co), gravel (Gr), sand (Sa), silt (Si), and clay (Cl) [35,36]. This diversity ensures representation of granulometries ranging from coarse gravels to fine silts and clays.

Virtual PSDs were generated using 50 equal-width bins on a logarithmic scale, with 100,000 particles per distribution. Figure 2 shows the resulting probability density functions (PDFs) while Figure 3 shows the corresponding cumulative distribution functions, with markers indicating d10, d50, and d90 percentiles.

The variability in curve shapes shown in both figures reflects the influence of soil texture and provenance: some distributions are coarse-dominated (gravels and sands), others fine-dominated (silts and clays).

Grouping by dominant fraction (coarse, medium, fine) illustrates systematic differences in size accumulation patterns. Fine-dominated soils exhibit steep CDF slopes at small diameters, indicating rapid accumulation of mass in the fine fraction. Medium-textured soils show gradual transitions, reflecting balanced contributions from sand and silt, while coarse-dominated soils display flatter initial slopes and delayed inflection points, consistent with gravel and cobble prevalence.

Hierarchical clustering, visualized in the dendrogram (Figure 4), reveals three primary clusters among the 27 soil PSDs. The clustering was performed using Ward's linkage and Euclidean distance based on d10, d50, and d90. Branch heights indicate increasing dissimilarity, with the highest merges separating coarse-, medium-, and fine-textured groups.

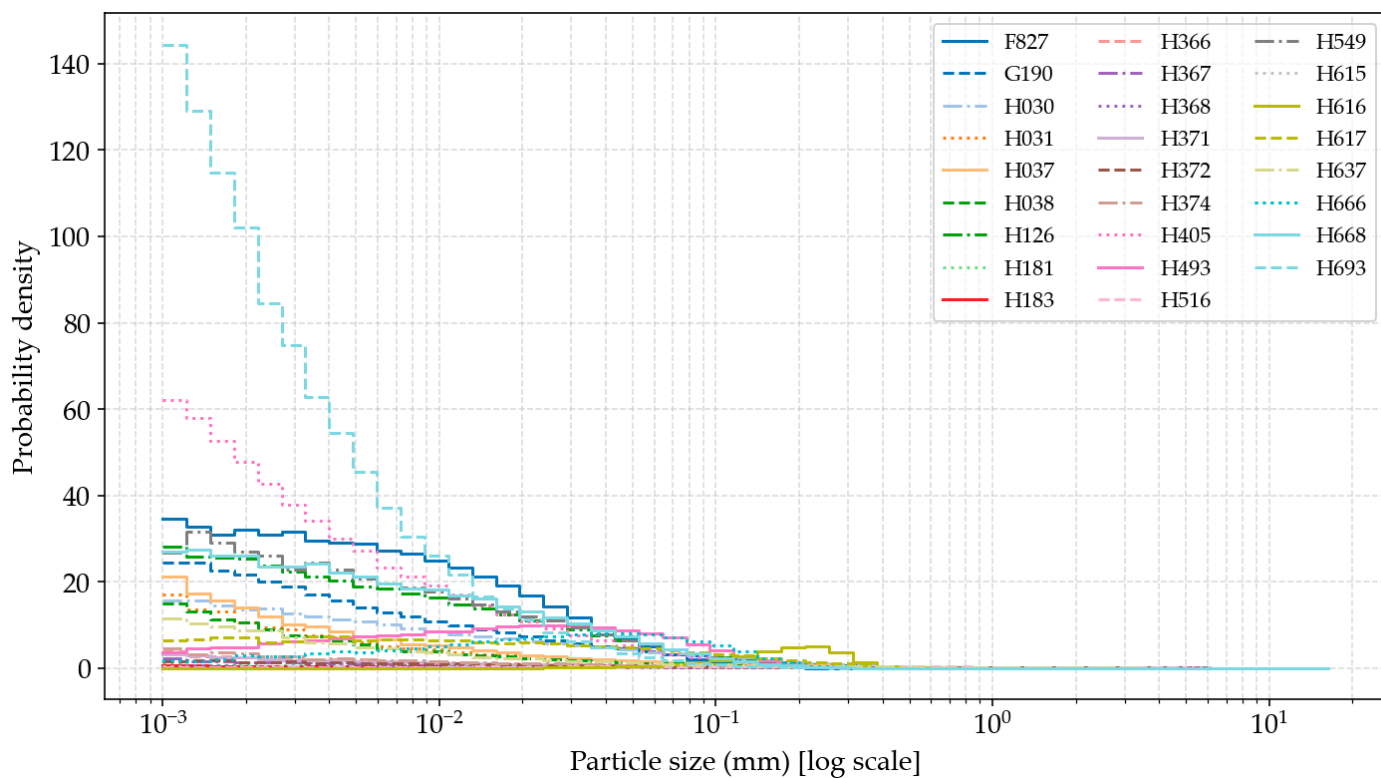


Figure 2. Family of probability density functions generated from Weibull distributions fitted to 27 natural soils.

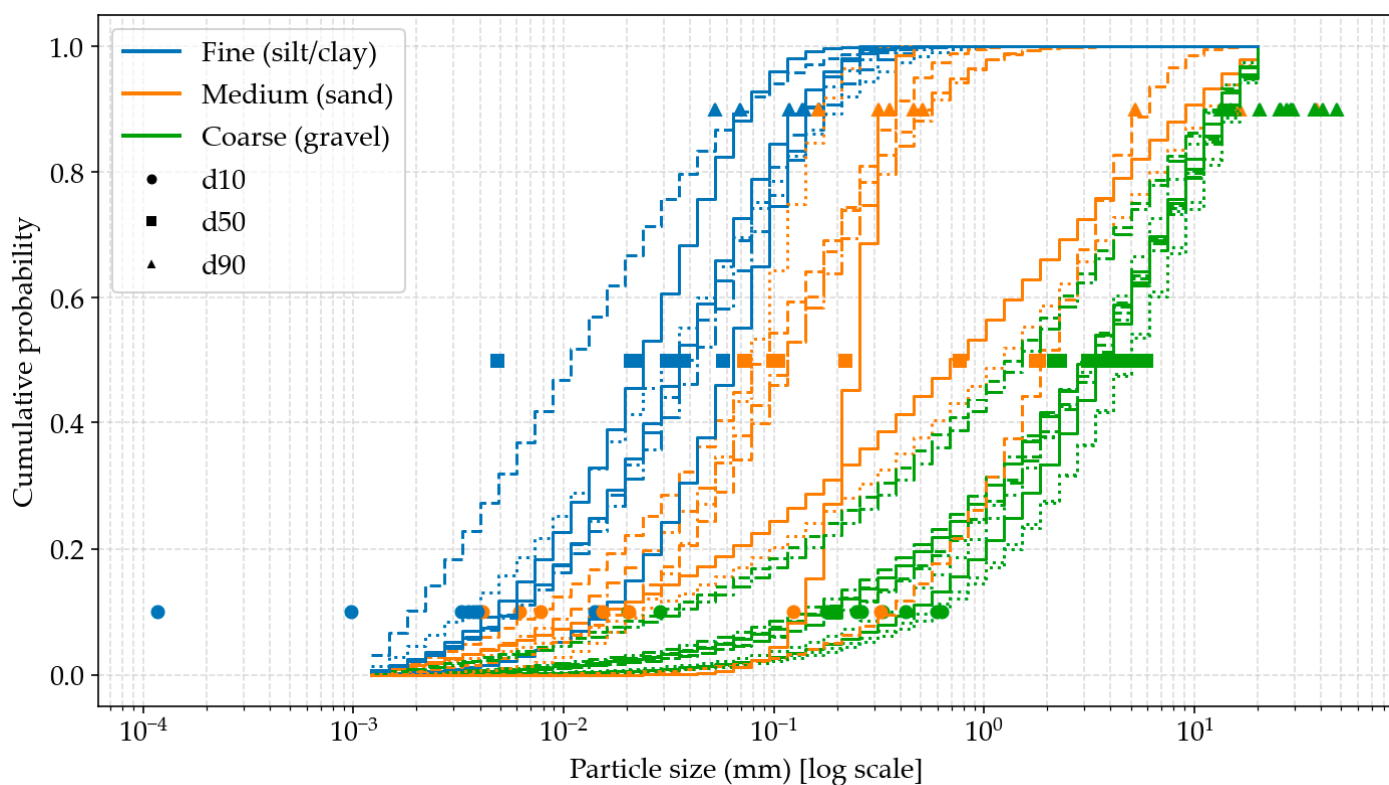


Figure 3. Family of cumulative distribution functions grouped by the dominant fraction (Fine, Medium, Coarse), markers on CDFs show d10 (circle), d50 (square), and d90 (triangle) percentiles.

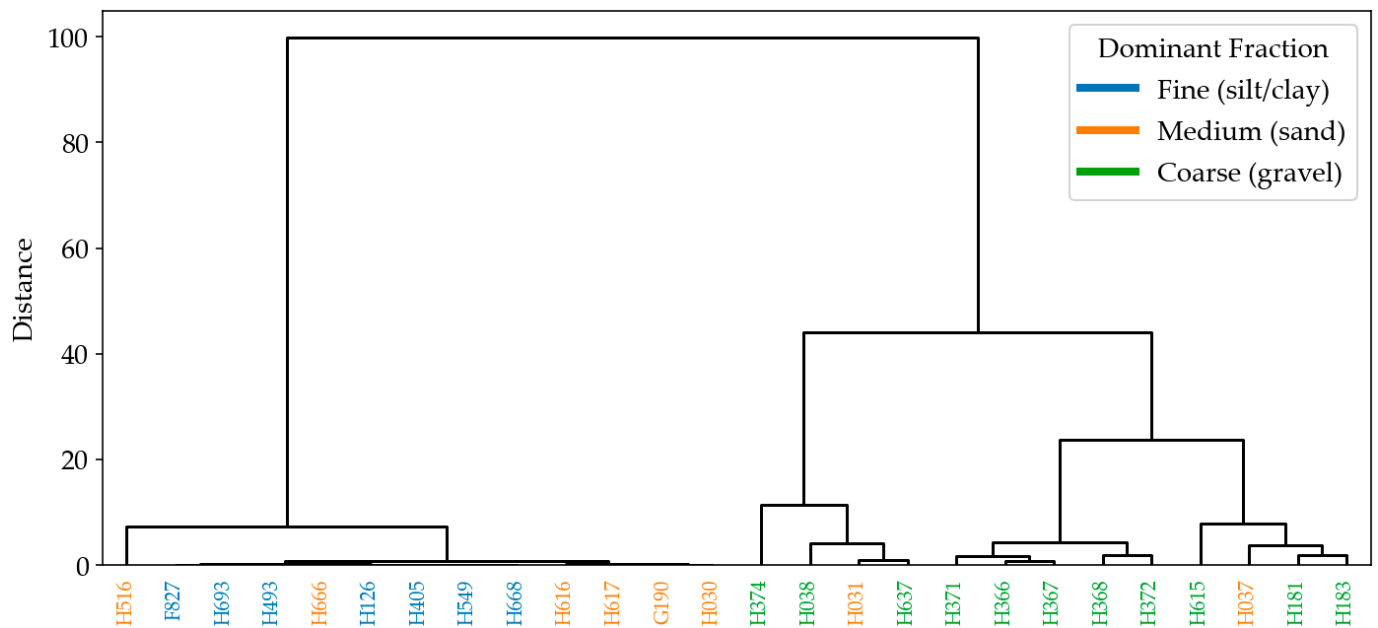


Figure 4. Hierarchical clustering dendrogram of 27 soil PSDs based on percentiles d10, d50, and d90. Three primary clusters are identified, corresponding to coarse-, medium-, and fine-grained soils.

The analysis of the dendrogram reveals a clear division of soil samples into three main groups, each corresponding to dominant grain size fractions.

The first group (left branch) consists of fine-grained soils with small particle sizes and a relatively narrow distribution. This group includes twelve samples that exhibit short branch lengths, indicating a high degree of internal similarity.

The second group (middle branch) represents medium-textured soils, suggesting a balanced granulometric composition. These samples differ significantly from the fine-grained group, reflecting distinct differences in grain structure.

The third group (right branch) comprises coarse-grained soils with larger particle sizes. This is the most heterogeneous group, further subdivided into smaller clusters that reflect the variability among the analyzed samples.

This classification demonstrates that Weibull parameters capture essential granulometric characteristics and, when combined with clustering, can effectively group soils by similarity, supporting predictive modeling and classification tasks.

The heatmap of percentiles and grain size spread (Figure 5) provides an additional perspective. The color gradient, ranging from light yellow (low values) to dark blue (high values), facilitates rapid visual assessment. Coarse soils exhibit the highest d90 and spread values, reflecting large particles and wide ranges. Fine soils display low percentiles and minimal spread, while medium soils occupy an intermediate position.

These findings confirm that Weibull parameters can be linked to soil texture, enabling the generation of synthetic PSDs that realistically represent natural variability. Representative parameter ranges for different soil types are summarized in Table 5.

Overall, this case study demonstrates that Weibull parameters systematically capture soil texture variability. Synthetic PSDs generated from these parameters reproduced characteristic percentiles (d10, d50, d90), enabling classification, clustering, and predictive analyses. This confirms the framework's applicability to geotechnical and hydrological contexts, where percentiles govern permeability, compressibility, and shear strength.

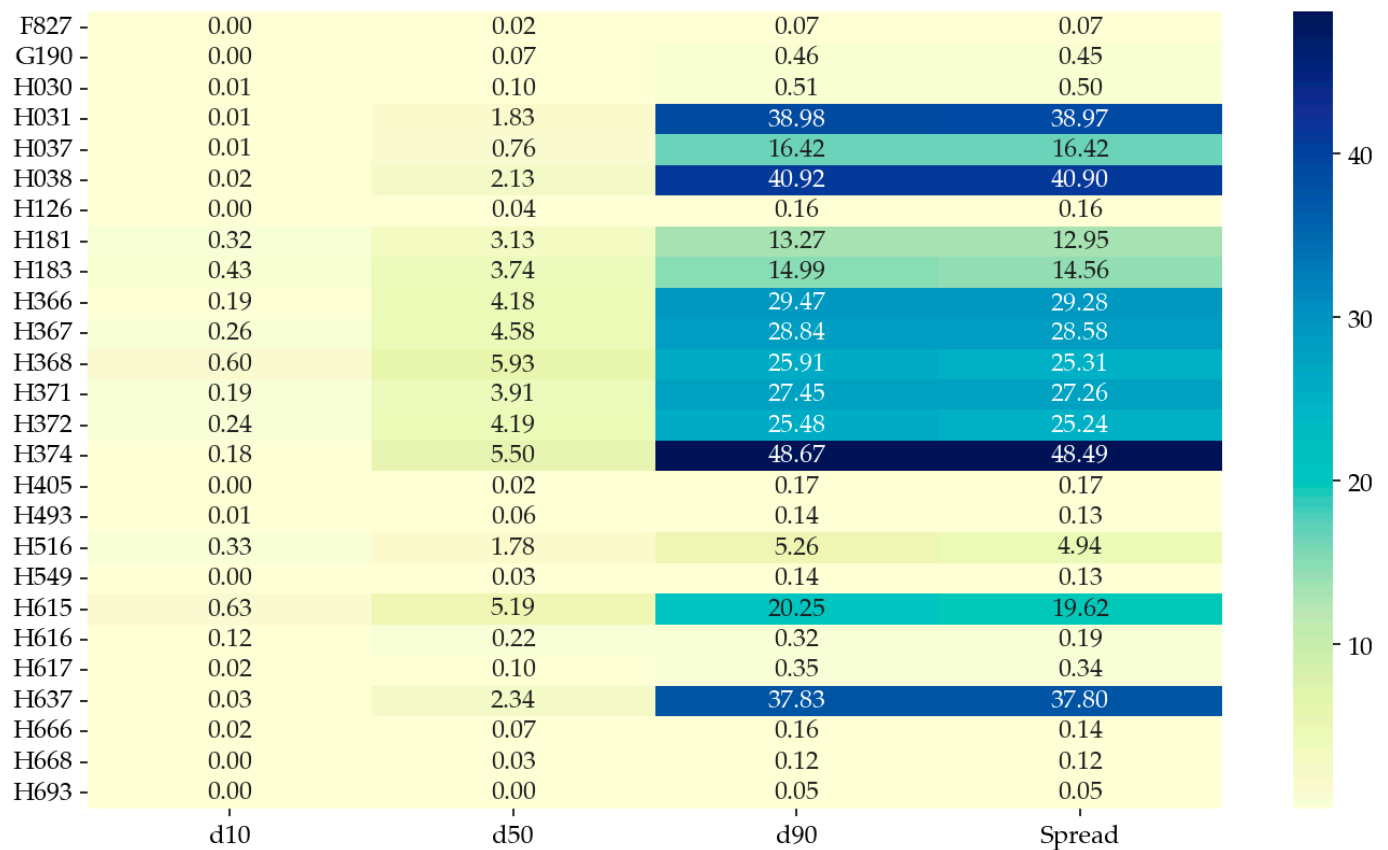


Figure 5. Heatmap of percentiles (d10, d50, d90) and grain size spread for all soils.

Table 5. Exemplary Weibull parameters (scale λ , shape k) for representative soil textures.

Soil Type	Scale Parameter λ (mm)	Shape Parameter k	Distribution Characteristics
high-gravel soils	5–10	0.4–0.8	broad distributions with dominant coarse fractions
uniform sands	0.2–0.3	>2.5	steep curves, narrow spread, well-sorted particle sizes
fine silty-clayey soils	<0.05	0.5–1.0	steep fine-dominated curves with extended tails in small sizes

5.3. Generation of Virtual Particle Size Distributions for Granular Materials Using the Gamma Distribution

The second case study demonstrates the framework's versatility for industrial and organic granular materials. The Gamma distribution, commonly used for positively skewed particle sizes, was applied to Tin, Gelatin, Iron, and Sodium Chloride. Parameters of the distributions, i.e., α (shape) and β (scale) were obtained from literature [37].

Virtual PSDs were generated using 100 logarithmically spaced bins across a particle size range of 1–1000 mm, with 100,000 particles per material. Figure 6 shows the resulting PDFs, each reflecting the influence of α and β : Tin and Sodium Chloride exhibited moderately skewed, narrow distributions, whereas Gelatin and Iron had broader, right-skewed distributions.

The corresponding CDFs are shown in Figure 7. They highlight cumulative size patterns, with higher α materials showing steeper slopes (more uniform particle sizes) and lower α materials exhibiting gradual accumulation (greater variability).

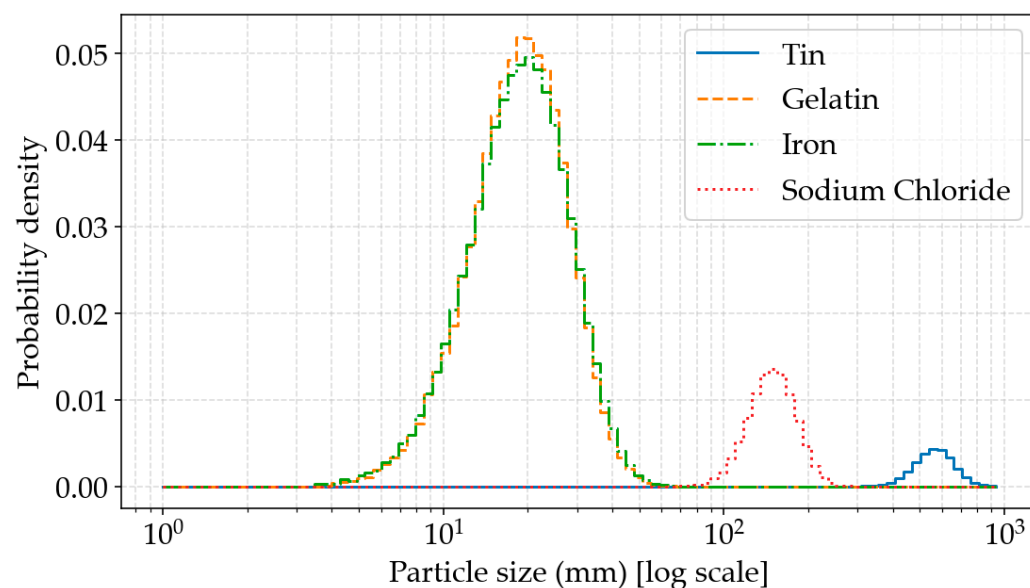


Figure 6. Probability density functions for Tin, Gelatin, Iron, and Sodium Chloride, generated using Gamma distributions with literature-derived parameters.

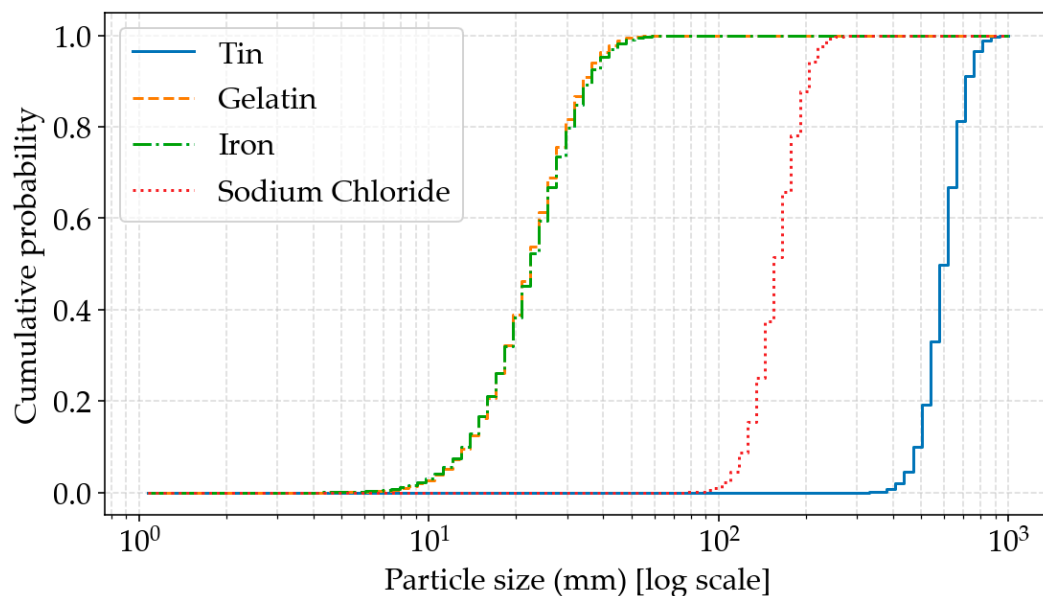


Figure 7. Cumulative distribution functions for the analyzed materials.

Key statistics, i.e., mean particle size, standard deviation, and skewness, are presented in Table 6. Gelatin and Iron displayed higher skewness, reflecting extended tails toward larger particles, whereas Tin and Sodium Chloride were more symmetric.

Table 6. Statistical parameters of Gamma-based particle size distributions for selected materials.

Material	Mean (mm)	Std Dev (mm)	Skewness
Tin	580.6	91.2	0.31
Gelatin	22.6	8.1	0.90
Iron	22.9	8.6	0.95
Sodium Chloride	155.4	29.5	0.34

The differences in mean and variance reflect the inherent size characteristics of the materials, while skewness captures the asymmetry of particle size distribution. Gelatin and

Iron show higher skewness, indicating a longer tail toward larger particle sizes, whereas Tin and Sodium Chloride distributions are more symmetric.

This case study illustrates several important aspects:

- Controlled reproduction of material-specific PSDs—adjusting α and β allows precise tailoring of particle size distributions without physical measurements;
- Quantitative characterization: PDF/CDF visualization combined with statistical descriptors ensures reproducible and complete description of particle systems;
- Efficiency and scalability—large datasets (100,000 particles) were generated rapidly, enabling simulations, probabilistic analyses, and machine learning applications;
- Universality—the framework is applicable beyond soils, covering industrial, chemical, and organic materials;
- Interpretation of distribution shape—high α yields narrow, uniform distributions, low α produces broad, skewed distributions, demonstrating flexibility in modeling particle heterogeneity.

Overall, the Gamma-based case study confirms that the framework enables statistically representative, reproducible, and scalable generation of virtual granular datasets, supporting simulation and analysis of diverse engineering and industrial applications.

5.4. Generation of Virtual Particle Size Distributions for Food Powders Using the Log-Normal Distribution

To illustrate the applicability of the framework to fine granular materials in the food industry, a third case study was conducted using log-normal distributions. Food powders such as sugar, corn meal, and instant milk were selected based on available literature data [38].

Virtual PSDs were generated with 100 logarithmically spaced bins over a particle size range of 10–10,000 μm , and 100,000 particles per material. Figure 8 shows the PDFs: sugar and corn meal have narrow, nearly symmetric distributions, while instant milk exhibits a broader, right-skewed distribution due to higher σ .

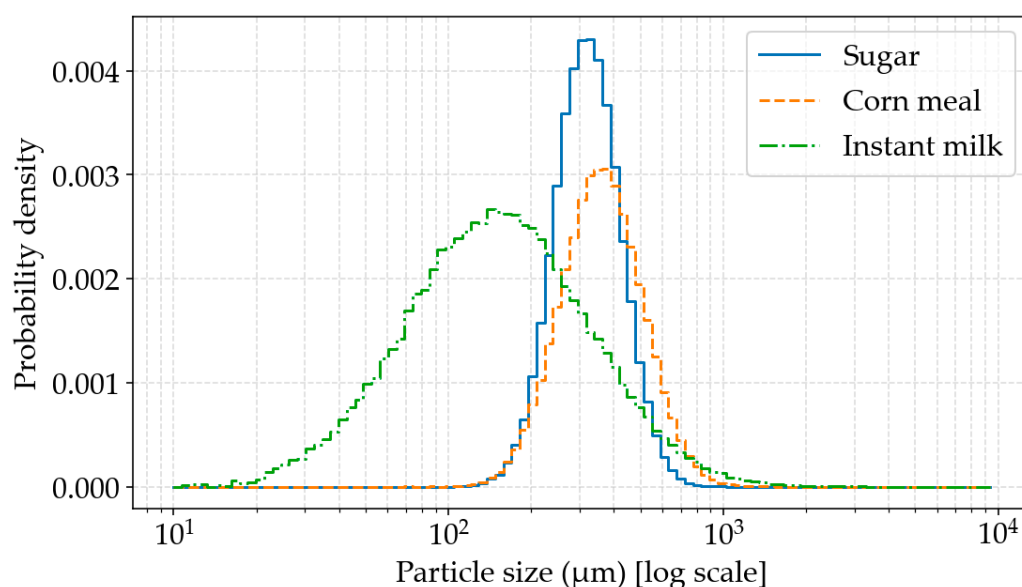


Figure 8. Probability density functions for sugar, corn meal, and instant milk, generated using log-normal distributions.

Corresponding CDFs (Figure 9) reflect cumulative particle size patterns, with sugar and corn meal showing steep slopes (homogeneous particles) and instant milk accumulating more gradually (higher variability).

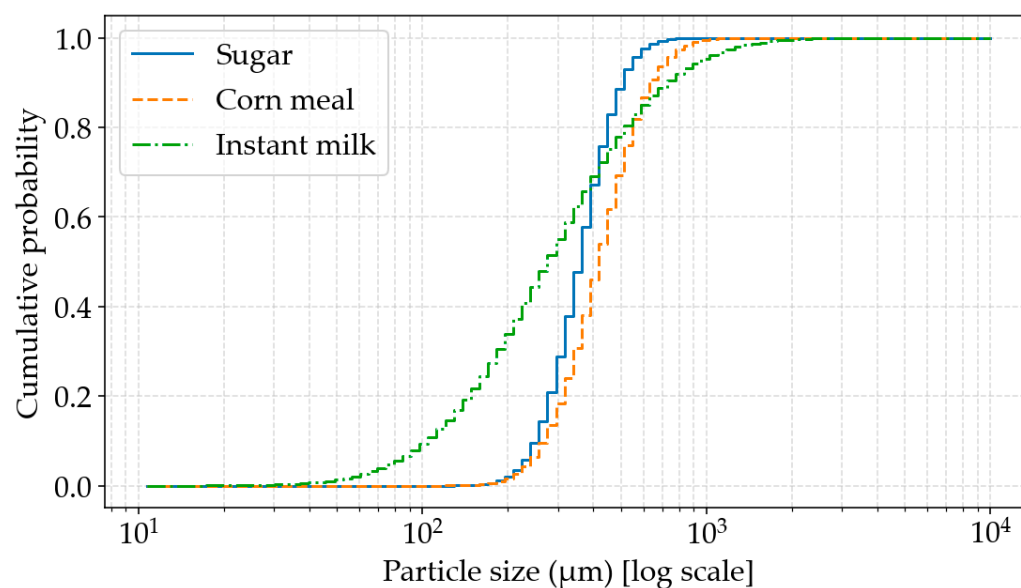


Figure 9. Cumulative distribution functions for the three analyzed food powders.

Understanding these distributions is important for optimizing mixing, transport, and dissolution processes. For instance, narrow distributions ensure consistent flow and packing, while broad distributions require careful handling to prevent segregation and maintain product uniformity.

From a practical standpoint, these results can directly inform process design and quality control in the food industry. For powders like sugar and corn meal with narrow, uniform distributions, standard handling and mixing procedures are sufficient to maintain consistent product quality. In contrast, powders like instant milk, with broad and skewed distributions, require tailored strategies, such as controlled feeding, careful blending, or sieving, to prevent segregation and ensure homogeneity in final products. The ability to rapidly generate virtual PSDs allows to simulate different scenarios, optimize equipment settings, and predict potential challenges in handling and processing granular materials.

To further illustrate the framework's capabilities, heterogeneous mixtures of sugar and instant milk were simulated at seven ratios: 100:0, 85:15, 70:30, 50:50, 30:70, 15:85, and 0:100. Each mixture contained 100,000 particles sampled according to the specified proportions.

Figure 10 shows the resulting PDFs. Increasing the fraction of instant milk progressively broadened and skewed the distributions. The 100:0 mixture (pure sugar) remained narrow and symmetric, while the 0:100 mixture (pure instant milk) was broad and highly skewed. Intermediate mixtures reflected gradual transitions in distribution shape.

This simulation demonstrates that mixture composition strongly influences PSD shape, variability, and cumulative patterns, which in turn affect flowability, mixing efficiency, and dissolution behavior. By systematically generating mixtures, the framework enables predictive simulations for process design and quality control.

Overall, this case study confirms that the methodology accommodates fine powders with different skewness and spread and can simulate realistic heterogeneous mixtures. Importantly, the framework can generate mixtures of multiple components, effectively producing multimodal particle size distributions that reflect complex material granulometries. The approach is fully reproducible, scalable, and allows rapid generation of virtual PSDs, reinforcing the generality and practical applicability of the framework across diverse granular systems, from single-component powders to heterogeneous, multimodal mixtures.

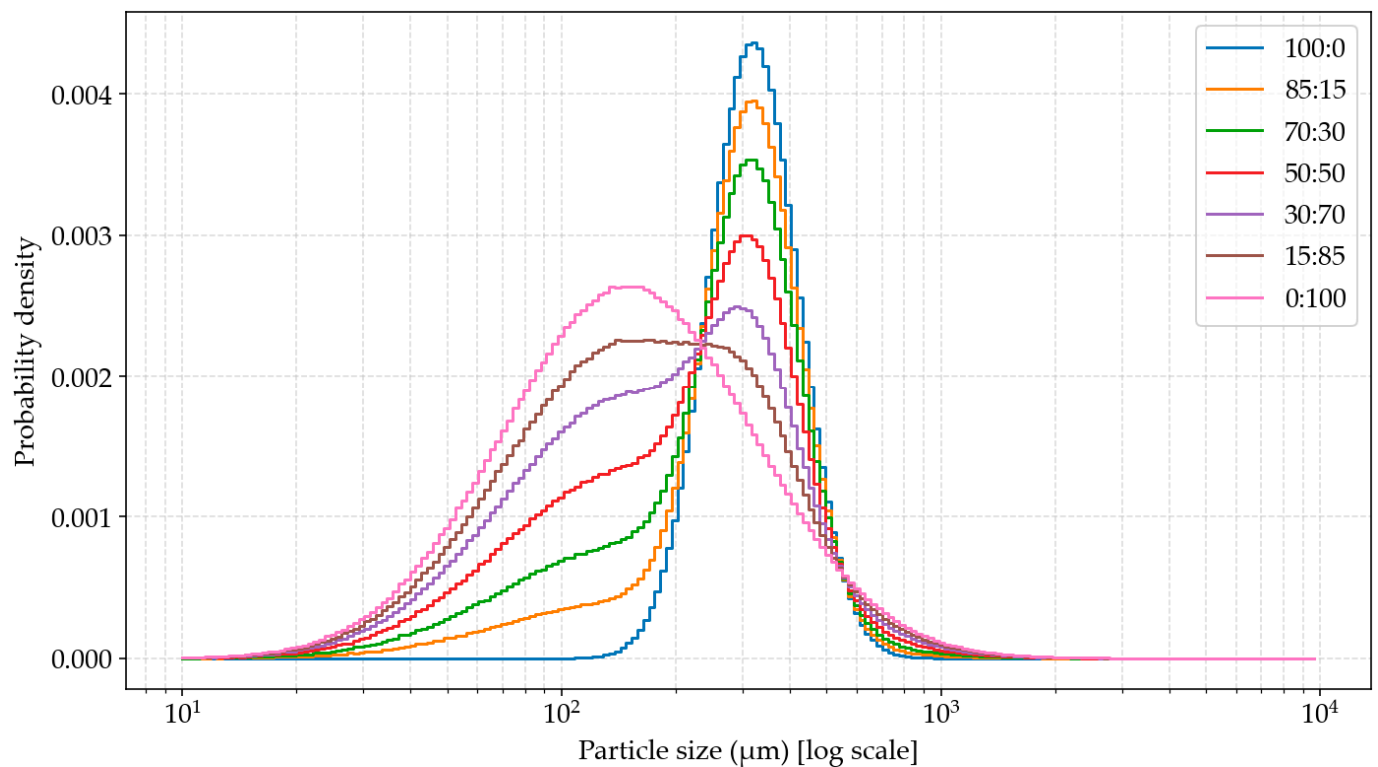


Figure 10. Probability density functions of sugar + instant milk mixtures at seven different ratios.

5.5. Computational Performance of Histogram Generation Methods

Benchmarking the two histogram-generation procedures revealed clear differences in execution time. For five repeated runs using a log-normal distribution (15 bins, sample sizes from $M = 10^3$ to 10^6 , the equal-width method showed consistently low and nearly constant execution times, typically between 5×10^{-5} and 5×10^{-4} s, indicating negligible scaling effect.

In contrast, the equal-probability method was systematically slower, with computation times increasing from approximately 3×10^{-4} s at $M = 10^3$ to 5×10^{-2} – 8×10^{-2} s at $M = 10^6$. The resulting performance ratio ranged from 1.2 to 36, with typical values between 10 and 20 for $M \geq 10^5$.

Additional benchmarks with 100 bins confirmed this trend. The equal-width method remained consistently faster, while speed ratios increased from about 6–7 for small sample sizes ($M = 10^3$ – 10^4) to approximately 15–20 for large samples ($M \geq 10^6$). These results indicate that the relative performance advantage of the equal-width method is robust across different histogram resolutions.

In summary, both methods produce statistically consistent PSDs, but the equal-width approach is markedly more efficient and therefore preferable for large-scale or iterative simulation workflows. The equal-probability method, while computationally more demanding, may be reserved for applications where bin adaptivity and quantile-based resolution outweigh performance considerations.

5.6. Discussion of Case Studies, Limitations and Future Work

The three case studies demonstrate that the proposed methodology yields reproducible and statistically controlled virtual particle size distributions. The generated synthetic PSDs are suitable for numerical simulations, sensitivity analyses, benchmarking, and virtual dataset creation, thereby bridging the gap between empirical measurements and computational modeling. By reproducing the analytical form of the selected distribution models,

the framework ensures consistency across different granular materials and enhances comparability between simulation-based studies.

A key aspect of the presented examples is that they rely on literature-derived parameters rather than newly collected experimental data. This choice reflects the methodological objective of the study, which was to evaluate the generality, reproducibility, and model-agnostic nature of the proposed framework. Nevertheless, the method can be directly applied to laboratory measurements, enabling users to generate reproducible synthetic PSDs corresponding to empirical samples. In future work, the framework will be systematically validated using newly acquired experimental datasets to assess accuracy, quantify deviations, and demonstrate practical applicability in laboratory settings.

Despite these advantages, several limitations must be acknowledged.

First, the present study focuses on unimodal grain-size distributions to maintain clarity and computational tractability. In future work, the framework can be extended to multimodal distributions by combining multiple parametric models into mixture formulations. This enhancement would enable accurate representation of materials with complex granulometric signatures, such as bimodal soils, blended industrial powders, and composite particulate systems, thereby broadening the applicability of the approach.

Second, the methodology depends on accurate estimates of distribution parameters, which in practice may be affected by measurement noise, instrument resolution, or fitting procedures. Incorporating parameter uncertainty or Bayesian estimation presents a promising direction for future research.

Third, the method generates only particle sizes, without accounting for morphological characteristics such as particle shape, angularity, roundness, or surface texture. These properties are known to significantly influence mechanical and hydraulic behavior in granular systems. Although beyond the scope of the present work, the framework may be extended in the future by coupling PSD generation with morphological descriptors obtained from imaging-based analyses or empirical correlations.

Fourth, although the equal-probability approach offers excellent statistical representativeness, it incurs a higher computational cost due to repeated quantile function evaluations. In the revised manuscript, representative generation times and scaling behavior have been provided to guide users working with large datasets.

Finally, the current validation was performed on literature-based PSD models. While sufficient for demonstrating numerical correctness and generality, comprehensive experimental benchmarking will be essential to fully establish robustness, applicability, and transferability across different material classes.

By outlining these limitations and potential extensions, this section highlights both the flexibility and the current boundaries of the proposed framework. Its ability to generate reproducible, application-ready PSD datasets provides a foundation for standardized benchmarking protocols, improved DEM and CFD simulations, and broader adoption of open-science practices in granular and geoscientific research.

6. Conclusions

This paper introduced a systematic and reproducible framework for generating synthetic particle size distributions for virtual modeling and simulation of granular materials. By reviewing commonly used PSD models, the study identified those with well-defined cumulative distribution functions as particularly suitable for reproducible dataset generation through inverse transform sampling.

Two complementary procedures for histogram construction were proposed: the equal-width method, which aligns with conventional PSD representation and facilitates direct comparison with sieve analysis, and the equal-probability method, which ensures uniform

representation of the probability space and highlights distribution tails. Together, these strategies balance interpretability with statistical rigor and reproducibility.

The framework was implemented in Python and demonstrated through case studies for soils (Weibull), sedimentary and industrial materials (Gamma), and food powders (log-normal), showing its versatility and applicability across diverse material classes. The generated datasets were statistically controlled, reproducible, and directly usable for model initialization, sensitivity analysis, and benchmarking in DEM, CFD, or geostatistical workflows. They also enable exploration of hypothetical or extreme conditions where experimental data are limited or inconsistent.

While the present work focuses on unimodal systems, the methodology can be naturally extended to multimodal, anisotropic, or spatially correlated particle systems by combining multiple distributions or introducing additional descriptors. Future developments may include automated parameter estimation from experimental datasets and standardized protocols for synthetic PSD benchmarking, further strengthening reproducibility and comparability across studies.

Overall, the proposed framework provides a flexible and transparent computational tool for bridging empirical grain-size data and virtual simulations. It supports data-driven research on soils, sediments, and particulate media, contributing to reproducible modeling practices and enhanced understanding of granular processes in geoscientific applications.

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Abbreviations

The following abbreviations are used in this manuscript:

CDF	Cumulative distribution function
PDF	Probability density function
PSD	Particle size distribution

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