Minimal discrete matches for target grain size distributions

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Abstract

Soil is fundamentally a discrete material that is, nevertheless, commonly modeled as a continuum in part because of the computational expense of large-scale discrete element models (DEMs). Even at lab specimen scales, DEM's computational cost may be substantial depending on the grain sizes being modeled. Despite these limitations, discrete models have proven useful in furthering our understanding of soil mechanics because they can spontaneously replicate realistic soil behavior as an emergent macro-scale property from a collection of particles following relatively simple interaction rules. This makes DEM an attractive tool for a multiscale modeling approach where the constitutive behavior of a representative volume element (RVE) is characterized with a discrete model and applied at a larger scale through a continuum model. The ability of the RVE to represent a soil depends strongly on an appropriate grain size distribution match. However, in order to achieve computationally feasible models, even at lab scales, DEM simulations often use larger minimum particle sizes and more uniform distributions than their intended targets. Intuitively, discrete matches of different grain size distributions (GSDs) will require vastly different numbers of particles. But the precise relationship between GSD characteristics and the number of particles needed to match the distribution (and by extension the associated computational cost associated) is not intuitive. In this paper, we present the minimal discrete match (MDM) concept. The minimal packing set is the smallest set of discrete particles needed to match a given GSD. We present a method for determining the MDM for any GSD and discuss strategies for finding the smallest MDM within a set of tolerances on the GSD. A mapping of USCS classification and MDM reveals a broad distribution of computational cost over several orders of magnitude for granular soils.

Keywords

Discrete soil description, analytical solutions, open-source algorithms, computational cost

Introduction

Soil is a fundamentally discrete granular material whose complex mechanical behavior emerges from the numerous interactions between its constituent parts. The discrete element method (DEM), introduced by Cundall and Strack (1979), has proven to be a powerful tool in exploring the inter-particle interactions of granular assemblies. With DEM, a vast parametric space exists where grain sizes, shapes, contact models, etc. can be systematically varied and their influences on macro-scale assembly behavior can be quantified.

These models pose several challenges that must be managed in order for their benefits to be realized. Due to the number of elements involved in typical DEM simulations, both the computational resources needed to run them and the ability to characterize and interpret them are non-trivial. Over the years, the number of particles used in DEM simulations has increased, but not proportionally to the reduction in costs of computational resources. O'Sullivan (2014) showed that the order of magnitude of average number of particles in DEM simulations increased substantially from 1998 to 2014, from approx. $\mathcal{O}(10^3)$ to $\mathcal{O}(10^5)$, but fell far short of the $\mathcal{O}(10^7)$ predicted by Cundall (2001) for "easy" geomechanics problems by 2011. More recent publications in DEM have shown that orders ranging from $\mathcal{O}(10^6)$ (Sufian et al. (2021), Dong, Yan, and Cui (2022)) to $\mathcal{O}(10^8)$ (Fang et al. (2021), Zhang et al. (2024)) are possible, but rare and require high performance computing resources.

Because of the computational cost, DEM simulations whose particles approach realistic grain sizes generally model at the representative volume element (RVE) scale. Several nuances to the RVE concept exist, but broadly speaking, the RVE represents the smallest volume of material to exhibit statistically consistent macro-scale behavior as its source material. In physical laboratory experiments and discrete numerical experiments, study samples sufficiently large to behave as an RVE is critical to the broader applicability of the results.

The RVE depends on several factors including the GSD and the behavior of interest. Samples with larger maximum particle sizes will have larger RVEs. Depending on the GSD, loading conditions, and behavior of interest, the minimum particle size expected to participate mechanically in the soil matrix may be substantially smaller than the largest particle size. Intuitively then, with increasing GSD breadth, the number of particles needed in a DEM simulation of granular assemblies will also increase. The ratio of minimum and maximum particle sizes is, therefore, a significant and often reported parameter in describing DEM models. Often, matching the true GSD of interest (e.g., from a physical soil sample) is sacrificed for computational efficiency, for example by upscaling the target GSD (Zeraati-Shamsabadi and Sadrekarimi 2025).

While the insights we gain from DEM simulations with upscaled or truncated GSDs are valuable, they come with acknowledged limitations on their broader applicability to natural soil fabrics. It becomes an important experimental design consideration, then, to understand the relative computational costs associated with different grain size distributions. The number of particles needed to represent a GSD can be calculated for specific assumed distributions (e.g., self-similar fractal distributions Tyler and Wheatcraft (1992)). However, these methods

assume a representative particle size within a given range, rather than optimizing it and are not applicable to GSDs not fitting their underlying shape assumptions. For general GSDs, particularly when a specific physical soil is being modeled, an ideal approach would be an analytical solution to the minimum number of particles required to reproduce the GSD.

This paper introduces such an approach through the minimal discrete match (MDM) concept. The minimal packing set is the smallest set of discrete particles needed to match a given grain size distribution by mass. Note that the MDM is based on mass-volume relationships only, not mechanical behavior. Therefore, it represents an important component to determining RVE and relative computational cost, but it is not equivalent to an RVE. In order to characterize the MDM, descriptions of grain size distributions and granular samples are presented as mathematical sets and the rules describing several relationships between the sets are defined. Using these definitions, a simple algorithm is shown to efficiently identify the MDM. The results show a broad range of MDM magnitudes over several GSDs of interest in geotechnical engineering. The MDM algorithm is implemented in an open-source Python module, available on GitHub.

Discrete definitions

Identifying the minimal discrete match requires rigorous mathematical definitions for particulate samples, S, and grain size distributions, G. Conceptually, each of these are collections of items (i.e., sets) with specific restrictions.

Sample definition

A sample, S is an indexed set describing its particles as pairs of size, X_S , and quantity, Q_S . X_S is an ordered (i.e., each entry is larger than the previous) set of unique values of positive real numbers. Q_S is an unordered set of positive integers related to X_S by a shared indexing set for the sample, I_S .

$$S = \{(X, Q) \in I_S\} \tag{1}$$

where:

$$X_S = \{x_i : i \in I_S\} \text{ with } x_1 < x_2 < \dots < x_{n_S}$$
 (2)

$$Q = \{q_i : i \in I_S\} \tag{3}$$

$$X_S \subset \mathbb{R}^+ \text{ and } Q \subset \mathbb{Z}^+$$
 (4)

Grain size distribution definition

A grain size distribution, G, has a similar structure. It is and indexed set describing size boundaries, X_G , and masses, M_G . Like X_S , X_G is an ordered set of unique values, however, it's domain also includes zero (representing the pan in a typical sieve analysis). Like Q_S , M_G shares an index (I_G) with the size set, but it's domain is not restricted to integers, only to non-negative real numbers. The values in M_G represent the masses retained on a sieve with opening size X_G .

$$G = \{(X_G, M_G) \in I_G\} \tag{5}$$

where:

$$X_G = \{x_j : j \in I_G\} \text{ where } x_1 < x_2 < \dots < x_{n_G}$$
 (6)

$$M = \{m_j : j \in I_G\} \tag{7}$$

$$X_G \subset \mathbb{R}^{non-neg} \; ; \; V \subset \mathbb{R}^{non-neg}$$
 (8)

Comparison definition

The relationship between S and G cad be defined in terms of how G describes S. In the context of DEM modeling, this may seem backward because typically in DEM modeling, a target GSD is defined first and a sample generated to match it. On the other hand, a discrete sample (either physical or numerical) exists on its own, whereas a GSD only has meaning when interpreted as a description of a sample. Therefore the relationship between S and G will be defined in terms of G's description of S. In a later section, the topic of finding an instance of S that matches a target G will be addressed.

The relationship between S and G is formalized in three conditions described as follows:

Condition 1: G is complete if and only if the final entry in M_G is zero:

$$G$$
 is complete $\Leftrightarrow m_{n_G} = 0$ (9)

This condition ensures that x_{nG} provides an upper bound to the sizes described by G. This is analogous to the limitation of scope in ASTM D6913 to grain sizes passing a 75-mm sieve (D18 Committee, n.d.).

Condition 2: G describes S (denoted $G \longrightarrow S$) if and only if Cond1 is met and the its smallest size is smaller than any size in S and its largest size is larger than any size in S:

$$G \longrightarrow S \Leftrightarrow \operatorname{Cond1} \wedge \min(X_G) < \min(X_S) \wedge \max(X_G) \ge \max(X_S)$$
 (10)

Condition 3: G describes S articulately if Cond2 is met and for all consecutive pairs of sizes in X_S there exists at least one size in X_G between them.

$$G \xrightarrow{\text{articulately}} S \Leftrightarrow \text{Cond2} \land \forall (x_i, x_{i+1}) \in X_S \exists (x_i < x_i \in X_G \le x_{i+1})$$
 (11)

Condition 4: G describes S accurately if Cond2 is met and the combined masses of all the particles with sizes between every pair of sizes in X_G is equal to the retained mass on the lower of the size pairs in G:

$$G \xrightarrow{\text{accurately}} S \Leftrightarrow \text{Cond2} \land \sum_{\substack{i \in I_S \\ x_j < x_i \le x_{j+1}}} q_i \cdot f(x_i) = m_j$$
 (12)

where f(x) is a scaling function that converts size to mass. As indicated in Equation 12, a size in X_S is considered between two sizes in X_G if it is larger than the x_j and smaller than or equal to x_{j+1} . This is physically analogous to assuming a particle will pass through an opening equal to its own size.

Note that Cond3 is not required for Cond4 to be satisfied. Equation 8

Physical interpretation

In physical terms, some assumptions are required in order for S and G to be interpreted as a physical sample and sieve analysis (or a numerical version of the same). First, the sizes in X_G are assumed to represent smallest enclosing diameter of whatever shapes the particles in S are. Second, the particles in S are assumed to be of the same shape such that a single scaling function, f(x), can represent the size-mass relationship for all of S. For spherical particles with of constant density (ρ) , this is a straightforward definition:

$$f(x) = \frac{\rho \pi}{6} x^3$$

Note, however, that the use of this particular scaling function is not required in general. It is only necessary that f(x) be some mapping of $x \mapsto m$. It would be possible to combine sets of differently shaped particles with respective mapping functions, but this paper will limit itself to assuming uniform, spherical particles.

Grain sizes evaluated

This paper will analyze several grain size distributions in the range of interest in geotechnical engineering (although the methods are applicable over a wider range). Specifically, randomized GSDs based on normal distributions across the sieve set specified in ASTM D6913 (14 opening sizes from 0.075-mm to 75-mm). For classification purposes, articles smaller than 0.075 are assumed to be silt, regardless of their size. Table 1 summarizes the GSDs used in this study using several traditional characteristics including coefficient of curvature, C_c , and coefficient of uniformity, C_u . The grain size index, I_{GS} , as defined by Erguler (2016) and a new parameter, the curvature index, I_C , are also presented. The curvature index is conceptually similar to the grain size index in that it is a ratio of areas related to the cumulative distribution function (in percent passing, log size space) of the GSD. I_C normalizes the area under the GSD curve to the trapezoidal area bounded by the percent passing the smallest size above the pan (x_{min+1}) and the largest size (x_{max}) . Figure 1 shows a small subset of the GSDs considered and illustrates the definition of I_C on an example GSD.

Some traditional grain size distribution characteristics

Table 1: Grain size distribution parameters in this study

Parameter	Value(s) in study
$\overline{x_{min+1}}$	0.075 to 25 mm
x_{max}	9.5 to 75 mm
Sieves in G	5 to 14
Instances of G	2750
C_c	0.2 to 25.5
C_u	1.2 to 214.5
I_{GS}	0.03 to 0.60
I_C	0.29 to 1.57

Minimal discrete match solution

For any given S, finding G that accurately describes S is no more complicated that following the grain size analysis procedure described in ASTM D6913 (D18 Committee, n.d.). The reverse, finding a solution for S that is accurately described by some target G, is non-trivial. One of the reasons is that unlike a grain size analysis, the sizes of the solution (X_S) are bounded, but not explicitly defined. Additionally, the goal for this procedure is not only to find any S that is accurately described by G, but the minimal packing set S_{min} that is accurately described by G.

As a starting point, assuming that G is an articulate description of S and selecting any valid values for X_S , an indexed set of mass ratios, Φ , and volume ratios, Z can be defined:

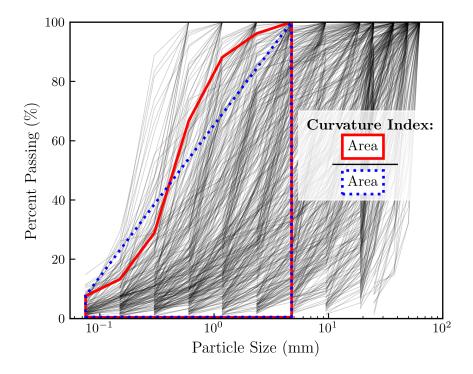


Figure 1: Grain size distributions evaluated. The area ratio defining the curvature index is shown. The example curve has a curvature index of 1.09.

$$\Phi = \left\{ \frac{m_j}{m_{n_G-1}} : j \in I_G \right\}; \text{ with elements } \phi_j$$

$$Z = \left\{ \frac{f(x_{nS})}{f(x_i)} : i \in I_S \right\}; \text{ with elements } \zeta_i$$

The mass ratio Φ describes the masses in M_G relative the the mass of the largest size retaining mass. Consequently, ϕ_{nG-1} will always equal 1. The volume ratio Z describes the relative volume of each particle size to that of the largest particle size in S. Consequently, ζ_{nS} will always equal 1. Note that Z is referred to as a volume ratio to avoid confusion with Φ despite the fact that the mapping function f(x) converts size to mass. Interpreting Z as a volume ratio is valid under a constant density assumption.

Since Φ describes relative masses of each size and Z describes the relative volume (and mass) per particle of each size, a quantity ratio, K, can be defined by the product of Φ and Z.

$$K = \{\phi_i \times \zeta_i : i \in I_S\}$$
; with elements κ_i

The quantity ratio K is the relative number of particles of each size for any S accurately described by G. It is directly proportional to the key target parameter, Q. Unfortunately, with the exception of κ_{nS} , the entries in K are not guaranteed to be integers, which is a requirement for Q. Rounding each element in K to the nearest integer provides a first-order, approximate solution for the minimal discrete match.

$$S_{approx} = \{(X, \text{int}(K)) \in I_S \cong S_{min}\}$$

Checking Cond4 against S_{approx} and G shows how much error there is in the approximate solution. Depending on the application and acceptable error tolerance, S_{approx} may be a suitable substitute for S_{min} . If a closer fit is needed, iteratively multiplying K by integers greater than 1 can be used to reduce the error to tolerable levels.

But since the sizes in X_S are only bounded by X_G and not explicitly defined, the opportunity exists to find a better selection of entries in X_S that will minimize Q_S . This approach is equivalent to dropping the articulate description (Cond3) requirement from the initial attempt because it allows for any sizes bounded by the respective sieve sizes in G. For this study, the maximum particle size is assumed to be fixed at it's minimum allowable size, however, the procedure will work for any allowable choice for maximum particle size.

The best allowable sizes for X_S can be found using the following spanned integer (SI) algorithm:

1) Find the quantity ratios associated with the minimum (-) and maximum (+) allowable sizes in x_1 through x_{nS-1} (i.e. K_- and K_+).

- 2) Check whether an integer is spanned between each entry in K_{-} and K_{+} .
- 3) If a spanned integer (SI) does not exist for each entry, repeat Steps 1 and 2 with incrementally larger sizes for x_{nS} .
- 4) If, after reaching the maximum allowable particle size for x_{nS} , an SI does not exist between each entry in K_{-} and K_{+} , iteratively multiply K_{-} and K_{+} by integers greater than 1 and repeat Steps 1 to 3 until the span between each entry contains an integer.
- 5) When an integer quantity exists between each entry in K_{-} and K_{+} , these integers can be used to populate the spanned integer quantity ratio, K_{SI} , which can now be interpreted as Q_{SI} .
- 6) Invert the mass scaling function f(x) on the ratio Φ / K_{SI} to identify the compatible sizes for the spanned integer quantities: in X_S .

$$X_{SI} = f^{-1} \left(\frac{\Phi}{Q_{SI}} \right) \tag{13}$$

Because Q_{SI} was generated using the allowable sizes of X and the mass ratios of the target G, the resulting X_{SI} satisfies Cond4 with Q_{SI} as the smallest possible quantity of particles, or the minimal discrete match:

$$MDM = S_{min} = \{X_{SI}, Q_{SI}\}$$

The total number of particles in the MDM is the sum of the quantities in Q_{SI} :

$$N_{MDM} = \sum_{i \in I_S} q_{SI,i} \tag{14}$$

The effectiveness of the spanned integer algorithm is shown in the rapid convergence to numerical zero error compared to a fixed-size approximation in Figure 2. The figure shows both approaches attempting to find a suitable sample for each of the GSDs shown in Figure 1 with an allowable error tolerance of 1 percent. In nearly all cases, the spanned integer approach requires no iteration (i.e., Step 4 is skipped). Where iteration is needed, it converges to numerical zero within one or two iterations. The fixed size approach converges with between 1 and 15 iterations and retains measurable error. This difference is significant, not because the spanned integer algorithm itself is computationally expensive, but because each iteration represents an increase in total particles in the final discrete sample.

If the fixed size approach, with its many iterations produce larger solutions for a "minimal" set than a different algorithm, can its solutions even be considered valid? They are, in fact, valid solutions, but to an over-constrained version of the problem at hand. This differently constrained solution serves at least two potential purposes. First, there are scenarios in which very specific, pre-determined sizes are required. For example, in space-filling solutions, such as presented by Botet, Kwok, and Cabane (2021), particle size is rigidly constrained and the

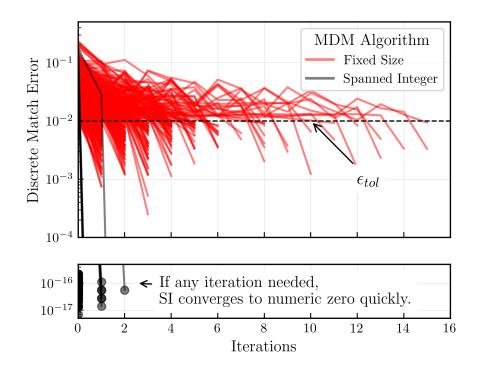


Figure 2: Packing Algorithm Convergence

spanned integer algorithm would not be appropriate. Second, comparing the "minimal" solution sizes from the fixed size and spanned integer algorithms provides a measure of how brittle the minimal discrete match problem is.

Results

The minimal discrete matches for the grain size distributions described in Table 1 range in magnitude from $\mathcal{O}(10^1)$ to $\mathcal{O}(10^{10})$ particles. As intuition suggests, increasing the percent mass of the smallest particle sizes or the ratio of the largest to the smallest particle sizes both tend to increase N_{MDM} . Figure 3 illustrates a scattered linear relationship between ϕ_1 (subscript 1 indicates the smallest particle size) and N_{MDM} in log-log space for constant volume ratio, ζ_1 . For $\phi_1 \approx 0.4$, $\log_{10} \zeta_1$ correlates roughly 1:1 with N_{MDM} .

A similar pattern exists between N_{MDM} , ζ_1 , and I_C as shown in Figure 4. At a given volume ratio, an increase in curvature index tends to result in an increased N_{MDM} . For $I_C \approx 0.7$, $\log_{10} \zeta_1$ provides a very rough 1:1 correlation with N_{MDM} .

The grain size parameters C_c , C_u , and I_{GS} were found to not correlate well with N_{MDM} . However, I_{GS} is helpful for visualizing the breadth of correlation between N_{MDM} and USCS classifications. Figure 5 shows the range of N_{MDM} associated with the granular USCS classifications in this study. The lower boundary of the data results indicate that all but the broadest distributions have instances that can be matched with N_{MDM} magnitudes of $\mathcal{O}(10^2)$ or lower. Yet even the classifications with the smallest observed matches also have numerous instances requiring magnitudes from $\mathcal{O}(10^6)$ to $\mathcal{O}(10^9)$.

Relative to "poorly graded gravel", "well-graded gravel" tends to have larger N_{MDM} . Where "with sand" is applicable to the gravel group name, the trend and lower limit of N_{MDM} remains the same, but the upper range of N_{MDM} is higher. Instances where "with silt and sand" are applicable to the gravel group name were rare in the generated GSDs and had very high values of N_{MDM} . The rarity and large N_{MDM} for these gradations are due to strict requirements for these group names, which only a small range of values across a broad range of particle sizes can satisfy.

Relative to "poorly graded sand", "well-graded sand" tends to have a similar (and quite broad) range of N_{MDM} . The addition of "with gravel" or "with silt" makes very little difference in the range of N_{MDM} at similar ranges of I_{GS} (although a small increase in lower bound is apparent in "well-graded sand with gravel". Even "silty sand" appears to share orders of magnitude with "poorly graded sand" at comparable ranges of I_{GS} . Similar to the trends for gravels, sands whose group names include both silt and gravel were rare in the generated GSDs and had high values of N_{MDM} .

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Discussion

The spanned integer algorithm component of the approach presented here is effective in finding the MDM. However, some caution is warranted in using the full flexibility allowed by a GSD on the discrete particle sizes. While traditional sieve analyses, and the analogous mathematical representation presented herein do not provide any additional constraints, natural soil grain distributions are known to be broadly distributed between sieves (Ghalib and Hryciw 1999). Modelers should inspect the MDM sizes of their target GSDs for results that would indicate abnormal underlying characteristics (e.g., repeated adjacent discrete sizes converging at the sieve boundary). Approximate solutions to the MDM, which give greater control over particle sizes, may be sufficient depending on the application and the desired rigor in the S:G match.

It is important to note that an MDM does not constitute an RVE. An MDM is defined purely in terms of discrete mass-volume relationships. An RVE has additional requirements about the mechanical behavior. Nevertheless, the mechanical behavior of granular materials is strongly influenced by its GSD, so the discrete mass-volume relationship is an integral part of the RVE. In this sense, the MDM can be thought of as a building block and minimum bound on the particle count in RVE, which can be useful in assessing computational cost.

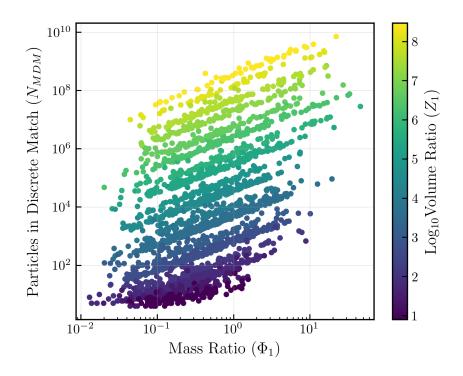


Figure 3: Change in total number of MPS Particles with mass ratio.

To some extent, the number of particles used to study geomechanics may simply be limited by the number of particles needed to capture the behavior of interest. For example, studies have shown that for certain combinations of grain size distribution (GSD) and density, there may be significant portions of the soil mass that are not mechanically engaged with the soil matrix. This may lead to thresholds of particle size that can be omitted from a given simulation without significant impact on the behavior being studied. This depends, of course, on what the behavior of interest is. DEM studies focusing on shearing resistance will have different needs than those focused on permeability, for example.

Conclusions

This paper described algorithms to 1) find a first-order approximation of a minimal discrete match (MDM) to general grain size distributions, 2) quantify the error in approximate minimal packings, and 3) find a rigorous solution for an MDM with a spanned integer approach. Depending on the relative size of the RVE and MDM and whether the modeling application calls for a rigorous match between a target GSD and its DEM representation, either a rigorous or approximate approach may be appropriate.

The MDM is to a valuable tool in quantifying the computational cost and assessing the feasibility of building DEM models of different grain size distributions. The MDM results for a

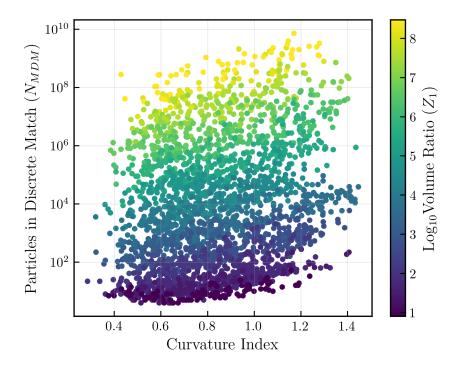


Figure 4: Change in total number of MPS Particles with curvature index.

large distribution of USCS show several trends: increasing the ratio of maximum to minimum particle size, the relative mass of the smallest particles, and the curvature index all increase the size of the MDM.

The distribution of MDM size across USCS classifications indicates that a wide range of realistic granular soils are feasibile for DEM modeling. The distribution also indicates that neither USCS classification, curvature index, size, and mass ratios alone are sufficient to characterize MDM size. This indicates that MDM magnitudes for specific GSDs of interest should calculated rather than estimated based on index parameters.

Data and code availability

The Python code used to generate data, solve for minimal discrete matches, and plot figures are available on GitHub.

Botet, Robert, Sylvie Kwok, and Bernard Cabane. 2021. "Filling Space with Polydisperse Spheres in a Non-Apollonian Way." *Journal of Physics A: Mathematical and Theoretical* 54 (19): 195201. https://doi.org/10.1088/1751-8121/abef81.

- Y Poorly graded gravel
- Y Poorly graded gravel with sand
- Y Poorly graded gravel with silt and sand
- **y** Well-graded gravel
- Y Well-graded gravel with sand
- Y Well-graded gravel with silt and sand
- Poorly graded sand
- Poorly graded sand with gravel
- Poorly graded sand with silt
- Poorly graded sand with silt and gravel
- Well-graded sand
- Well-graded sand with gravel
- Well-graded sand with silt
- Well-graded sand with silt and gravel
- Silty sand
- Silty sand with gravel

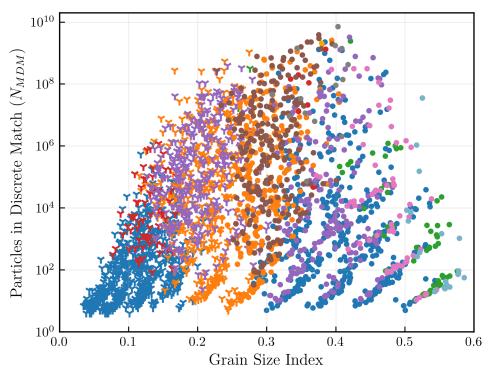


Figure 5: USCS classifications of the MPS data.

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