

Generation of 2-D Porous Media for a Study of Macroscopic Properties

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ABSTRACT

We investigate the hypothesis that the macroscopic properties of a porous material can be determined from limited morphological information. Specifically, we investigate this hypothesis for the Minkowski functionals of two-phase media in 2-D. We look at two methods for generating samples with desired Minkowski functionals: the Gibbs sampler and the Metropolis-Hastings algorithm. The Metropolis-Hastings algorithm allows for the production of samples with any possible Minkowski functionals. Macroscopic properties of these samples will be measured in a future project.

I. INTRODUCTION

Any solid phase possessing pore space falls into the category of porous media. Porous media encompass many common substances including foam, soil, bones, and concrete. Since these substances, among other porous media, are intimately connected with our lives, there exists motivation to understand the underlying physics of these substances. Investigating porous media is nothing new; yet, there are open questions in the field.

It has been hypothesized that the macroscopic properties of a material can be determined from limited morphological information about that material¹. However, morphological information is not necessarily unique to every structure. Indeed, two different structures can give rise to the same morphological values, which means, if the hypothesis is correct, that fundamentally different structures can result in the same macroscopic properties.

In order to evaluate the validity of the aforementioned hypothesis, we investigate a sufficient spread of values for a particular morphological property, namely the Minkowski functionals. Additionally, we consider an adequate number of samples, each

with unique structure, that satisfy the investigated morphological values. Our samples are simulated as 2-D lattices of 1's and 0's, which represent phase one and phase zero, respectively. We require closed samples, which means that the boundaries of the samples wrap around.

Markov Chain Monte Carlo simulations provide a clear and relatively simple means for generating samples with desired morphological properties. In particular, there are two types of simulations that fit the needs of this task: Gibbs sampling and the Metropolis-Hastings algorithm. The Metropolis-Hastings algorithm proves better suited for the production of samples in this regard, because complications with the Gibbs sampler prevent the production of substances with a large enough span of morphological properties.

The macroscopic properties of these substances will soon be tested. It is our expectation that the results of those calculations will determine whether or not the macroscopic properties of a substance can indeed be determined from limited morphological information.

II. MORPHOLOGICAL INFORMATION

Morphological information pertains to the physical shape, form, or structure of a substance. Some examples of morphological information include the number of clumps of a particular phase, the relative area of phases and the boundary length between phases. There are a variety of measurements used to obtain morphological properties of a substance, including: the two-point autocorrelation function, the lineal-path function²,

the chord-length distribution function³ and the Minkowski functionals. We choose the Minkowski functionals for our investigation.

In 2-D, the Minkowski functionals for a two-phase substance describe the area and the Euler characteristic of a particular phase, as well as the boundary length between the two phases. For this study, the Minkowski functionals are measured with respect to phase one. Thus, the area functional, v_0 , is the number of lattice points that are in phase one; the boundary length, v_1 , is the total length of boundary needed to isolate the two phases; and the Euler characteristic, v_2 , is the net number of “blobs” of phase one. For a given substance, a blob of phase one inside phase zero adds one to the net Euler characteristic. Conversely, a blob of phase zero inside phase one subtracts one from the net Euler characteristic.

Additionally, we are interested in the values of the Minkowski functionals per lattice point because these values are independent of the dimensions of a substance. To attain the normalized Minkowski functionals, we divide the total functionals by the number of points in the lattice.

Clearly, calculating Minkowski functionals for a sample of small dimensions is straightforward and can be done by visual inspection, but that method is not practical for samples with a large number of lattice points. The necessity for large scale computations requires the introduction of an iterative process for calculating the functionals. For this purpose, we define a process that iterates through each two-by-two square in the lattice and updates the total Minkowski functionals at each of those structures. Figure 1 shows the possible structures, as well as their contributions to the total Minkowski functionals, where black squares represent phase one and white squares represent phase zero. Note

that Figure 1 only shows unique structures, and rotations of those structures produce the same contributions to the total Minkowski functionals.

The iterative method for calculating the contributions to the total Minkowski functionals at each two-by-two square has the inherent problem of over-counting both lattice points and internal boundaries. Each lattice point is counted four times and each internal boundary is counted two times. Thus, to alleviate the problem of over-counting, it is necessary to divide both the total area and Euler characteristic by four and the boundary length by two. Now, with the correct total functionals, dividing by the total number of lattice points will yield the normalized Minkowski functionals. Now that we are able to calculate the normalized Minkowski functionals for a sample, we need to produce many samples with the desired values for the functionals.

III. RECONSTRUCTION

It is not possible to directly produce samples that satisfy specified values for the Minkowski functionals, so it is necessary to implement an indirect method for generation. Markov Chain Monte Carlo methods are widely used throughout computational physics to indirectly generate samples from a distribution when direct generation from the distribution is either costly or impossible. We attempt two different Markov Chain Monte Carlo simulations, namely the Gibbs Sampler and the Metropolis-Hastings algorithm. Both of these methods are commonly used in physical simulations, but each has its own advantages and disadvantages.

A. GIBBS SAMPLER

Generally, Gibbs sampling solves the problem of producing a sample from a distribution function when direct generation from the distribution is not practical, but when generations from the conditional distributions are easy. The production of a sample from the desired distribution rests on successive generations from the conditional distributions. Some advantages of the Gibbs sampler are that it is easy to implement numerically and that convergence to the target distribution is guaranteed as long as the conditional distributions are correctly defined. Unfortunately, the conditional distributions are not always trivial, or even possible to figure out. Without the conditional distributions, the Gibbs sampler is of no value.

Specifically, we want to sample from all possible structures consistent with a set of Minkowski functionals. The Minkowski functionals are not the components of a probability distribution; so, we consider the respective densities of the possible two-by-two squares (Figure 1). There are a total of six unique structures, which we designate as S_0, \dots, S_5 . The distribution of interest is $\pi(\vec{S})$, where $\vec{S} = (S_0, \dots, S_5)$. However, we do not know how to directly sample from this distribution. On the other hand, we may be able to sample from the full conditional probability distributions, $\pi_i(S_i) = \pi(S_i | \vec{S}_{-i})$, $i = 0, \dots, 5$. If this is the case, then we set the initial values for \vec{S} and begin the Gibbs sampling. The initial values for \vec{S} are set by generating a random lattice of 1's and 0's and calculating each S_i .

In order to define the conditional distributions we assume that the individual two-by-two squares in the lattice are independent of one another. Subsequently, we look at a lattice point in the r^{th} row and c^{th} column of our lattice, $p_{r,c}$, and calculate the

probability that the point is in phase one. This probability is based on the conditional probabilities and $p_{r+1,c}$, $p_{r,c+1}$, $p_{r+1,c+1}$. However, knowing $p_{r+1,c}$, $p_{r,c+1}$, and $p_{r+1,c+1}$ narrows down the dependence of the probabilities to just two S_i values. Assuming the two-by-two square created by $p_{r,c}$ being in phase one has a probability of S_j and that the square created by $p_{r,c}$ being in phase zero has a probability of S_k , then

$$\Pr(p_{r,c} = 1 | S_j, S_k) = \frac{S_j}{S_j + S_k}, \quad (1)$$

where s_j is defined as S_j divided by the total number of rotational degeneracies of the j^{th} structure. Then, a random number on the interval (0,1) is generated and compared to the probability from Equation (1). If the random number is less than the probability from Equation (1) then we set $p_{r,c} = 1$. Otherwise, we set $p_{r,c} = 0$. We then move to another point on the lattice; and the process of calculating probabilities and switching points to different phases is repeated until convergence is attained. The movement from one point to another can either be random or ordered. Both methods are used in physical simulations, but there is some debate as to which one is more efficient. Both methods result in convergence, but the speed of convergence can depend on the method implemented.

Given a random lattice, every lattice point is independent of the remaining lattice points. So, each two-by-two square in the lattice is independent of the other squares save for the shared lattice points. Besides this correlation, there are no other correlations between squares within the sample. Consequently, the conditional distributions from Equation (1) should be good approximations to the right conditional distribution. Figure

2 shows that using Equation (1) works perfectly for the reconstruction of a random lattice. Note that the target values for the Minkowski functionals and the values produced by the Gibbs sampling are so close that they are barely distinguishable in the figure.

Unfortunately, for a lattice that is not random, the individual lattice points are not independent of one another. This dependence between lattice points introduces correlations between the two-by-two squares used for calculating Minkowski functionals. Equation (1) is no longer sufficient for defining the correct conditional distributions. Correcting the conditional distributions for these correlations has proven to be nontrivial and we are not able to reformulate Equation (1) into an effective form. Consequently, we cannot implement the Gibbs sampler over a wide range of Minkowski functionals. Hence, we cannot produce a wide range of samples; so, it is necessary to try another generation method.

B. METROPOLIS-HASTINGS ALGORITHM

Similar to the Gibbs sampler, the Metropolis-Hastings algorithm is only useful if a non-iterative generation of a sample from the desired distribution is not possible. The Metropolis-Hastings algorithm is similar to the physical process of freezing a substance into a particular state. The process begins at a high enough temperature such that the substance is in the liquid phase. By slowly lowering the temperature, the substance freezes into a particular state. Some advantages of the Metropolis-Hastings algorithm are that it is known to work well for physical simulations and again, like the Gibbs sampler,

it is fairly easy to implement. The disadvantages of this method are that convergence is not guaranteed and that there are many initial parameters to set.

For our setup, we choose to maintain the correct area of the phases throughout the iterative process. So, we generate a lattice of phase zero and then switch random lattice points to phase one until we have attained the correct areas of the two phases. At this point, we calculate the energy of the system,

$$E = \sum_{i=0}^2 (v_i^t - v_i^0)^2, \quad (2)$$

where v_i^t is the i^{th} target Minkowski functional and v_i^0 is the i^{th} Minkowski functional of our lattice. To evolve our system towards v_i^t , or in other words, to minimize the energy of our system, we interchange the phase of two randomly selected points from different phases. As noted earlier, we want to maintain the correct area of the phases in our system; and that is undoubtedly fulfilled by this method of switching the phases of two points. After the phases are switched, we calculate the new energy of the system E' using Equation (2). The energy difference between the two consecutive states is evaluated as $\Delta E = E' - E$. The new phase is then accepted with probability $\text{Pr}(\Delta E)$ as

$$\text{Pr}(\Delta E) = \begin{cases} 1, & \Delta E \leq 0 \\ \exp(-\Delta E / T), & \Delta E > 0, \end{cases} \quad (3)$$

where T is the “temperature”. As T is lowered, this method causes our system to gradually converge to a system that is a sample with the desired Minkowski functionals.

There are several cooling schedules that are frequently used with Metropolis-Hastings algorithm; but, we choose a cooling schedule of the form

$$T = T_0 \left(\frac{T_f}{T_0} \right)^{(i/N)}, \quad (4)$$

where T_0 is the initial temperature, T_f is the final temperature, i designates the current cycle and N is the total number of cycles. We choose T_0 such that the system is initially in the “liquid phase” and allowed to move freely through any of the possible states. T_f is chosen such that it is low enough for the system to freeze into a final state. Also, N must be large enough such that the system does not cool too quickly and become mired in an energy local minimum.

Furthermore, the system must sit at any given temperature for enough time to thoroughly sample all possible states. Requiring this ensures an even sampling from all possible states. After a sufficient number of runs have been completed, the temperature of the system is lowered according to Equation (4). This process of switching the phase of points is repeated until the energy of our system is below some tolerance limit or the system becomes stuck in a local energy minimum. If the algorithm is run successfully, then our final state is a sample with the desired Minkowski functionals.

Unlike the Gibbs sampler, the Metropolis-Hastings algorithm works with all possible Minkowski functionals, whether there are correlations between individual lattice points or not. Figure 3 shows both the target sample and the sample obtained from the Metropolis-Hastings algorithm. Note that the samples have the same Minkowski functionals, but they are not exactly the same structure. However, they are very similar. By visual inspection, the samples appear to have roughly the same Euler characteristic and the shapes of the two phases are similar.

IV. MACROSCOPIC PROPERTIES

Now that we have established a tool for creating samples with desired Minkowski functionals, we are ready to confront the primary question: can macroscopic properties be determined from limited morphological information? Figure 4 is a plot of the heat flux for various Minkowski functionals with a fixed Euler characteristic. The plot has some definite structure, which suggests that the hypothesis under investigation has promise. The samples tested for this plot were generated using a method that is not the Metropolis-Hastings algorithm. However, using the Metropolis-Hastings algorithm will allow us to fill in empty spots on the plot, to determine the boundaries of possible Minkowski functionals, and to produce more samples with functionals that have already been plotted. This process will be repeated after fixing the Euler characteristic at more values. After this lengthy process is completed, the validity of the hypothesis driving this work can finally be evaluated.


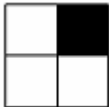




V. CONCLUSION

Since porous media are a part of almost everything with which we interact on a daily basis, understanding how porous media work is both pragmatic and attractive. Accordingly, it is hypothesized that the macroscopic properties of a substance can be determined from limited morphological information. In this paper, the morphological information that we investigate are the Minkowski functionals. The Minkowski functionals for a two-phase material in 2-D describe the area and Euler characteristic of a particular phase and the boundary length between the two phases. This is a significant amount of information, though it is not completely descriptive as multiple samples with different structures can have identical Minkowski functionals.

Testing the hypothesis requires the generation of many samples that span the possible Minkowski functionals. A Markov Chain Monte Carlo method is an effective means for accomplishing this purpose because direct generation from a distribution is not possible. After testing both the Gibbs sampler and the Metropolis-Hastings algorithm, we decide against the Gibbs sampler due to the difficulties of properly defining the conditional distributions. On the other hand, we are successful with the Metropolis-Hastings algorithm, and it suits our purposes for this investigation.

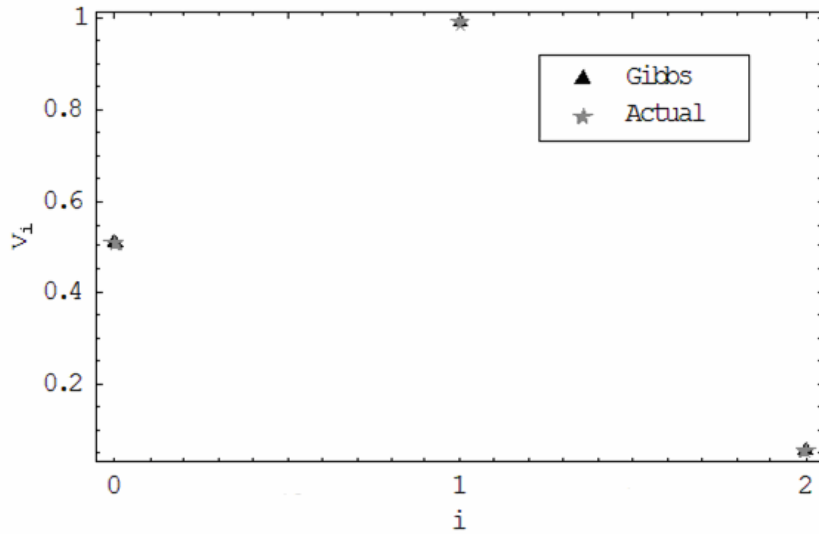
Now that we are able to produce as many samples as are needed with desired Minkowski functionals, different macroscopic properties of the samples can be measured. Plots similar to that in Figure 4 will tell the tale. These computations are currently underway, and the results will soon be reported.

FIGURE 1:

	Area	Boundary	Euler
	v_0	v_1	v_2
	0	0	0
	1	2	1
	2	2	0
	2	4	2
	3	2	-1
	4	0	0

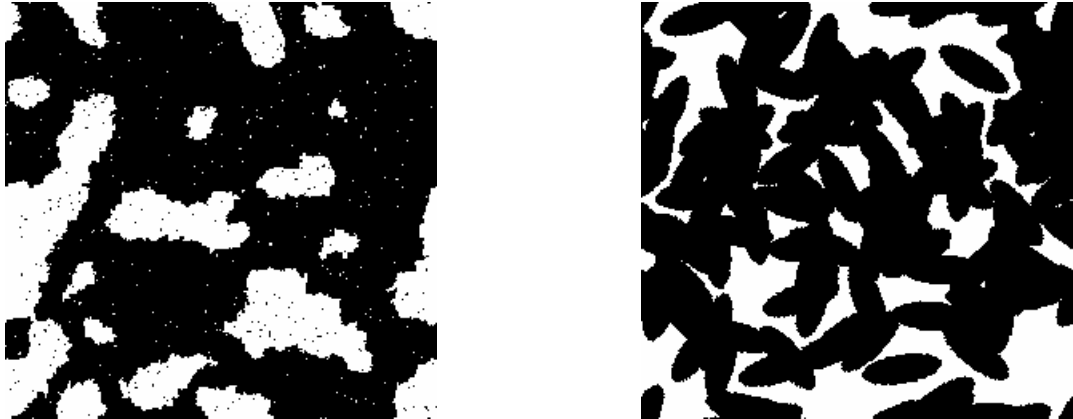
Possible two-by-two squares in a lattice with their respective contributions to the total Minkowski functionals. The rotational degeneracies of these structures are repressed as they make the same contributions to the total Minkowski functionals.

FIGURE 2:



Plot of the actual Minkowski functionals against the Minkowski functionals obtained from the Gibbs sampler from reconstruction of a random lattice. The actual Minkowski functionals are $v_0 = 0.5080$, $v_1 = 0.9864$, $v_2 = 0.0544$ and the values obtained from the Gibbs sampler are $v_0 = 0.5080$, $v_1 = 0.9864$, $v_2 = 0.056$. The values produced by the Gibbs sampler are so close to the actual values that the points on the plot are indistinguishable.

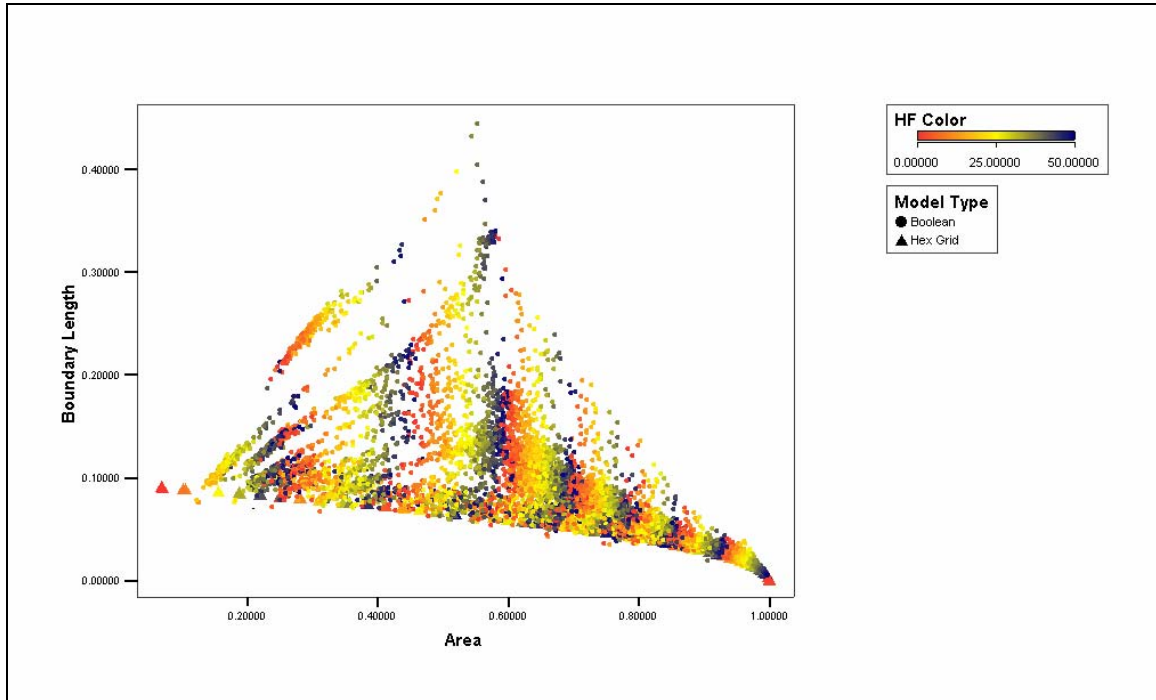
FIGURE 3:



The sample on the left is obtained from the Metropolis-Hastings algorithm and the sample on the right is the sample we use to get the target Minkowski functionals. The Minkowski functionals are identical for these samples. The functionals are

$$v_0 = .705028490028490, v_1 = .07410256410256410, v_2 = -0.0004273504273504270.$$

FIGURE 4:



Plot of the heat flux for structures with various Minkowski functionals and a fixed Euler characteristic. The boolean method for producing desired functionals involves placing ellipses of phase one into a lattice of phase zero. The hexagonal method uses a honeycomb lattice where the boundaries between hexagons are in phase one.

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