




# Procedural Multiscale Geometry Modeling using Implicit Surfaces (supplemental)

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1 This document covers additional details of the modeling of the  
2 multiscale geometry in Sec. 1, the optimization of the sphere tracing  
3 algorithm for visualization of the multiscale geometry in Sec. 2, and  
4 the reconstruction of the multiscale geometry in Sec. 3.

## 5 1. Multiscale geometry modeling

6 This section covers additional details and analysis of multiscale  
7 geometry modeling.

### 8 1.1. Tiling and Issues

9 Tiling introduces regularity artifacts between tiles, and continuous  
10 spatial variations using the tiling approach also introduce artifacts  
11 and breaks between the tiles. In addition, density variations using  
12 tiling produce inconsistent shading. In Fig. 1 we illustrate the tiling  
13 artifacts.

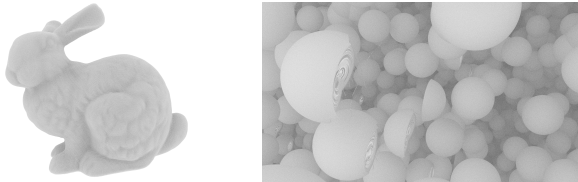


Figure 1: Tiling artifacts. Tiling introduces regularity artifacts and generates errors between tiles, making it impossible to create continuous spatial variations.

### 14 1.2. Point Distribution

15 The following is a way we can generate the seed for the random num-  
16 ber generator and add the random vector to the particle in the grid  
17 cell  $\mathbf{q}$  to create a random distribution in the eight neighbors (adding  
18  $(0,0,0)$ ,  $(1,0,0)$ ,  $(0,1,0)$ ,  $(1,1,0)$ ,  $(0,0,1)$ ,  $(1,0,1)$ ,  $(0,1,1)$ ,  $(1,1,1)$ ) to the  
19 point  $\mathbf{p}$  to get the grid cell  $\mathbf{q}$  of the point  $\mathbf{q}$ .

$$t = N \sum_{i=0}^1 \sum_{j=0}^1 \sum_{k=0}^1 a_{ijk} q_x^i q_y^j q_z^k \quad (1)$$

$$(\xi_1, \dots, \xi_N) = \text{rnd}(t, N) \quad (2)$$

$$[\mathbf{x}, s] = [\mathbf{q} + (\xi_1, \xi_2, \xi_3), \xi_4], \quad (3)$$

20 The pseudorandom number generator (PRNG), denoted as  $\text{rnd}$ ,  
21 produces  $N$  random numbers that are uniformly distributed within  
22 the interval  $[0, 1)$ . The coefficients  $a_{ijk}$  are chosen to remove regular-  
23 ity artifacts in the distribution of particles that result in the process of  
24 generating particle clouds. Choosing prime numbers as coefficients  
25 eliminates the regularity artifacts in a better way.

### 26 1.3. Multi-phase Particle Cloud

27 We use spatial transformations of points to generate multiphase  
28 particles within a volume. The following transformation generates  
29 particles with various shapes, smoothly transitioning between each  
30 type of shape in the volume, where each shape is considered a  
31 different phase. This works as a frequency modulation of the signal,  
32 and it almost generates the Phasor noise [TEZ\*19] effect. These  
33 transformed points are used to generate the particle cloud.



Figure 2: Inspired by a photo of air bubbles in ice (right), we used our multi-phase particle cloud approach to model a similar material (left). Our model has ice as the host medium and contains air particles that vary in size and shape with the spatial location in the medium, transitioning from spherical to non-spherical.

34 We can create a particle cloud containing specific regions where  
35 some regions are isotropic and others are anisotropic, with smooth  
36 transitions between these regions, see Fig. 2. This concept is simi-  
37 lar to positional encoding, where particular regions in the volume  
38 behave in a specific manner. To achieve this, the transformed point

$$\mathbf{p}' = \mathbf{p}\mathbf{T}, \quad \text{with } \mathbf{T} = \mathbf{A}\mathbf{D}, \quad (4)$$

39 is used as the input point for the particulate material generation. This  
40 generates effects like phasor noise, where the signal's frequency

41 depends on spatial coordinates. The matrices

$$\mathbf{A} = \begin{bmatrix} A_1 & A_2 & A_3 \\ A_4 & A_5 & A_6 \\ A_7 & A_8 & A_9 \end{bmatrix}, \quad \mathbf{D} = \begin{bmatrix} \sin(p_y) & \sin(p_z) & \sin(p_x) \\ \sin(p_z) & \sin(p_x) & \sin(p_y) \\ \sin(p_x) & \sin(p_y) & \sin(p_z) \end{bmatrix}, \quad (5)$$

42 contribute to these phasor noise generation effects. The matrix  $\mathbf{A}$   
43 acts as an amplitude matrix, typically with values between 0 and 1.  
44 Essentially, we use the original point to generate a noise matrix or  
45 turbulence [PH89] matrix ( $\mathbf{T}$ ), which is a circulant-type matrix that  
46 is symmetric and every row is a left circular shift of the previous  
47 row.

#### 48 1.4. Mesoscale Surface Patterns on the Macrosurface

49 The following distance approximations can be used to generate  
50 mesoscale surface patterns on macroscopic objects with thickness  
51 control.

$$d(\mathbf{p}, w) = \begin{cases} d_g(\mathbf{p}, w), & \text{if } \exists \mathbf{q}_k \text{ such that } l_i < P_i(\mathbf{q}_k) < r_i, \\ \frac{w}{2}, & \forall k = 0, \dots, 26, \\ \frac{w}{2}, & \text{otherwise.} \end{cases} \quad (6)$$

52 where,

$$d_g(\mathbf{p}, w) = f(\mathbf{p}) + \min_{\substack{k=0 \\ \exists \mathbf{q}_k, l_i < P_i(\mathbf{q}_k) < r_i}}^{26} d_{\mathbf{q}_k} \left( \frac{1}{w} (\mathbf{p} + \mathbf{h}(\mathbf{p})) \right), \quad (7)$$

53 In this condition, the terms  $l_i$  and  $r_i$  represent the minimum and  
54 maximum bounds of the corresponding polynomial values  $P_i(\mathbf{q}_k)$   
55 when the  $i$ -th polynomial is evaluated with the point  $\mathbf{q}_k$ . The interval  
56 length  $(l_i, r_i)$  controls the width (or thickness) of the macroscopic  
57 object. In some cases, it may be necessary to use  $R$  instead of  $P$ .  
58 These polynomials can be used to create the macro-shape of the  
59 object based on the roots of the polynomials; basically, the particle  
60 jittering follows these polynomial functions. When the roots of  
61 these polynomials are true, the microgeometry on the surface can  
62 be generated using the distance bound  $d_g(\mathbf{p}, w)$ .

63 For instance, the mesoscale geometry on the macrosurface is  
64 shown in Fig. 3. The following polynomial can then be used to  
65 generate the macrosurface with microstructure.

$$P(\mathbf{q}) = 2q_x + q_y^2 + q_z^2 - q_x q_y - q_y q_z - q_z q_x. \quad (8)$$

#### 66 1.5. Implicit Periodic Functions

67 Implicit periodic functions, such as sine and cosine, can avoid grid  
68 discretizations and improve performance, as they do not require  
69 geometry evaluation in neighboring grid cells. Many geometric  
70 structures, such as fibers, can be represented by combinations of  
71 these functions with varying frequencies and amplitudes following  
72 the Fourier Series. In addition, periodic functions are more suitable  
73 for continuous optimization.

74 The general formula which can be used to generate various struc-  
75 tures with sine and cosine functions defined is

$$SC(\mathbf{p}) = \sum_{i=1}^u \prod_{j=1}^v T_{ij}(\mathbf{p})^{k_{ij}} + w, \quad (9)$$

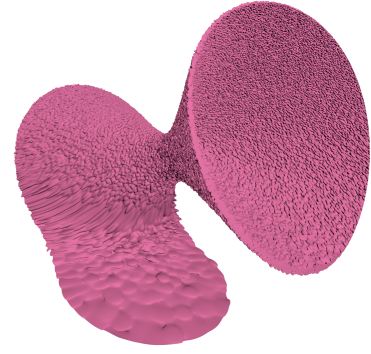


Figure 3: Mesoscale texture patterns on the macrosurface, where mesoscale patterns follow the macrosurface geometry. The same Implicit function can generate both the mesoscale geometry and the second-order macro surface, with control over thickness through particle agglomeration. As a result, we can see mesoscale geometry at the surface level.

76 where  $w$  represents the width of the microstructure and  $k_{ij} \geq 0$  are  
77 the powers associated with each trigonometric term  $T_{ij}(\mathbf{p})$  defined  
78 by

$$T_{ij}(\mathbf{p}) \in \{A_k \cdot f(\omega_k p_d + \phi_k) \mid f \in \{\sin, \cos\}, p_d \in \{p_x, p_y, p_z\}\}.$$

79 where  $A_k$  is the amplitude,  $\omega_k$  is the frequency, and  $\phi_k$  is the phase  
80 shift of the trigonometric function.

81 One collection of such functions that we use in our system is the  
82 family of Triply Periodic Minimal Surfaces (TPMS); for instance,  
83 the Gyroid, Diamond, and Primitive functions [HC18], see Sec. 3.1  
84 for equations of these structures.

85 Many microstructures can be defined using these trigonometric  
86 functions: Let us consider a  $3 \times 3$  matrix  $\mathbf{T}$ , which performs affine  
87 transformations such as scaling, rotation, and translation. Some-  
88 times, one or more of these operations are combined in the  $3 \times 3$   
89 matrix using octaves. Each entry in this matrix is generated from  
90 the summation of multiple sine and cosine waves with varying am-  
91 plitudes and frequencies, and typically, each value is normalized  
92 between  $-1$  and  $1$ , see Sec. 3.1.4.

#### 93 1.6. Particle Piling

94 In this section, we report additional experiments for piling structures  
95 with our framework. The implicit surfaces for the particle material  
96 can be changed in the following manner for the generation of particle  
97 piling:

$$d_g(\mathbf{p}, w) = f(\mathbf{p}) + \min_{i=0, \dots, 26} d_{\mathbf{q}_i} \left( \frac{1}{w} ((\mathbf{R}_\theta \mathbf{p}) + \mathbf{P}(\mathbf{p}) \mathbf{N}(\mathbf{p})) \right), \quad (10)$$

98 where  $f(p)$  is an arbitrary function for spatially varying surface  
99 offsetting. The term  $\mathbf{R}_\theta$  refers to the rotation matrix with angle  
100  $\theta$ . The term  $\mathbf{P}(\mathbf{p}) \mathbf{N}(\mathbf{p})$  generates the implicit surface deformation  
101 using a product of the control polynomial function  $P(\mathbf{p})$  and the  
102 noise function  $N(\mathbf{p})$ . The term  $P(\mathbf{p})$  in the above equation controls  
103 the degree of convexity to the concavity of the grains in the same

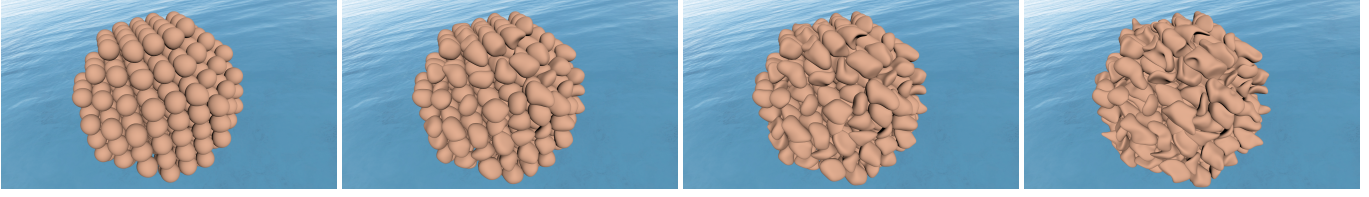


Figure 4: Starting from a regular cubic lattice of spherical grains (first column), slowly adding different levels of sparse convolution noise [FW07] as  $N(\mathbf{p})$  in the eq. 14 in the main document for the implicit surface deformation generates grains similar to rock piles with contact points. Increasing the level of deformation generates more concave grains. Here, the rotation angle with respect to the y-axis used is  $15^\circ$ . We can utilize any deformation function that deforms the implicit surface in a specific manner for targeted applications.



Figure 5: Our framework can generate multiscale granular media with grains in settled positions. In the left image, the generated rockpile shows smaller grains at the bottom and larger ones at the top, with well-defined contact points even across scales. The right image illustrates the same cloud, but with an additional polynomial function applied to the rotation angle,  $\theta = 15 + p_z$ , as defined in Eq. 14 of the main document.

127 we use something for  $h(\mathbf{p})$  like Perlin noise in Eq. 3 in the main  
128 document, we do not need to change the Lipschitz bounds [Har96].

129 Another important transformation we use is the scaling of the  
130 point coordinates to achieve anisotropy in shape. Suppose we use  
131 the following scaling operation on point coordinates [Har96]:

$$\mathbf{p}' = (c_1 p_x, c_2 p_y, c_3 p_z). \quad (11)$$

132 The value of the Lipschitz bound is then  $\max(c_1, c_2, c_3)$ .

133 Linear deformation of shapes is achieved by multiplying the  
134 transformation matrix  $\mathbf{T}$  with the point  $\mathbf{p}$ , resulting in spatially  
135 varying shapes. In Sec. 1.3, the transformed point  $\mathbf{p}'$  is obtained  
136 using this type of transformation. The value of the Lipschitz bound  
137 for this case is the largest eigenvalue of the matrix  $\mathbf{T}$  [Har96], and  
138 we can find this using the power method [Ger04].

139 For example, we used the turbulence matrix  $\mathbf{T}$  for the linear de-  
140 formation in Sec. 1.3. This turbulence matrix is dependent on the  
141 point  $\mathbf{p}$  each time. For the Lipschitz bound, we need to calculate the  
142 maximum eigenvalue of this matrix each time, which is computa-  
143 tionally expensive. Instead of calculating it every time for matrices  
144 that change, we can calculate it only once for the matrix with all  
145 entries set to the maximum possible values. In this case, it is the  
146 value one for all entries in the matrix. The maximum eigenvalue of  
147 this matrix, using the power method, is 3. This value serves as the  
148 Lipschitz bound for the transformation involving  $\mathbf{T}$ .

104 particle cloud, where the smooth transition between convexity and  
105 concavity happens in the same cloud.

106 In Fig. 4, we show how different levels of deformation affect  
107 an initial particle cloud of spheres. This approach is useful for  
108 modeling granular media, such as rock piles, as can be seen in the  
109 last column. Fig. 5 illustrates the versatility of our framework to  
110 generate multiscale granular patterns on the fly without the need for  
111 any pre-computation or collision detection methods.

## 112 2. Multiscale Geometry Rendering

113 In this section, we provide additional details about Lipschitz bounds  
114 2.1 for the transformed objects and the multiscale sphere tracing  
115 algorithm 2.2.

### 116 2.1. Lipschitz Bounds for the Transformed Objects

117 The Lipschitz constant of the sum of two functions is, at most,  
118 the sum of their Lipschitz constants. The Lipschitz constant of the  
119 composite function is the product of the Lipschitz constant of each  
120 of the component function's Lipschitz constants [Har96].

121 The transformations, rotations, translations, and reflections are  
122 called isometries, and if the transformation  $\mathbf{T}$  is an isometry, then the  
123 distances for the implicit function need no adjustment, meaning the  
124 distances are preserved when we perform these isometric transfor-  
125 mations. For example, in our case, the warping function  $h(\mathbf{p})$  is an  
126 isometry transformation, essentially a translation. Therefore, when

### 149 2.2. Multiscale Sphere Tracing

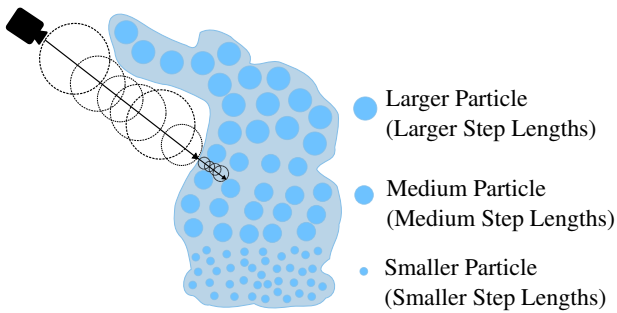
150 In this paper, we present an optimized sphere-tracing algorithm  
151 aimed at improving the performance of sphere tracing for multiscale  
152 grid variations as illustrated in Alg. 1 and Fig. 6.

**Algorithm 1** Optimized sphere tracing with adaptive step factors based on gradients of the implicit surface and the polynomial function  $D(\mathbf{p})$  for sparse sampling. IS denotes the implicit surface.

```

1: function COMPUTEGRIDSACLE( $\mathbf{p}$ )
2:    $\epsilon \leftarrow 0.01$ 
3:    $dp_x \leftarrow (\epsilon, 0, 0)$ 
4:    $dp_y \leftarrow (0, \epsilon, 0)$ 
5:    $dp_z \leftarrow (0, 0, \epsilon)$ 
6:    $gp_x \leftarrow |\text{IS}(p + dp_x) - \text{IS}(p - dp_x)|$ 
7:    $gp_y \leftarrow |\text{IS}(p + dp_y) - \text{IS}(p - dp_y)|$ 
8:    $gp_z \leftarrow |\text{IS}(p + dp_z) - \text{IS}(p - dp_z)|$ 
9:    $|\nabla d| \leftarrow \sqrt{gp_x^2 + gp_y^2 + gp_z^2}$ 
10:   $scale \leftarrow \text{clamp}(|\nabla d| \cdot 0.5, 0.0, 1.0)$ 
11:  return  $scale$ 
12: end function
13: function MULTISCALE-SPHERE-TRACING( $ro, rd, t_{\min}, t_{\max}$ )
14:   $t \leftarrow t_{\min}$ 
15:   $d \leftarrow \text{IS}(ro + t \cdot rd)$ 
16:   $s \leftarrow \text{sign}(d)$ 
17:   $lastScale \leftarrow \text{ComputeGridScale}(ro + t \cdot rd)$ 
18:  for  $i = 0$  to  $n$  do
19:    if  $|d| < \text{precision} \cdot t$  or  $t > t_{\max}$  then
20:      break
21:    end if
22:    if  $D(\mathbf{p}) = 1$  then  $\triangleright$  Evaluate gradient only when
    polynomial checks  $D(\mathbf{p})$  is true
23:       $lastScale \leftarrow \text{ComputeGridScale}(ro + t \cdot rd)$ 
24:    end if
25:     $stepFactor \leftarrow \text{LERP}(\delta_{\min}, 1.0, lastScale)$ 
26:     $t \leftarrow t + s \cdot d \cdot stepFactor$ 
27:     $d \leftarrow \text{IS}(ro + t \cdot rd)$ 
28:  end for
29:  return  $t$ 
30: end function

```



**Figure 6:** (Camera Ready: We improve the efficiency of the sphere tracing algorithm using adaptive step lengths controlled by the magnitude of the implicit surface gradients. Polynomial checks allow sparse sampling of gradients, reducing the number of expensive gradient evaluations while still capturing grid-scale variations. This enables finer grids to use shorter steps and coarser grids to use longer steps, improving overall performance. An example of a polynomial condition is  $\sin(p_x) \cos(p_y) + \sin(p_y) \cos(p_z) + \sin(p_z) \cos(p_x) = 0.5$ .)

In the above algorithm, on line 22, we can use any other condition to reduce the gradient computations and improve performance during sphere-tracing steps. For instance, we can check this using the following condition, where we examine gradients to track variations in grid scale for every  $m$ -step length.

$$\text{If } i \bmod m = 0, \text{ where } m < n$$

For instance, we use something like the following functions (in Eqs. 12 and 13) for the  $D(\mathbf{p})$  in the above algorithm to track the gradient changes. Essentially, we are sampling sparse points throughout the volume to track the grid scale variations effectively. The polynomial conditional check  $D(\mathbf{p})$  is a method to reduce the number of gradient evaluations in sphere tracing iterations.

$$D(\mathbf{p}) = \begin{cases} 1, & \text{if } |\text{fmod}(p_y, n_1)| = 0.0 \\ & \vee (|\text{fmod}(p_z, n_2)| = 0.0 \wedge |\text{fmod}(p_x, n_3)| = 0.0) \\ 0, & \text{otherwise} \end{cases} \quad (12)$$

Step Factor	RTX 4090		RTX A2000	
	RT (ms)	FPS	RT (ms)	FPS
Fixed global bound	9.3	105.7	50	20
Bisection based	9.0	108.5	45	22.1
Fully Adaptive (N = 1)	44.1	22.6	240	4
Adaptive (N = 10)	11.5	85.8	60.6	16.2
Adaptive (N = 100)	8.1	121.1	44	22.8
Adaptive (N = 500)	8.1	121.5	42.7	23.1
Adaptive ( $D(\mathbf{p}) = 1$ )	7.8	124.5	42.2	23.5

**Table 1:** (Camera Ready: Performance comparison of different step-length strategies for sphere tracing in multiscale particulate media made of Lambertian particles. We evaluate fixed stepping (classical sphere tracing), the bisection method, fully adaptive stepping (update every step), adaptive stepping with gradient checks every  $N$  steps (10, 100 and 500), and adaptive stepping with polynomial-based gradient checks for 1500 steps. Longer steps are more effective for macroscopic scales, shorter steps for microscopic scales, and intermediate steps for mesoscopic scales. Adaptive stepping with polynomial checks achieves the best performance, improving rendering efficiency by 16% over fixed and bisection methods.)

$$D(\mathbf{p}) = \begin{cases} 1, & \text{if } \sin(p_x) \cos(p_y) + \sin(p_y) \cos(p_z) \\ & + \sin(p_z) \cos(p_x) = 0.5 \\ 0, & \text{otherwise} \end{cases} \quad (13)$$

These methods can improve performance, but using polynomial checks to track variations in the grid scale is particularly effective. It allows smaller step lengths in finer grid-scale regions and larger ones in coarser grid scales. In Table 1, we report the performance comparison of different sampling strategies for the step length across multiple GPUs. Fig. 7 presents the renderings obtained with the multiscale sphere tracing algorithm, demonstrating that the use of polynomial checks yields a significant performance boost without introducing noticeable visual differences.



Figure 7: Visualization of the rendered multiscale grid variational geometry with different step length methods. The results are shown for fixed step lengths, as well as for the two polynomial checks  $D(\mathbf{p})$  (as referenced in equations 12 and 13) used for adaptive step lengths, respectively. The performance values for these three cases are as follows: for the fixed lengths case, the results are (RT - 8.6 ms, FPS - 112.3). For the polynomial-based gradient checks with the equation in 12, where the values of  $n_1, n_2, n_3$  are 11, 5, and 7, the results are (RT - 7.0 ms, FPS - 140.1). With the equation in 13, the results are (RT - 6.9 ms, FPS - 141.6). It clearly shows that polynomial-based gradient checks for tracking grid scale variations within the sphere tracing algorithm improve performance.

### 173 3. Multiscale Geometry Reconstruction

174 Inverse procedural modeling promises to overcome some of the main  
 175 limitations of procedural modeling, such as parameter tweaking to  
 176 create a given real target exemplar. In this section, we focus on recon-  
 177 structing procedural microstructures generated by our framework.  
 178 We explore two modalities: implicit surfaces, potentially extracted  
 179 from noisy MicroCT scans, and RGB images, potentially obtained  
 180 from Transmission Electron Microscopy (TEM) or Scanning Elec-  
 181 tron Microscopy (SEM) samples. First, we create a synthetic dataset  
 182 of representative microstructures that serves as a proof of concept.  
 183 For the first modality, we apply direct parameter fitting to find the  
 184 parameters of our procedural microstructures with observed data.  
 185 For the second modality, we employ analysis-by-synthesis, iteratively  
 186 refining reconstructions by comparing a simulated image with  
 187 a reference image. We also show that the reconstruction of synthetic  
 188 microstructures is not a trivial task by trying to reconstruct implicit  
 189 functions using popular network architectures to represent signals  
 190 such as NeRF [MST\*21] and SIREN [SMB\*20], and a physically-  
 191 based differentiable rendering algorithm for SDF [VSJ22].

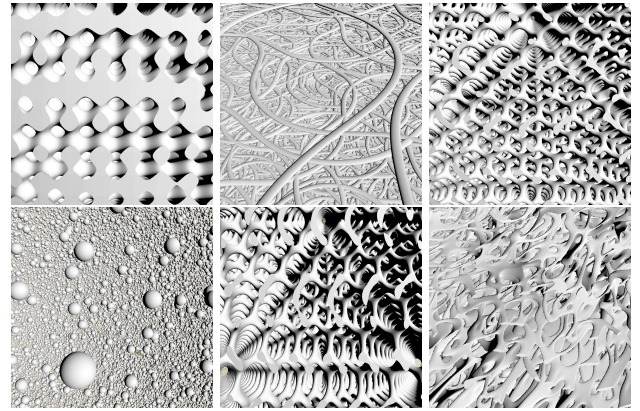


Figure 8: Instances of exemplar renders (*top row*) Gyroid [1D] 14, Fibers [2D] 25, Gyroid [3D] 15 respectively. Rest of the renders (*bottom row*) are Spheres [2D] 22, Gyroid [5D] 18, Porous [28D] 28 respectively. The number inside the parentheses corresponds to the number of parameters, i.e., the dimensionality of the space search.

#### 192 3.1. Synthetic Dataset

193 For the proof of concept and more control over the experiments, we  
 194 evaluate our algorithms on representative synthetic examples that  
 195 resemble SEM/TEM images. The dataset consists of six microstruc-  
 196 tures, where each microstructure is defined by an implicit function  $\hat{f}$   
 197 with  $n$  parameters, denoted as  $\phi$ . All ground-truth parameter values  
 198 presented in the dataset were selected for their convenience and to  
 199 ensure they fit in the defined domain range.

##### 200 3.1.1. Gyroid Family

201 The first family of microstructures are the gyroid microstructures.  
 202 These consist of periodic fully deterministic patterns created using  
 203 trigonometric functions. Our dataset includes three such microstruc-  
 204 tures with 1, 3, and 5 degrees of freedom, respectively. The simplest  
 205 example is the Gyroid [1D]. The only parameter is a scalar variable  
 206  $\eta \in \mathbb{R}$ . We refer to  $\eta$  as the noise scale. The  $\eta$  variable controls  
 207 the density of the microgeometry. We create the ground-truth using

208  $\eta = 100$ :

$$\hat{f}(\mathbf{x} | \eta) = \sum_i^3 \sin(x_i \cdot \eta) / \eta. \quad (14)$$

209 The second element from the set of gyroid functions, Gyroid [3D],  
 210 is guided by  $\eta \in \mathbb{R}$ , and  $k = 2 \cdot \pi / a \in \mathbb{R}, t \in \mathbb{R}$ . The  $a$  represents  
 211 the cell size of the gyroid structure,  $t$  represents the wall thickness.  
 212 We create the ground-truth using the setting of  $\eta = 100.0, a = 7.0,$   
 213  $t = 1.2$  as follows

$$\hat{f}(\mathbf{x} | \eta, k, t) = g(\mathbf{x} \cdot \eta | k, t) / \eta, \quad (15)$$

$$g(\mathbf{x} | k, t) = \sin(kx_0) \cos(kx_1) + \quad (16)$$

$$\sin(kx_1) \cos(kx_2) + \sin(kx_2) \cos(kx_0) + t. \quad (17)$$

214 Finally, the last exemplar, the Gyroid [5D], closely resembles the Gy-  
 215 roid [3D] problem. The only difference is the division of the  $\mathbf{a} \in \mathbb{R}^3$   
 216 parameter into three variables  $k_i = 2 \cdot \pi / a_i$ , each controlling the cell  
 217 size of the gyroid in the  $x, y,$  and  $z$  directions respectively. We create

218 the ground-truth using the setting  $\eta = 100.0$ ,  $\mathbf{a} = (7.0, 10.0, 15.0)$ , 253  
 219  $t = 1.2$ . The formulation ins this case is:

$$\hat{f}(\mathbf{x} | \eta, \mathbf{k}, t) = r(\mathbf{x} \cdot \boldsymbol{\eta} | \mathbf{k}, t) / \eta, \quad (18) \quad 254$$

$$r(\mathbf{x} | \mathbf{k}, t) = \sin(k_1 x_0) \cos(k_2 x_1) + \quad (19) \quad 255$$

$$\sin(k_2 x_1) \cos(k_3 x_2) + \sin(k_3 x_2) \cos(k_1 x_0) + t, \quad (20) \quad 256$$

### 220 3.1.2. Spherical Microstructure

221 Spherical microstructure consists of an implicit function for ran- 260  
 222 domly placed spheres. We generate a granular material microgeome- 261  
 223 try using a space-filling grid-based random variable of points. A grid 262  
 224 cell index, computed from its floored location, is used to generate a 263  
 225 seed  $t$  for the PRNG. A multilinear hash function defining the seed 264  
 226 looks as follows:

$$t_l(\mathbf{x}) = M \sum_{i=0}^1 \sum_{j=0}^1 \sum_{k=0}^1 a_{ijk} q_l(x_0)^i q_l(x_1)^j q_l(x_2)^k, \quad (21)$$

227 where grid indices  $(q_l(x_0), q_l(x_1), q_l(x_2))$  are computed in eight 262  
 228 directions using binary offsets and the floor operation.  $M$  and all 263  
 229  $a_{ijk}$  were selected such that regularity artifacts are avoided. A seed 264  
 230  $t_l$  is later used as an input to PRNG, generating a pseudo-random 265  
 231 number in the interval  $[0, 1)$ . We then add the randomly generated 266  
 232 number to the grid position to obtain the center of a random sphere 267  
 233 in the current grid. We repeat the described procedure a total of 8 268  
 234 times (once for each potential overlapping grid cell). Finally, the 269  
 235 implicit function is calculated by finding the minimum distance to 270  
 236 all spheres, taking into account their radius. The variables are the 271  
 237 density-controlling  $\eta \in \mathbb{R}$  and the radius of the spheres  $r \in \mathbb{R}$ . The 272  
 238 procedure can be mathematically described as follows:

$$\hat{f}(\mathbf{x} | \eta, r) = \left( \min_{l=1}^8 \|c_l(\boldsymbol{\eta} \cdot \mathbf{x}, t_l(\boldsymbol{\eta} \cdot \mathbf{x})) - \mathbf{x}\|_2 - r \right) / \eta, \quad (22)$$

$$c_l(\boldsymbol{\eta} \cdot \mathbf{x}, t_l(\boldsymbol{\eta} \cdot \mathbf{x})) = \mathbf{q}_l(\boldsymbol{\eta} \cdot \mathbf{x}) + \text{PRNG}(t_l(\boldsymbol{\eta} \cdot \mathbf{x})), \quad (23) \quad 273$$

$$\mathbf{q}_l(\boldsymbol{\eta} \cdot \mathbf{x}) = \lfloor \boldsymbol{\eta} \cdot \mathbf{x} \rfloor + \mathcal{U}_l, \quad (24)$$

239 where  $\mathbf{x}$ ,  $t_l(\mathbf{x})$ ,  $c_l(\mathbf{x}, t_l(\mathbf{x}))$ ,  $\mathcal{U}_l$  are a point of evaluation, a random seed, 274  
 240 the center of a random sphere, and the  $l$ -th element of the unit cube 275  
 241 vertices  $\mathcal{U} = \{(v_1, v_2, v_3) \mid v_i \in \{0, 1\}\}$ , respectively. The PRNG is 276  
 242 not differentiable, making  $\hat{f}$  a non-differentiable function. We use 277  
 243 the following setting to create the ground-truth  $\eta = 30.0$ ,  $r = 0.08$ .

### 244 3.1.3. Fibrous Microstructure

245 Fibrous microstructures can be obtained by a union of two rotated 281  
 246 sets of fibers parallel to the  $y$ -axis arranged in layers. To achieve 282  
 247 this, we need a rotation transformation matrix  $T_\varphi$  along the axis  $y$  by 283  
 248 an angle  $\varphi \in [0, 2\pi]$ , which is a parameter. Thanks to the symmetry 284  
 249 of the problem, we can constrain the  $\varphi \in [0, \pi]$ . We also need a 285  
 250 function  $u: \mathbb{R}^3 \rightarrow \mathbb{R}$  defining the fibers. The last parameter is the 286  
 251  $\eta \in \mathbb{R}$  controlling the density of the fibers. The microstructure Fibers 287  
 252 [2D] is then defined by:

$$\hat{f}(\mathbf{x} | \eta, \phi) = h(\mathbf{x} \cdot \boldsymbol{\eta} | \phi) / \eta, \quad (25) \quad 287$$

$$h(\mathbf{x} | \phi) = \min \left( u(\mathbf{x}) + u((x_1, x_1, x_1)), u(T_\phi(\mathbf{x})) + u(T_\phi(x_1, x_1, x_1)) \right), \quad (26) \quad 288$$

$$u(x) = (\sin(x_0) \cos(x_1) + \sin(x_1) \cos(x_2) + \sin(x_2) \cos(x_0))^2. \quad (27) \quad 289$$

To create the ground truth, we set  $\eta = 100$ ,  $\varphi = \pi/4$ .

### 3.1.4. Porous Microstructure

255 Lastly, we present the function defining a porous microstructure  
 256 named Porous [28D]. The first parameter,  $\eta \in \mathbb{R}$ , controls the den-  
 257 sity of the material. The implicit function is composed of the sum-  
 258 mation of several sine and cosine waves with different amplitudes  
 259 and frequencies, resulting in a complex material structure. Three-  
 260 parameter transformation matrices determine the frequencies, den-  
 261 oted as  $\mathbf{T} \in \mathbb{R}^{3 \times 3 \times 3}$ . The final distance is then computed by

$$\hat{f}(\mathbf{x} | \eta, \mathbf{T}) = \min \left( \epsilon, v(\boldsymbol{\eta} \mathbf{T}_1 \mathbf{x}) + w(\boldsymbol{\eta} \mathbf{T}_2 \mathbf{x}) \cdot v(\boldsymbol{\eta} \mathbf{T}_3 \mathbf{x}) \right) / \eta, \quad (28)$$

$$v(\mathbf{x}) = \left( \sin(x_0) \cos(x_1) + \sin(x_1) \cos(x_2) + \sin(x_2) \cos(x_0) \right)^2, \quad (29)$$

$$w(\mathbf{x}) = \left( \sin(x_0) \sin(x_1) + \sin(x_1) \sin(x_2) + \sin(x_2) \sin(x_0) \right)^2, \quad (30)$$

where  $\epsilon$  is a small positive number. The ground truth is created with  
 a fixed  $\eta = 30$  and the  $\mathbf{T} \in [-4, 7]^{3 \times 3 \times 3}$ .

### 3.2. Parameter Fitting

265 This approach formulates microstructure reconstruction as a model-  
 266 fitting task, where the goal is to optimize the parameters of a pro-  
 267 cedural implicit surface to match the microstructure's ground truth  
 268 accurately. Given a set of spatial coordinates  $\Omega = \{\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^3\}$ , a  
 269 ground-truth SDF  $\hat{S}: \mathbb{R}^3 \rightarrow \mathbb{R}$  describing the surface at the point  
 270  $x$ , a bounded parameter space  $\Phi = [a_1, b_1] \times [a_2, b_2] \times \dots \times [a_n, b_n]$   
 271 with  $n$  parameters, and a loss function  $\mathcal{L}: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ , the problem  
 272 is defined as minimizing the discrepancy between the fitted function  
 273  $f$  and the ground truth  $\hat{S}$  across the domain:

$$\min_{\Phi \in \Phi} \int_{\Omega} \mathcal{L}(f(\mathbf{x}, \Phi), \hat{S}(\mathbf{x})) d\mathbf{x}. \quad (31)$$

274 Procedural implicit surfaces allow efficient extrapolation of the mi-  
 275 crostructure beyond the optimization domain without modifying the  
 276 fitted function. Additionally, our compact, parametrized microstruc-  
 277 tures are described using a relatively low number of parameters. We  
 278 propose a loss function to evaluate discrepancies in the frequency  
 279 domain using the discrete Fourier transform (DFT), which considers  
 280 the periodic behavior common in many microstructures. The loss  
 281 function compares the amplitude and phase spectra of the Fourier  
 282 coefficients, using the logarithm of the mean squared error (MSE) as  
 283 an error metric. This metric is closely related to the spectral density  
 284 function commonly used in microstructure analysis [BZL\*18].

### 3.3. Analysis by Synthesis

286 The analysis-by-synthesis approach optimizes the SDF by iteratively  
 287 rendering it using a non-differentiable pipeline and comparing the  
 288 results in image space. The process is illustrated in Fig. 9. Given a  
 289 camera intrinsics  $\mathbf{K} \in \mathbb{R}^{3 \times 3}$  taken from a set of intrinsic matrices  $\mathcal{K}$ ,  
 290 the camera extrinsics  $\mathbf{E} = [\mathbf{R} \mid \mathbf{t}] \in \mathbb{R}^{3 \times 4}$  taken from a set of extrinsic  
 291 matrices  $\mathcal{E}$ , a labeling function  $\hat{S}: \mathbb{R}^3 \rightarrow \mathbb{R}$ , a bounded parameter  
 292 space  $\Phi = [a_1, b_1] \times [a_2, b_2] \times \dots \times [a_n, b_n]$  with  $n$  parameters, a  
 293 signed distance fitting function  $f: \mathbb{R}^3 \times \Phi \rightarrow \mathbb{R}$ , a loss function  $\mathcal{L}$ :

294  $\mathbb{R}^{W \times H \times 3} \times \mathbb{R}^{W \times H \times 3} \rightarrow \mathbb{R}$ , with  $W, H$  being width and the height  
 295 respectively, a set of functions  $\mathcal{A}$ , and finally the rendering function  
 296  $\mathcal{R} : \mathcal{A} \times \mathcal{K} \times \mathcal{E} \rightarrow \mathbb{R}^{W \times H \times 3}$ , we can express the optimization  
 297 problem as follows:

$$\min_{\phi \in \Phi} \mathcal{L}(\mathcal{R}(f(\cdot, \phi), \mathbf{K}, \mathbf{E}), \mathcal{R}(\hat{S}(\cdot), \mathbf{K}, \mathbf{E})). \quad (32)$$

298  $\mathcal{R}$  renders the microstructure bounded by a unit sphere from the  
 299 given view with the camera parameters using the sphere-tracing  
 300 algorithm [Har96] in the CUDA-based framework OptiX [PBD\*10].  
 301 For the loss function, we used the two-dimensional DFT to trans-  
 302 form the image signal into the frequency domain. By focusing on  
 303 the amplitudes of the Fourier coefficients, we capture the key peri-  
 304 odic features of the image, which are crucial for the effective global  
 305 optimization of microstructures. While a multi-view optimization is  
 306 possible, we opted for a single-view approach to minimize computa-  
 307 tional overhead.

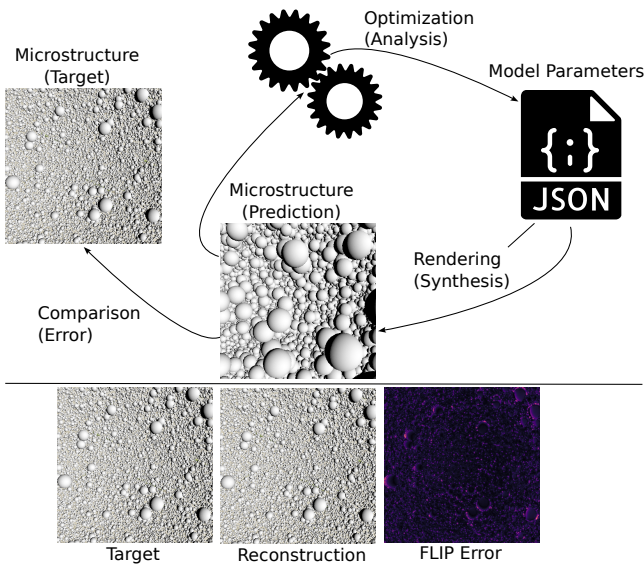


Figure 9: Analysis by synthesis schematic. Given a single target image (such as from SEM or TEM), we perform iterative optimization. At each step, we synthesize a microstructure using an implicit function and render a corresponding synthetic image using our rendering algorithm. We then compare this synthetic image to the target image and adjust the parameters of the synthetic microstructure to reduce the difference. This process continues until the synthetic image closely resembles the target.

### 3.4. Optimization Algorithms

309 Selecting a suitable optimization algorithm is critical for solving  
 310 unconstrained global optimization problems. The loss function  
 311 used in parameter fitting is differentiable, allowing us to use  
 312 gradient-based optimization algorithms, as the operations involved  
 313 are differentiable, including the discrete Fourier transform (DFT).  
 314 In this paper, we consider two first-order methods that utilize  
 315 gradient information: Basin-Hopping (BH) [Wal03] and Simplicial  
 316 Homology Global Optimization (SHGO) [ESF18] algorithms. The  
 317 BH algorithm is particularly effective for problems with funnel-like

loss functions. Its key hyperparameters include the step size  $s$   
 and the temperature  $T$ , which define the bounds of the uniformly  
 distributed random perturbations and the acceptance probability for  
 the candidate function, respectively. SHGO global optimization  
 algorithm approximates locally convex subdomains using homology  
 groups. The main hyperparameters for SHGO include the number  
 of iterations,  $l$ , and the number of samples,  $m$ , for building  
 the complex. The Fourier loss functions are differentiable, but  
 certain microstructures defined by procedural implicit surfaces  
 and the rendering function  $\mathcal{R}$  are non-differentiable, leading to  
 non-differentiability of the final composite function. We consider  
 two gradient-free optimization algorithms: the Covariance Matrix  
 Adaptation Evolutionary Strategy (CMA-ES) algorithm [HAB19]  
 and the modified Powell method [PVTf88, Pow64]. The CMA-ES  
 algorithm is highly effective, particularly for problems that are  
 rugged, noisy, and non-differentiable. Its key hyperparameters are  
 the population size  $\mathcal{P}$  and the initial  $\sigma_0$  of the covariance matrix,  
 typically chosen depending on the complexity and dimensionality  
 of the problem. The modified Powell method [PVTf88, Pow64] is a  
 local optimizer without hyperparameters that can be effective when  
 a reasonably close initialization is provided.

### 3.5. Neural networks

In this section, we describe how we use neural network to reconstruct  
 the synthetic microstructures from incomplete exemplars of surface  
 points and volumes.

**Problem Formulation** Given a set of point coordinates  $\Omega = \{\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^3\}$ , a signed distance labeling function  $\hat{S} : \mathbb{R}^3 \rightarrow \mathbb{R}$  that provides the ground truth signed distance from the surface at a point, a parameter space  $\Theta$  with  $h$  parameters, a neural network  $f : \mathbb{R}^3 \times \Theta \rightarrow \mathbb{R}$ , and finally a loss function  $\mathcal{L} : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ , the problem can be formulated as follows:

$$\min_{\theta \in \Theta} \int_{\Omega} \mathcal{L}(f(\mathbf{x}, \theta), \hat{S}(\mathbf{x})) d\mathbf{x}. \quad (33)$$

In contrast to the parameter fitting and analysis by synthesis approaches, there is no need for a manual selection of a suitable fitting function for the current problem. One drawback of the neural network is its inability to extrapolate outside of the training domain, which could be potentially solved in the future by tiling the fitted volume. In this section, we assume the use of a truncated SDF within a unit sphere, meaning that the SDF is only relevant inside the unit sphere and is truncated beyond it.

**Loss Function and Optimization** We adopt the loss function for optimizing 3D shapes from the SIREN paper [SMB\*20], which evaluates ground truth distances and gradients only at zero-level set points, while enforcing non-zero distances elsewhere. The loss also includes the Eikonal constraint to ensure the gradient magnitude is 1, making the function behave like a true distance function. The loss is formulated as follow:

$$\mathcal{L}_{\text{sur}} = \lambda_1 \int_{\Omega} \left( \|\nabla_{\mathbf{x}} f(\mathbf{x})\| - 1 \right) d\mathbf{x} + \lambda_2 \int_{\Omega_0} |f(\mathbf{x})| d\mathbf{x} + \lambda_3 \int_{\Omega_0} \left( 1 - \nabla_{\mathbf{x}} f(\mathbf{x})^T \nabla_{\mathbf{x}} \hat{S}(\mathbf{x}) \right) d\mathbf{x} + \lambda_4 \int_{\Omega \setminus \Omega_0} \psi(f(\mathbf{x})) d\mathbf{x}, \quad (34)$$

365 where  $\Omega_0$  denotes the surface points,  $\nabla_{\mathbf{x}}f(\mathbf{x})$  represents the gradient 414  
 366 of  $f$  with respect to  $\mathbf{x}$  in  $\mathbf{x}$ , and  $\nabla_{\mathbf{x}}\hat{S}(\mathbf{x})$  here is the normal at a given 415  
 367 surface point. The function  $\psi(\mathbf{x}) = \exp(-100 \cdot |f(\mathbf{x})|)$  encourages 416  
 368 off-surface points to maintain a non-zero distance. The first term 417  
 369 enforces the Eikonal constraint, constraining the gradient norm to 418  
 370 be 1. The second term forces zero-level set points to have a value 419  
 371 of zero. The third term aligns the normals of the function  $f$  with 420  
 372 the ground truth normals. We adopt the the hyperparameters from 421  
 373 the paper as follows:  $\lambda_1 = 50, \lambda_2 = 3000, \lambda_3 = 100, \lambda_4 = 100$ . 422  
 374 During training, for each point with a known ground truth signed 423  
 375 distance and normal from  $\mathbf{x} \in \Omega_0$ , an additional random off-surface 424  
 376 point  $\mathbf{x} \in \Omega \setminus \Omega_0$  is sampled. 425

377 In the second loss function, we use the fact that the signed distance 426  
 378 function is well-defined not only at the zero-level set points but also 427  
 379 available at the entire volume. Therefore, we propose a loss that 428  
 380 forces the network to learn the signed distances and gradients in the 429  
 381 entire domain: 430

$$\mathcal{L}_{\text{vol}} = \lambda_1 \int_{\Omega} \left| \|\nabla_{\mathbf{x}}f(\mathbf{x})\| - 1 \right| d\mathbf{x} + \lambda_2 \int_{\Omega} |f(\mathbf{x}) - \hat{S}(\mathbf{x})| d\mathbf{x} + \lambda_3 \int_{\Omega} \left( 1 - \nabla_{\mathbf{x}}f(\mathbf{x})^T \nabla_{\mathbf{x}}\hat{S}(\mathbf{x}) \right) d\mathbf{x}. \quad (35)$$

382 We use the same  $\lambda$  values as in the loss 34. Note that we do not 431  
 383 normalize the signed distances  $\hat{S}(\mathbf{x})$ . To find the minima of the loss 432  
 384 functions 34, 35, we use the ADAM optimizer [KB14] with the 433  
 385  $\alpha = 10^{-4}$  and  $\beta_1 = 0.9, \beta_2 = 0.999$  for all our experiments. 434

386 **Data Generation** To generate the ground truth signed distances, we 435  
 387 use the same approach as the synthetic dataset. For the optimization 436  
 388 of neural networks, we also need to compute the gradients with 437  
 389 respect to the inputs. For the synthetic microstructures that are not 438  
 390 differentiable (e.g., spherical microstructures), we approximate the 439  
 391 gradients using the central differences scheme. We consider two 440  
 392 scenarios: surface-level points and volume-level points. Specifically, 441  
 393 a point  $\mathbf{x}$  is considered to belong to the surface  $\Omega_0$  if its signed 442  
 394 distance satisfies  $|f(\mathbf{x})| < \epsilon$ , with  $\epsilon = 10^{-3}$ . 443

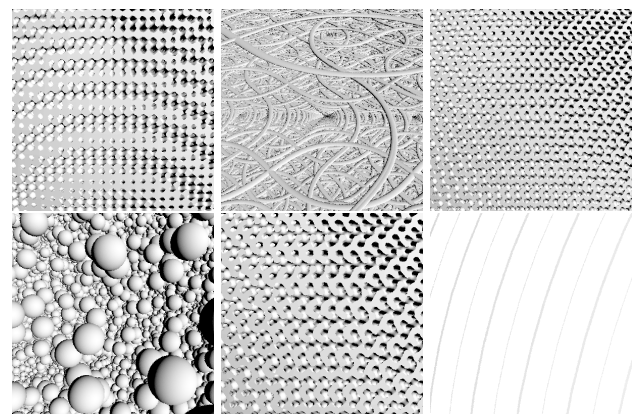
395 **Network Architectures** We consider two neural network architec- 444  
 396 tures. The first architecture is a standard MLP with ReLU as the 445  
 397 activation function, where we also use the positional encoding of the 446  
 398 input coordinates, adapted from NeRF [MST\*21]. This enables the 447  
 399 network to better represent higher frequency signals, such as sharp 448  
 400 details of the microstructure. We initialize the network using the He 449  
 401 initialization [HZRS15] and fix the number of hidden layers at five, 450  
 402 experimenting with 256 and 512 features per layer. The second net- 451  
 403 work architecture uses a periodic sine activation function instead of 452  
 404 the standard ReLU [SMB\*20]. We expect the periodic component, 453  
 405 similarly to positional encoding, would help the neural network to 454  
 406 encode the repetitive patterns of the microstructures. We use the 455  
 407 same initialization with  $\omega = 30$  as in the original SIREN paper 456  
 408 [SMB\*20]. To ensure a fair comparison with the MLP using 457  
 409 Positional Encoding, we also fixed the number of hidden layers at 458  
 410 five and experimented with 256 and 512 features per layer. 459

### 411 3.6. Reconstruction Results

412 In Fig. 10, we show the initial structures for the reconstruction 460  
 413 experiments. In Table 2, we report the performance of different 461

414 algorithms for different microstructures. In Table 3, we report 462  
 415 the initial parameters and the optimized parameters after the 463  
 416 reconstruction. In Fig. 11, we show the corresponding renders. 464  
 417 We set a maximum time limit of approximately 20 minutes for 465  
 418 optimization, as results typically do not improve significantly 466  
 419 beyond this point. The results show that no single optimization 467  
 420 algorithm consistently outperforms the others across all microstruc- 468  
 421 tures. SHGO-PF and BH-PF perform well for small-variable 469  
 422 problems but struggle with higher-dimensional cases (e.g., Gyroid 470  
 423 [5D], Porous [28D]) and cannot be applied to certain discrete 471  
 424 problems (e.g., Spheres [2D]). CMA-ES-PF demonstrates solid 472  
 425 performance across various microstructures, including discrete 473  
 426 ones such as spheres [2D]. As expected, parameter fitting methods 474  
 427 outperform analysis-by-synthesis in both accuracy and efficiency, 475  
 428 given the larger complexity of the latter. Interestingly, CMA-ES-AS 476  
 429 resembles Porous [28D] more than the other methods, highlighting 477  
 430 its potential for high-dimensional reconstructions. 478

431 In Table 4, we report the performance of different neural network 479  
 432 architectures. In Fig. 12 and Fig. 13, we include the corresponding 480  
 433 renders for the volume and surface reconstruction results, respec- 481  
 434 tively. Notice that all neural network architectures struggle to 482  
 435 recover the shapes given surface or volumetric points for the Fibers 483  
 436 [2D], Spheres[2D], and Porous [28D] microstructures. The discrete 484  
 437 nature of these microstructures and the non-differentiable search 485  
 438 spaces make the optimization with neural networks particularly 486  
 439 challenging. The results show that the SIREN architecture 487  
 440 outperforms the MLP with Positional Encoding architecture in most 488  
 441 microstructures, particularly in recovering thin structures. Hybrid 489  
 442 models combining the strengths of both classical optimization 490  
 443 methods and neural networks present an interesting venue for future 491  
 444 work. 492



493 Figure 10: Initial structures (*top row*) Gyroid [1D] 14, Fibers [2D] 25, Gyroid [3D] 15 respectively. Rest of the initial structures (*bottom row*) are Spheres [2D] 22, Gyroid [5D] 18, Porous [28D] 28 respectively. 494

Microstructure	Metrics	SHGO-PF	BH-PF	CMA-ES-PF	CMA-ES-AS	Powell-AS
Gyroid [1D]	Val. Error $\downarrow$	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	$10^{-4}$	$10^{-6}$
	LPIPS $\downarrow$	<b>0.00</b>	<b>0.00</b>	<b>0.00</b>	0.02	<b>0.00</b>
	$\mathcal{H}$ LIP $\downarrow$	$3 \times 10^{-7}$	$1 \times 10^{-7}$	$1 \times 10^{-3}$	$2 \times 10^{-3}$	$2 \times 10^{-3}$
	Time $\downarrow$	<b>2.85s</b>	16.67s	<b>2.23s</b>	20m	7m
Fibers [2D]	Val. Error $\downarrow$	0.34	$1 \times 10^{-3}$	0.65	1.00	1.00
	LPIPS $\downarrow$	0.41	<b>0.13</b>	0.54	0.56	0.56
	$\mathcal{H}$ LIP $\downarrow$	0.3	<b>0.14</b>	0.42	0.40	0.43
	Time $\downarrow$	13m	20m	<b>6m</b>	20m	<b>5m</b>
Gyroid [3D]	Val. Error $\downarrow$	$1 \times 10^{-3}$	$6 \times 10^{-3}$	1.02	0.15	$2 \times 10^{-3}$
	LPIPS $\downarrow$	<b>0.01</b>	0.04	0.65	0.35	0.02
	$\mathcal{H}$ LIP $\downarrow$	<b>0.01</b>	0.05	0.61	0.42	0.03
	Time $\downarrow$	<b>22.7s</b>	20m	<b>7m</b>	14m	20m
Spheres [2D]	Val. Error $\downarrow$	N/A	N/A	$1 \times 10^{-5}$	1.01	1.01
	LPIPS $\downarrow$	N/A	N/A	<b>0.00</b>	0.53	0.53
	$\mathcal{H}$ LIP $\downarrow$	N/A	N/A	$3 \times 10^{-7}$	0.55	0.55
	time $\downarrow$	N/A	N/A	<b>4m</b>	20m	5m
Gyroid [5D]	Val. Error $\downarrow$	0.66	0.65	$3 \times 10^{-4}$	0.03	0.44
	LPIPS $\downarrow$	0.42	0.57	<b>0.00</b>	0.21	0.54
	$\mathcal{H}$ LIP $\downarrow$	0.42	0.62	$6 \times 10^{-3}$	0.28	0.60
	Time $\downarrow$	<b>2m</b>	15m	<b>11m</b>	20m	15m
Porous [28D]	Val. Error $\downarrow$	N/A	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>	<b>1.00</b>
	LPIPS $\downarrow$	N/A	0.64	0.64	0.64	<b>0.61</b>
	$\mathcal{H}$ LIP $\downarrow$	N/A	<b>0.51</b>	0.52	0.52	0.59
	Time $\downarrow$	N/A	<b>4m</b>	8m	20m	20m

458 optimization is an interesting opportunity for future work.  
459

Table 2: Reconstruction performance for different optimization algorithms (columns) and synthetic procedural microstructures (rows). We report for each microstructure the **a**) Validaton Error, **b**) LPIPS Perceptual loss, **c**)  $\mathcal{H}$ LIP error, **d**) Time of the optimization. We consider a numerical 0 to be a number below  $1 \times 10^{-7}$ . The N/A implies that the optimization method could not be applied for the corresponding microstructure. The best results are highlighted in orange, while the second-best results are marked in yellow.

Problem	Ground Truth	Init.	SHGO-PF	BH-PF	CMA-ES-PF	CMA-ES-AS	Powell-AS
Gyroid [1D]	$\eta$ : 100.0	300.0	<b>100.000</b>	<b>100.000</b>	<b>100.000</b>	100.001	<b>100.000</b>
Fibers [2D]	$\eta$ : 100.0	200.0	<b>100.000</b>	<b>100.000</b>	100.100	175.159	133.202
	$\theta$ : $\pi/4$	$\pi$	0.142	<b>0.785</b>	2.825	3.126	0.831
Gyroid [3D]	$\eta$ : 100.0	300.0	<b>116.633</b>	213.469	32.000	186.593	86.780
	$a$ : 7.0	6.0	8.164	14.942	11.010	12.958	<b>6.075</b>
	$t$ : 1.2	0.0	<b>1.200</b>	<b>1.200</b>	1.196	1.173	1.198
Spheres [2D]	$\eta$ : 30.0	150.0	N/A	N/A	<b>29.999</b>	291.739	300.964
	$r$ : 0.08	0.2	N/A	N/A	<b>0.079</b>	0.093	0.086
Gyroid [5D]	$\eta$ : 100.0	200.0	114.983	142.570	<b>97.668</b>	74.162	89.104
	$a$ : 7.0	6.0	8.051	9.979	<b>6.836</b>	5.180	6.319
	$t$ : 10.0	6.0	11.534	14.162	<b>9.766</b>	7.376	9.228
	$t$ : 15.0	6.0	<b>14.961</b>	14.778	14.650	11.062	13.125
	$t$ : 1.2	6.0	1.180	1.199	<b>1.200</b>	1.165	1.151
Porous [28D]	$\eta$ : 30.0	50.0	N/A	38.586	42.796	<b>28.268</b>	43.272

Table 3: Optimal function parameters  $\phi$  Table. Optimal parameters found by the specified global optimizers. These are the parameters used to compute the error metrics in Table 2. The parameters were rounded to 3 decimal points. We also specify the ground truth and the initialization of the variables.

### 447 3.7. Differentiable SDF Rendering

448 We verify that the current state of the art for differentiable  
449 physically-based SDF rendering [VSJ22] does not handle typical  
450 features for multiscale material reconstruction, such as multi-object  
451 reconstruction and porous structures. In Figure 14, we show  
452 an example of failures in the reconstruction of a small set of  
453 objects (two spheres in contact and three cubes) and a porous  
454 sphere. In addition, it is not always possible to guarantee that the  
455 microstructure mathematical formulation is always differentiable,  
456 making differentiable optimization not possible in some scenarios.  
457 Further investigation to extend the algorithm to support multi-object

Microstructure		SIREN-SUR-256	SIREN-SUR-512	SIREN-VOL-256	SIREN-VOL-512	MLP-PE-SUR-256	MLP-PE-SUR-512	MLP-PE-VOL-256	MLP-PE-VOL-512
Gyroid [1D]	Val. Error $\downarrow$	0.03	0.03	0.02	<b>0.01</b>	0.04	0.15	0.13	0.36
	LPIPS $\downarrow$	0.42	0.31	0.21	<b>0.19</b>	0.47	0.65	0.37	0.49
	$\mathcal{H}$ LIP $\downarrow$	0.28	0.22	0.18	<b>0.16</b>	0.32	0.46	0.19	0.25
	$\max \ \nabla f(x)\  \downarrow$	2.18	1.95	2.07	<b>1.91</b>	2.51	4.81	7.04	11.94
	$\Delta$ -loss $\uparrow$	130.31	149.31	289.02	387.23	17650.59	16391.40	23623.22	22462.19
Fibers [2D]	Val. Error $\downarrow$	1.00	1.00	1.00	1.00	1.07	0.60	<b>0.39</b>	0.43
	LPIPS $\downarrow$	0.72	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	<b>0.69</b>	0.71	0.73
	$\mathcal{H}$ LIP $\downarrow$	0.95	0.51	0.49	0.54	0.51	0.51	0.38	<b>0.37</b>
	$\max \ \nabla f(x)\  \downarrow$	3.58	4.73	5.43	3.88	<b>2.08</b>	2.79	2.75	4.31
	$\Delta$ -loss $\uparrow$	66.99	88.40	208.28	274.95	20743.34	17657.37	20647.70	23504.41
Gyroid [3D]	Val. Error $\downarrow$	0.12	0.10	0.09	<b>0.05</b>	0.06	0.13	0.08	0.15
	LPIPS $\downarrow$	0.41	<b>0.34</b>	0.61	0.59	0.47	0.52	0.65	0.72
	$\mathcal{H}$ LIP $\downarrow$	0.46	<b>0.40</b>	0.58	0.56	0.46	0.46	0.57	0.58
	$\max \ \nabla f(x)\  \downarrow$	3.41	2.86	2.83	3.42	<b>1.99</b>	2.77	2.90	3.69
	$\Delta$ -loss $\uparrow$	121.56	178.95	311.83	412.26	21315.19	19604.08	24535.98	20033.85
Spheres [2D]	Val. Error $\downarrow$	0.70	0.94	0.46	<b>0.36</b>	1.02	1.00	1.00	1.01
	LPIPS $\downarrow$	0.66	0.64	0.61	<b>0.59</b>	0.66	0.66	0.64	0.64
	$\mathcal{H}$ LIP $\downarrow$	0.57	0.58	<b>0.54</b>	<b>0.54</b>	<b>0.54</b>	<b>0.54</b>	<b>0.54</b>	<b>0.54</b>
	$\max \ \nabla f(x)\  \downarrow$	4.61	4.98	<b>2.67</b>	4.55	4.7	10.59	15.45	19.13
	$\epsilon$ -loss $\uparrow$	133.71	238.88	345.84	544.73	23633.08	21651.34	24528.74	25124.24
Gyroid [5D]	Val. Error $\downarrow$	0.11	0.08	<b>0.03</b>	0.04	1.02	1.04	0.46	0.30
	LPIPS $\downarrow$	0.33	0.35	<b>0.31</b>	0.33	0.67	0.67	0.66	0.69
	$\mathcal{H}$ LIP $\downarrow$	0.38	0.41	<b>0.36</b>	0.38	0.61	0.61	0.60	0.57
	$\max \ \nabla f(x)\  \downarrow$	2.66	2.37	2.81	<b>1.61</b>	2.89	2.89	4.41	4.40
	$\Delta$ -loss $\uparrow$	138.95	167.09	244.68	383.13	21584.95	17986.02	20003.56	22752.97
Porous [28D]	Val. Error $\downarrow$	0.91	1.00	0.79	<b>0.70</b>	0.92	0.94	1.00	1.00
	LPIPS $\downarrow$	0.63	0.63	<b>0.6</b>	<b>0.6</b>	0.77	0.71	0.79	0.8
	$\mathcal{H}$ LIP $\downarrow$	0.47	0.47	0.55	0.51	<b>0.46</b>	0.56	0.59	0.47
	$\max \ \nabla f(x)\  \downarrow$	3.77	3.92	4.23	4.18	<b>2.75</b>	3.19	3.57	3.92
	$\Delta$ -loss $\uparrow$	49.25	86.32	271.66	393.56	15319.12	17610.17	22234.11	22713.46

Table 4: Trained Networks. Table of comparison of the network architectures and the training domains used on our sythetic dataset 3.1. We show for each problem the following: **a)** Validaton Error, **b)** LPIPS Perceptual loss, **c)** Image  $\mathcal{H}$ LIP error, **d)** The maximum norm of the gradient inside of the learning domain, **e)** The difference between the loss at the beginning and at the end of the optimization process denoted as  $\Delta$ -loss. The best results are highlighted in orange, while the second-best results are marked in yellow.

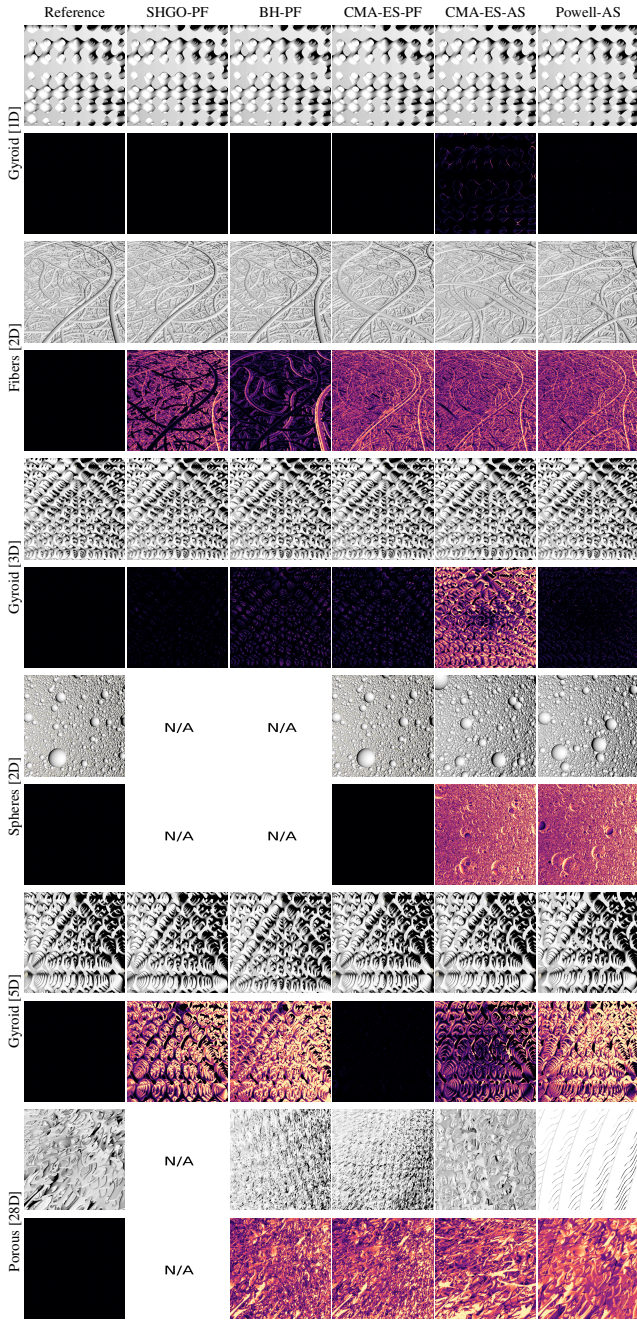


Figure 11: Reconstruction results for different optimization algorithms (columns) and synthetic procedural microstructures (rows). We show a comparison of rendered ground truth exemplars and the rendered approximations (*top row per microstructure*) with the measured  $\mathcal{FLIP}$  (*bottom row per microstructure*).

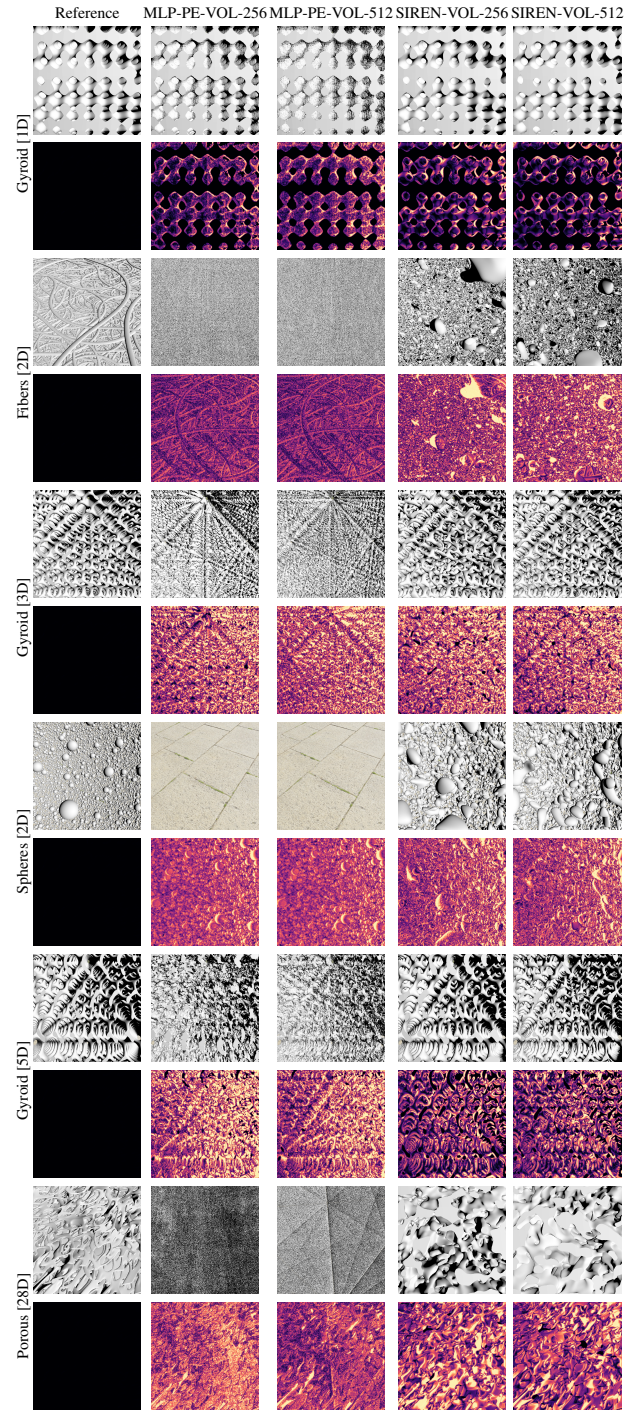


Figure 12: Volume reconstruction results for different neural network architectures (columns) and synthetic procedural microstructures (rows). We show a comparison of rendered ground truth exemplars and the rendered approximations (*top row per microstructure*) with the measured  $\mathcal{FLIP}$  (*bottom row per microstructure*).

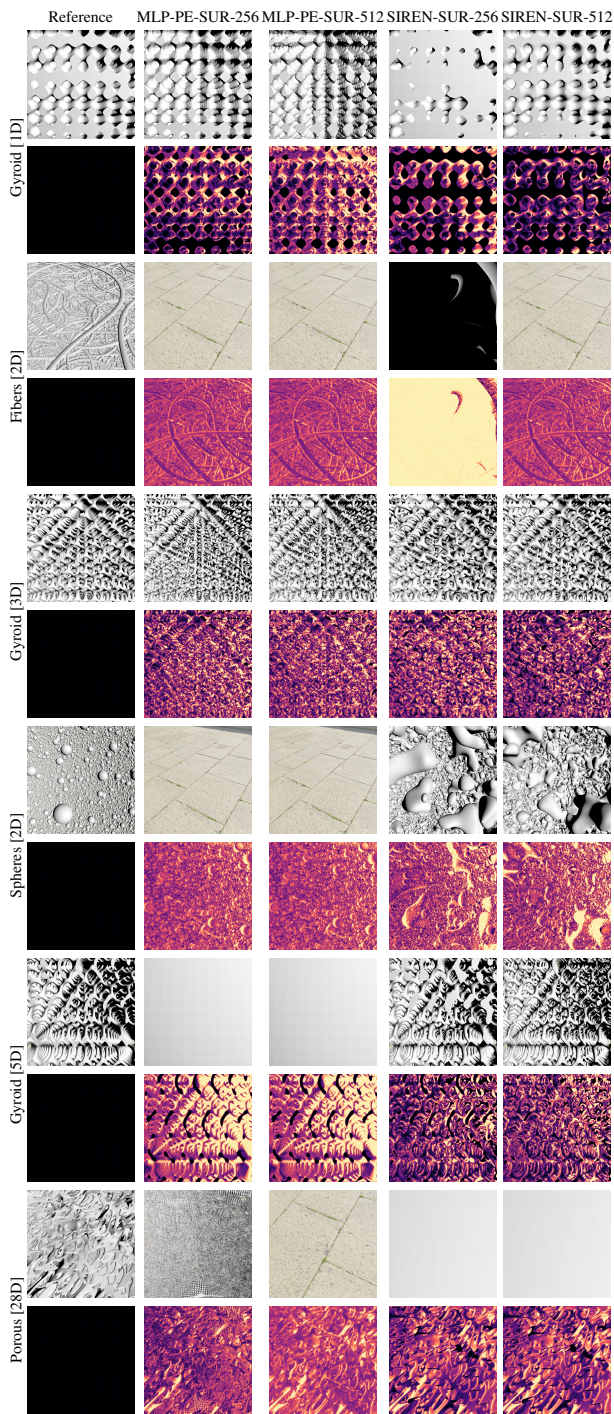


Figure 13: Surface reconstruction results for different neural network architectures (columns) and synthetic procedural microstructures (rows). We show a comparison of rendered ground truth exemplars and the rendered approximations (*top row per microstructure*) with the measured  $\mathcal{FLIP}$  (*bottom row per microstructure*).

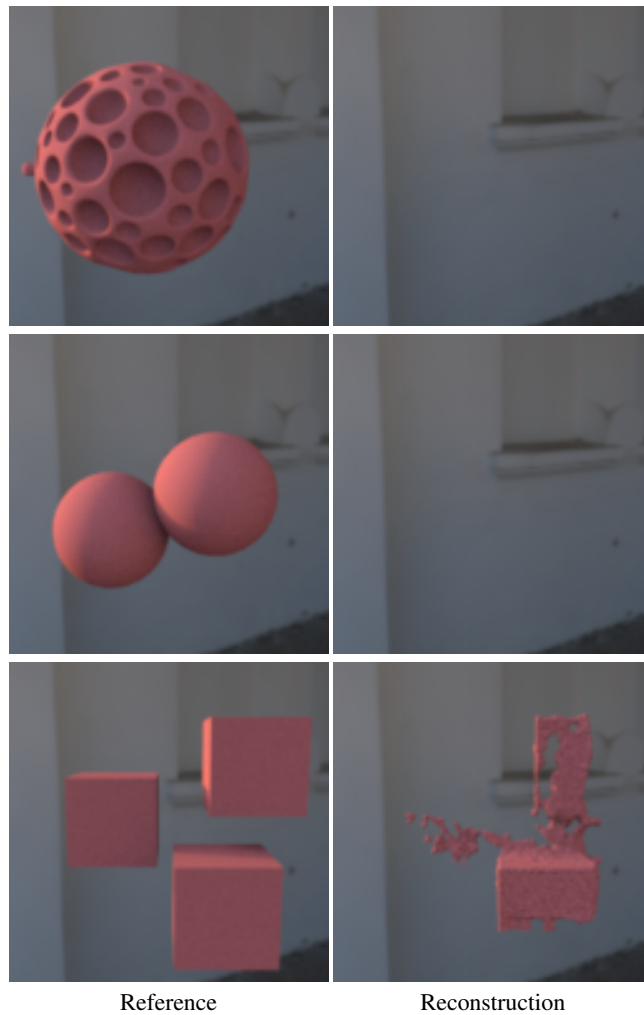


Figure 14: Results using a differentiable physically-based SDF rendering algorithm [VSJ22] for microstructure reconstruction including typical features such as multiple objects and porous structures. The algorithm fails after 512 iterations to reconstruct all cases, including empty solution for the first two rows and visible artifacts for the last row. The initialization is the unit sphere.

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