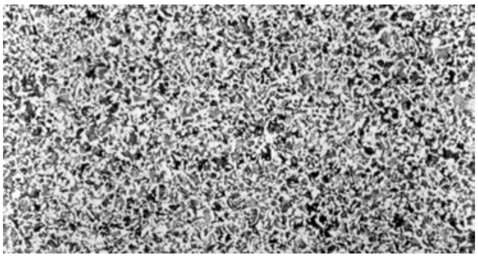
Electronic Supplementary Material (ESI) for Digital Discovery.

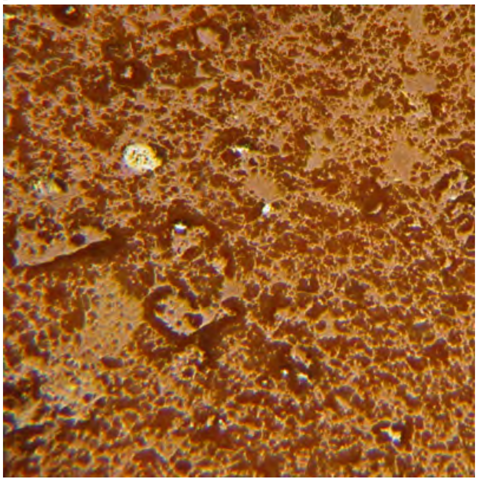
Supplementary Information

Training data

(a) Case 1 - 3-phase segmented SOFC micrograph [42]. 1326 × 2286 pixels.



(b) Case 2 - grayscale eutectic steel micrograph [43]. 795 × 418 pixels.

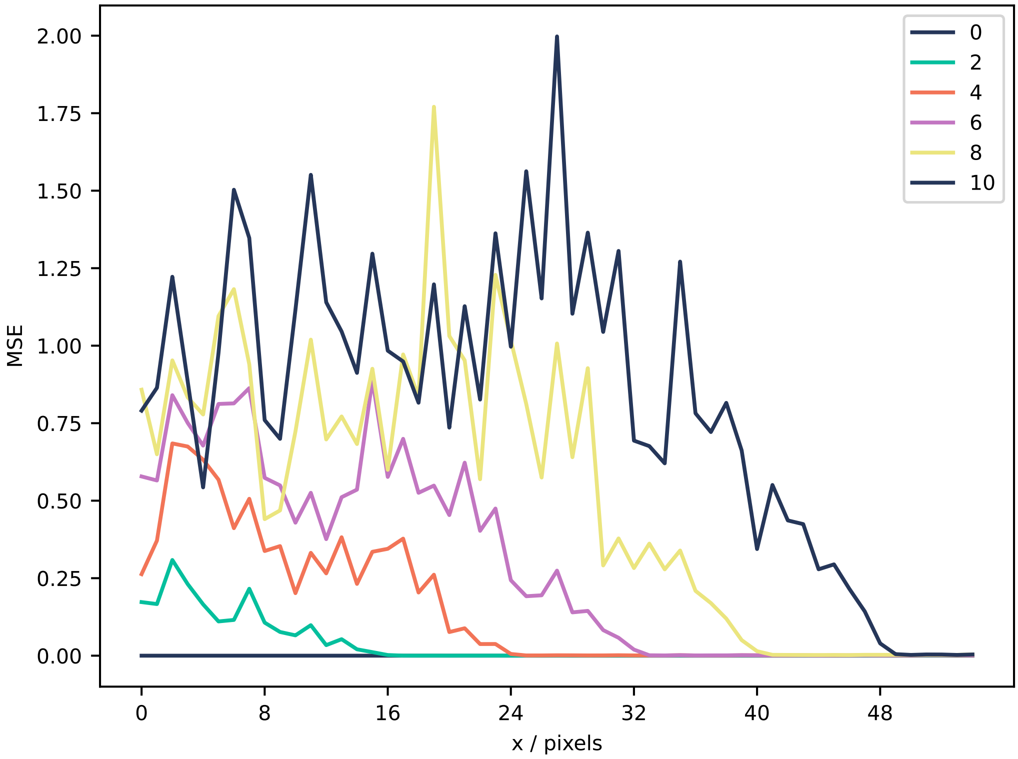


(c) Case 3 - colour terracotta pot micrograph [43]. 400×400 pixels.

Supplementary Figure 1: Full datasets used in training for each case study.

Seed propagation

The design of the architecture means that approximately one seed corresponds to an 8x8 region. However, this is not exactly the case and the reader is directed to convolv.in to explore the way different configurations of convolutions affect the output size of the network. To visualise the effect of changing seeds on the output of the generator, a baseline sample was generated from a single random seed. Then, marching outwards, the seed is changed one step at a time, and the difference between the resulting output and the baseline is taken. This is then summed in one spatial direction, and plotted in Figure 2. The central 2x2 region affects a region approximately 32^2, each step following roughly increases the effected region by 8 pixels on each side.



Supplementary Figure 2: A plot showing the MSE between a baseline image and a generated image with the seeds changed. The original size of the image is 112×112 pixels, generated from a 16×16 seed. The x-axis is moving away from the center of the image, and the different lines correspond to different $n \times n$ squares of seeds being changed in the center of the image.

Volume fraction KS tests

The p-values for the KS tests between the distribution of volume fractions for the three-phase SOFC material in case 1. To calculate these, a KS test was performed between the ground truth of each phase and the corresponding method.

Phase	G rand.	G fixed	Seed opt.	Seed rand.
Pore	0.73	1.2e-12	4.6e-08	0.43
Metal	0.91	2.3e-16	1.1e-45	0.022
Ceramic	0.97	7.3e-05	4.9e-50	0.022

Supplementary Table 1: KS test p-values of the volume fraction distributions for each of the methods for unoptimised and optimised cases across each three phases.

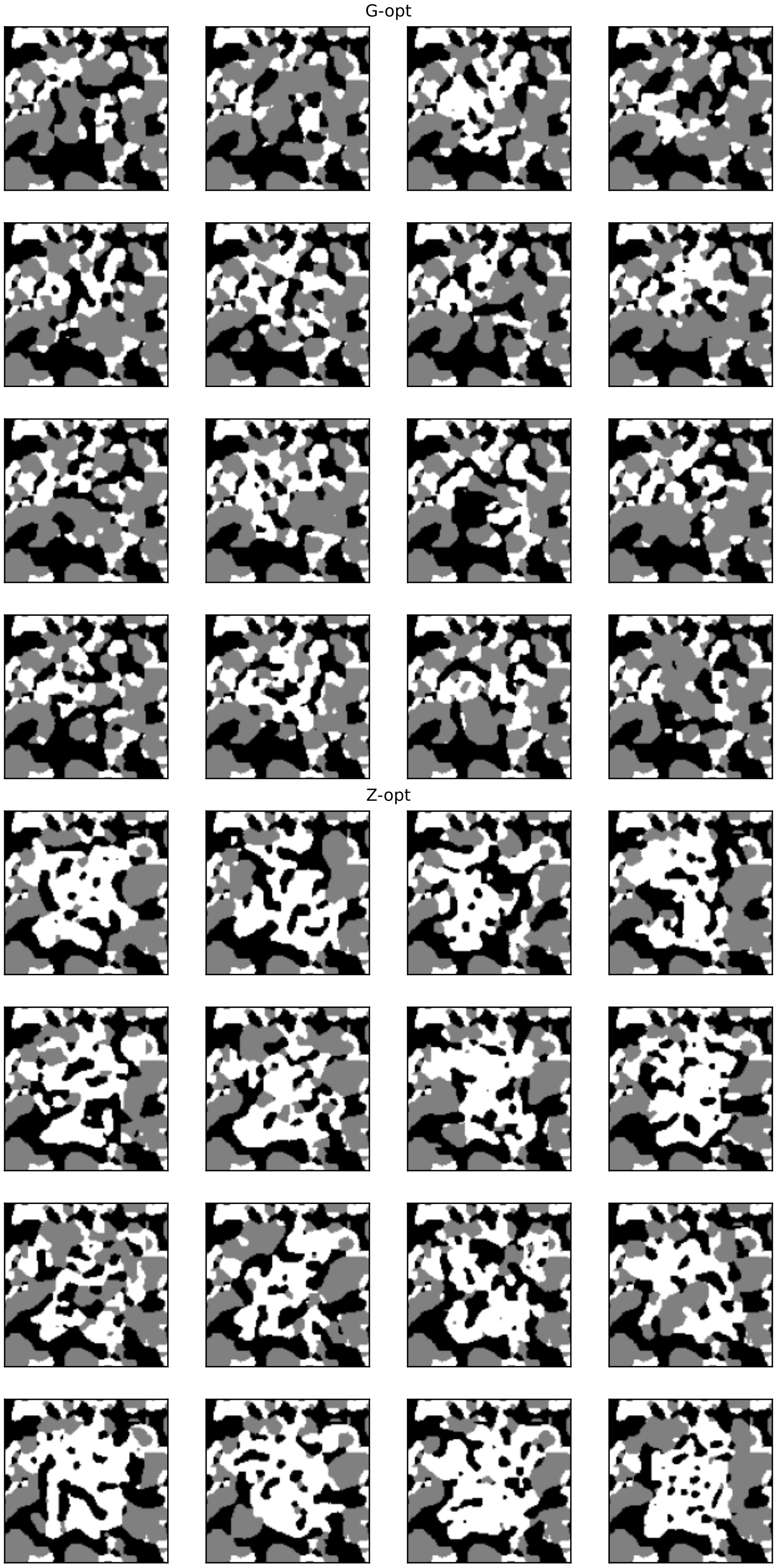
The results clearly show G rand performs the best, achieving a less significant result than the seed rand case. Although the G fixed method performs much worse than either random method, it achieves a p-value many orders of magnitude larger than the seed opt case, indicating that the seed opt distributions are more significantly different to the ground truth.

Network architecture

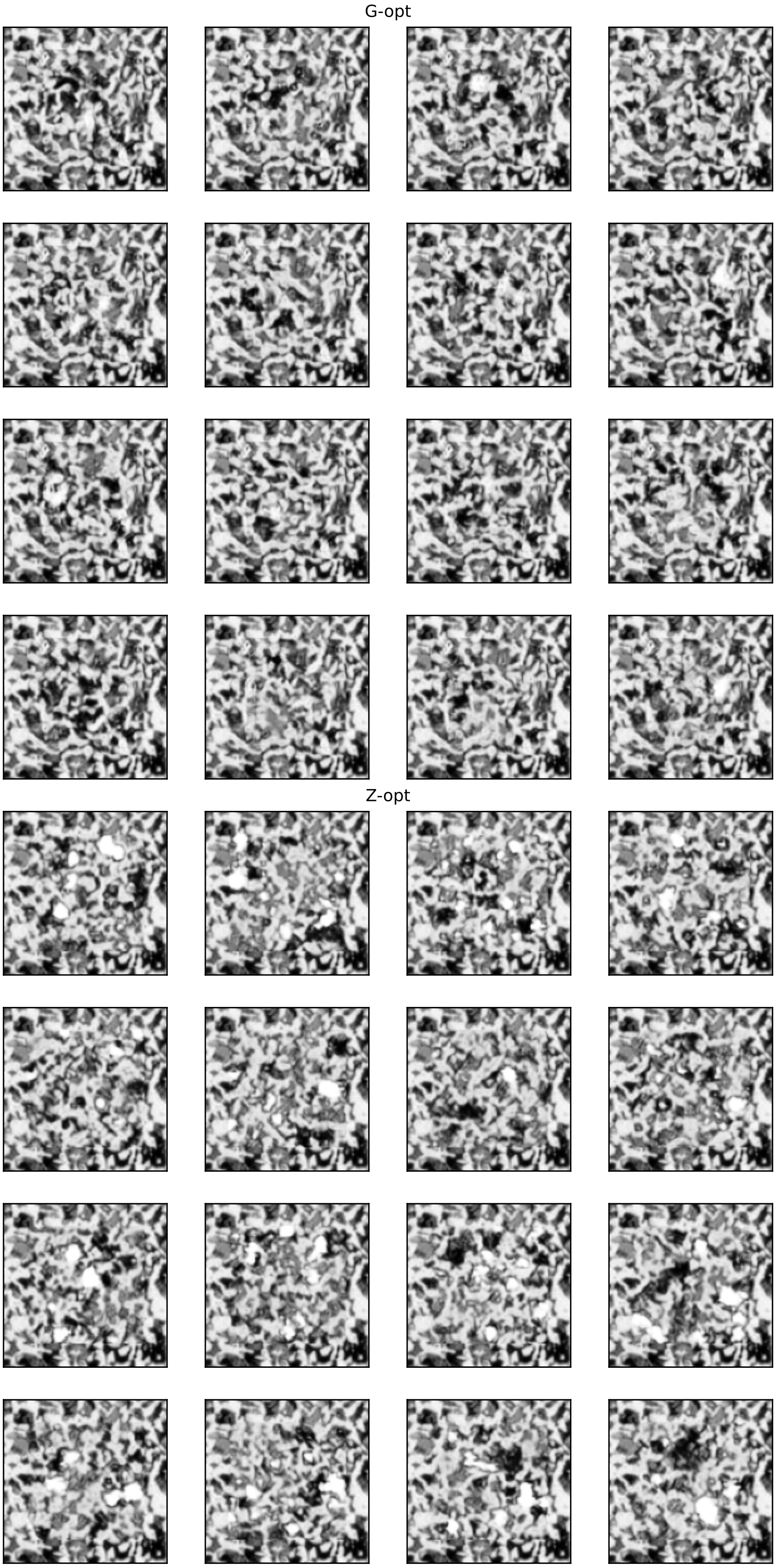
Layer	**Generator**	**Discriminator**
0	TransposeConvolution(100, 512, 4, 2, 2)	Convolution(n_{phases}, 64, 4, 2, 1)
1	TransposeConvolution(512, 256, 4, 2, 2)	Convolution(64, 128, 4, 2, 1)
2	Convolution(256, 128, 3, 1, 1), Upsample(size*2+2)	Convolution(128, 256, 4, 2, 1)
3	Convolution(128, n_{phases}, 3, 1, 1)	Convolution(256, 512, 4, 2, 1)
4		Convolution(512, 1, 4, 2, 1)

Supplementary Table 2: Network architecture and hyperparameters for both discriminator and generator networks. The number of phases (n_{phases}) is a parameter that varies depending on the input type. For *Convolution* and *TransposeConvolution* the order of the hyperparameters is *(input channels, ouput channels, kernel size, stride, padding)*. For *Upsample* the hyperparameter is *output size*, and the method used is a bilinear interpolation.

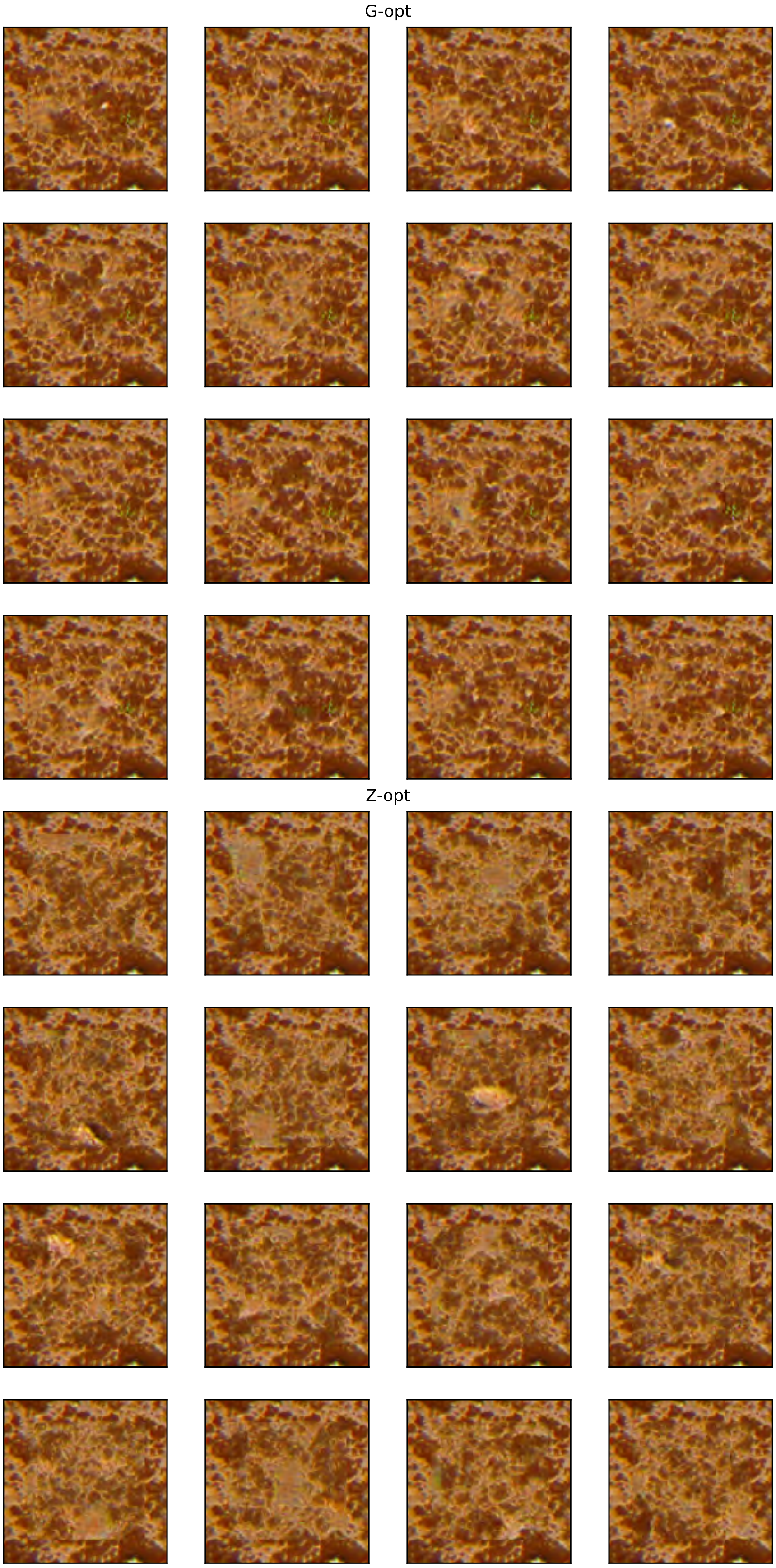
Generated examples



Supplementary Figure 3: 16 generated inpainting examples for each method. Case 1 - 3-phase segmented SOFC micrograph.



Supplementary Figure 4: 16 generated inpainting examples for each method. Case 2 - grayscale eutectic steel micrograph.



Supplementary Figure 5: 16 generated inpainting examples for each method. Case 3 - colour terracotta pot micrograph.