

Prediction of Atomic Stress Fields using Cycle-Consistent Adversarial Neural Networks based on Unpaired and Unmatched Sparse Datasets

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SUPPLEMENTARY INFORMATION

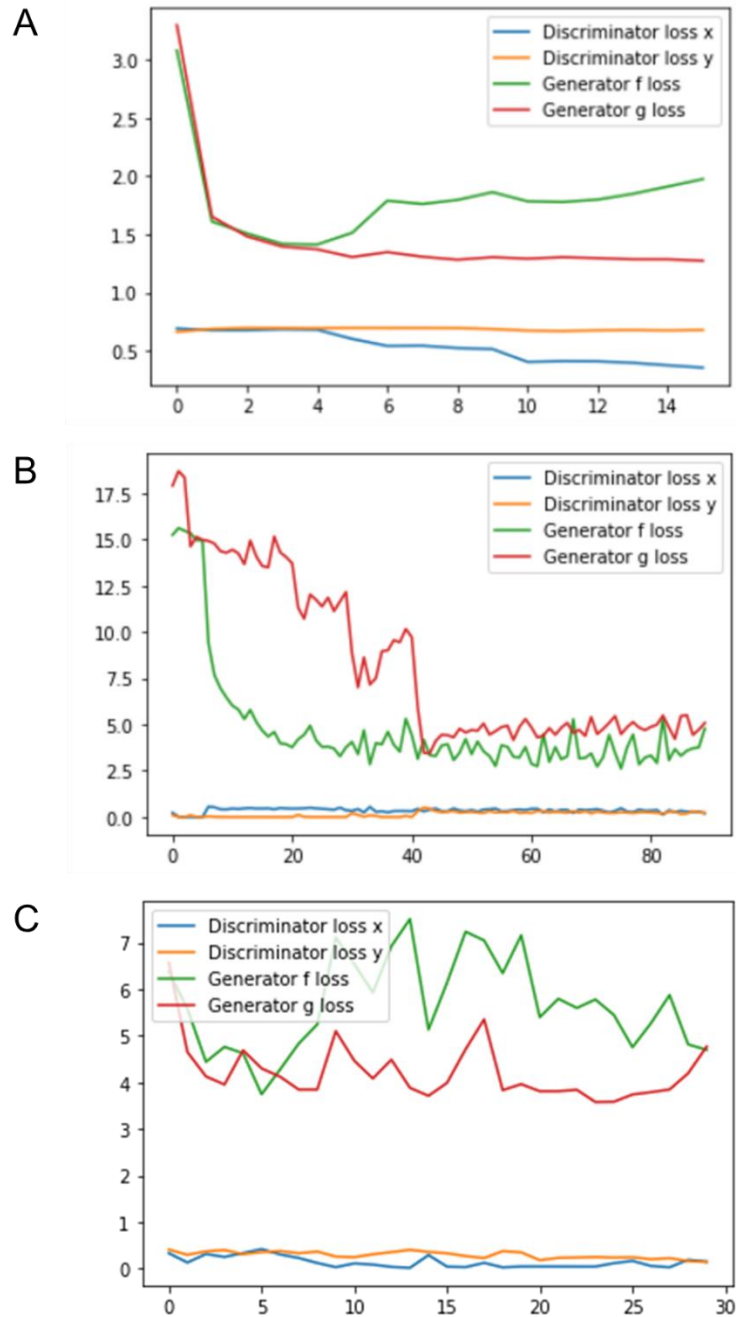


Figure S1: Training progression of the U-Net (A), ResNet (B), and U-Net-ResNet (C) neural networks. Note, the results shown in (C) are for the most challenging problem, training for deformation of the lattice while at the same time solving for the stress field. As can be seen, while training performance for A-B is generally good, performance for the third problem is more challenging.

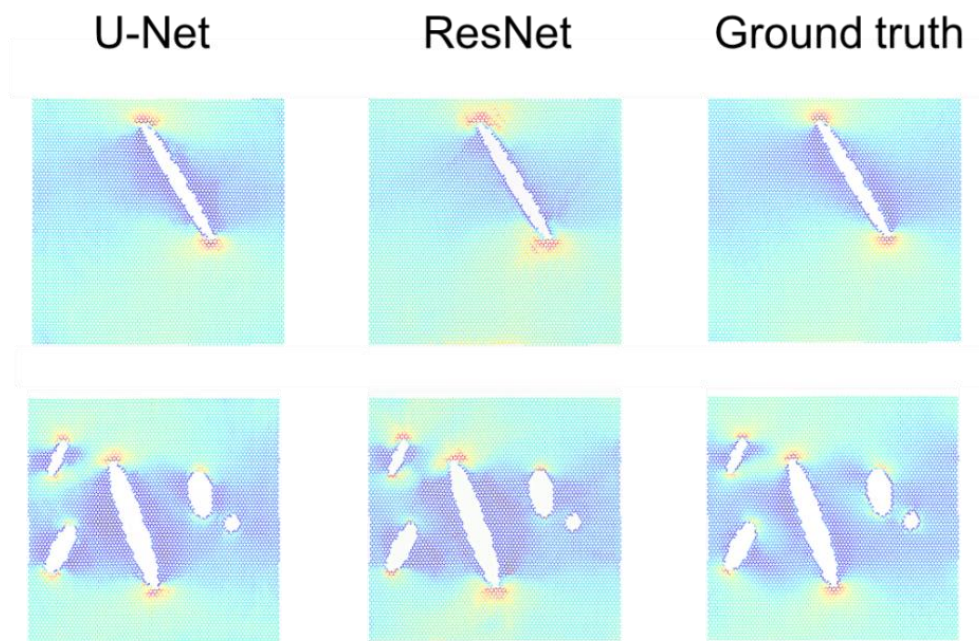


Figure S2: Direct comparison between predictions from the U-Net and ResNet generators, and comparison to ground truth data.

U-Net generator model:

Layer (type)	Output Shape	Param #	Connected to
input_1 (InputLayer)	(None, None, None, 0	0	
sequential (Sequential)	(None, None, None, 6	3072	input_1[0][0]
sequential_1 (Sequential)	(None, None, None, 1	131328	sequential[0][0]
sequential_2 (Sequential)	(None, None, None, 2	524800	sequential_1[0][0]
sequential_3 (Sequential)	(None, None, None, 5	2098176	sequential_2[0][0]
sequential_4 (Sequential)	(None, None, None, 5	4195328	sequential_3[0][0]
sequential_5 (Sequential)	(None, None, None, 1	8390656	sequential_4[0][0]
sequential_6 (Sequential)	(None, None, None, 1	16779264	sequential_5[0][0]
sequential_7 (Sequential)	(None, None, None, 1	16779264	sequential_6[0][0]
sequential_8 (Sequential)	(None, None, None, 1	16779264	sequential_7[0][0]
sequential_9 (Sequential)	(None, None, None, 1	16779264	sequential_8[0][0]
sequential_10 (Sequential)	(None, None, None, 1	16779264	sequential_9[0][0]
concatenate (Concatenate)	multiple	0	sequential_10[0][0] sequential_8[0][0] sequential_11[0][0] sequential_7[0][0] sequential_12[0][0] sequential_6[0][0] sequential_13[0][0] sequential_5[0][0] sequential_14[0][0] sequential_4[0][0] sequential_15[0][0] sequential_3[0][0] sequential_16[0][0] sequential_2[0][0] sequential_17[0][0] sequential_1[0][0] sequential_18[0][0] sequential[0][0]
sequential_11 (Sequential)	(None, None, None, 1	33556480	concatenate[0][0]
sequential_12 (Sequential)	(None, None, None, 1	33556480	concatenate[1][0]
sequential_13 (Sequential)	(None, None, None, 1	33556480	concatenate[2][0]
sequential_14 (Sequential)	(None, None, None, 1	33556480	concatenate[3][0]
sequential_15 (Sequential)	(None, None, None, 5	12583936	concatenate[4][0]
sequential_16 (Sequential)	(None, None, None, 5	8389632	concatenate[5][0]
sequential_17 (Sequential)	(None, None, None, 2	3146240	concatenate[6][0]
sequential_18 (Sequential)	(None, None, None, 1	786688	concatenate[7][0]
conv2d_transpose_10 (Conv2DTran	(None, None, None, 3	9219	concatenate[8][0]
Total params: 258,381,315			
Trainable params: 258,381,315			
Non-trainable params: 0			

Figure S3: U-Net generator architecture, featuring skip connections.

ResNet generator model:

Layer (type)	Output Shape	Param #	Connected to
input_1 (InputLayer)	(None, 1024, 1024, 0		
conv2d (Conv2D)	(None, 1024, 1024, 6 9472		input_1[0][0]
instance_normalization (Instanc	(None, 1024, 1024, 6 128		conv2d[0][0]
activation (Activation)	(None, 1024, 1024, 6 0		instance_normalization[0][0]
conv2d_1 (Conv2D)	(None, 512, 512, 128 73856		activation[0][0]
instance_normalization_1 (Insta	(None, 512, 512, 128 256		conv2d_1[0][0]
activation_1 (Activation)	(None, 512, 512, 128 0		instance_normalization_1[0][0]
conv2d_2 (Conv2D)	(None, 256, 256, 256 295168		activation_1[0][0]
instance_normalization_2 (Insta	(None, 256, 256, 256 512		conv2d_2[0][0]
activation_2 (Activation)	(None, 256, 256, 256 0		instance_normalization_2[0][0]
conv2d_3 (Conv2D)	(None, 256, 256, 256 590080		activation_2[0][0]
instance_normalization_3 (Insta	(None, 256, 256, 256 512		conv2d_3[0][0]
activation_3 (Activation)	(None, 256, 256, 256 0		instance_normalization_3[0][0]
conv2d_4 (Conv2D)	(None, 256, 256, 256 590080		activation_3[0][0]
instance_normalization_4 (Insta	(None, 256, 256, 256 512		conv2d_4[0][0]
concatenate (Concatenate)	(None, 256, 256, 512 0		instance_normalization_4[0][0] activation_2[0][0]
conv2d_5 (Conv2D)	(None, 256, 256, 256 1179904		concatenate[0][0]
instance_normalization_5 (Insta	(None, 256, 256, 256 512		conv2d_5[0][0]
activation_4 (Activation)	(None, 256, 256, 256 0		instance_normalization_5[0][0]
conv2d_6 (Conv2D)	(None, 256, 256, 256 590080		activation_4[0][0]
instance_normalization_6 (Insta	(None, 256, 256, 256 512		conv2d_6[0][0]
concatenate_1 (Concatenate)	(None, 256, 256, 768 0		instance_normalization_6[0][0] concatenate[0][0]
conv2d_7 (Conv2D)	(None, 256, 256, 256 1769728		concatenate_1[0][0]
instance_normalization_7 (Insta	(None, 256, 256, 256 512		conv2d_7[0][0]
activation_5 (Activation)	(None, 256, 256, 256 0		instance_normalization_7[0][0]
conv2d_8 (Conv2D)	(None, 256, 256, 256 590080		activation_5[0][0]
instance_normalization_8 (Insta	(None, 256, 256, 256 512		conv2d_8[0][0]
concatenate_2 (Concatenate)	(None, 256, 256, 102 0		instance_normalization_8[0][0] concatenate_1[0][0]
conv2d_9 (Conv2D)	(None, 256, 256, 256 2359552		concatenate_2[0][0]
instance_normalization_9 (Insta	(None, 256, 256, 256 512		conv2d_9[0][0]
activation_6 (Activation)	(None, 256, 256, 256 0		instance_normalization_9[0][0]
conv2d_10 (Conv2D)	(None, 256, 256, 256 590080		activation_6[0][0]
instance_normalization_10 (Inst	(None, 256, 256, 256 512		conv2d_10[0][0]
concatenate_3 (Concatenate)	(None, 256, 256, 128 0		instance_normalization_10[0][0] concatenate_2[0][0]
conv2d_11 (Conv2D)	(None, 256, 256, 256 2949376		concatenate_3[0][0]
instance_normalization_11 (Inst	(None, 256, 256, 256 512		conv2d_11[0][0]
activation_7 (Activation)	(None, 256, 256, 256 0		instance_normalization_11[0][0]
conv2d_12 (Conv2D)	(None, 256, 256, 256 590080		activation_7[0][0]
instance_normalization_12 (Inst	(None, 256, 256, 256 512		conv2d_12[0][0]
concatenate_4 (Concatenate)	(None, 256, 256, 153 0		instance_normalization_12[0][0] concatenate_3[0][0]
conv2d_13 (Conv2D)	(None, 256, 256, 256 3539200		concatenate_4[0][0]
instance_normalization_13 (Inst	(None, 256, 256, 256 512		conv2d_13[0][0]
activation_8 (Activation)	(None, 256, 256, 256 0		instance_normalization_13[0][0]
conv2d_14 (Conv2D)	(None, 256, 256, 256 590080		activation_8[0][0]
instance_normalization_14 (Inst	(None, 256, 256, 256 512		conv2d_14[0][0]
concatenate_5 (Concatenate)	(None, 256, 256, 179 0		instance_normalization_14[0][0] concatenate_4[0][0]
conv2d_15 (Conv2D)	(None, 256, 256, 256 4129024		concatenate_5[0][0]
instance_normalization_15 (Inst	(None, 256, 256, 256 512		conv2d_15[0][0]
activation_9 (Activation)	(None, 256, 256, 256 0		instance_normalization_15[0][0]
conv2d_16 (Conv2D)	(None, 256, 256, 256 590080		activation_9[0][0]
instance_normalization_16 (Inst	(None, 256, 256, 256 512		conv2d_16[0][0]
concatenate_6 (Concatenate)	(None, 256, 256, 204 0		instance_normalization_16[0][0] concatenate_5[0][0]
conv2d_17 (Conv2D)	(None, 256, 256, 256 4718848		concatenate_6[0][0]

instance_normalization_17 (Inst	(None, 256, 256, 256 512	conv2d_17[0][0]
activation_10 (Activation)	(None, 256, 256, 256 0	instance_normalization_17[0][0]
conv2d_18 (Conv2D)	(None, 256, 256, 256 590080	activation_10[0][0]
instance_normalization_18 (Inst	(None, 256, 256, 256 512	conv2d_18[0][0]
concatenate_7 (Concatenate)	(None, 256, 256, 230 0	instance_normalization_18[0][0] concatenate_6[0][0]
conv2d_19 (Conv2D)	(None, 256, 256, 256 5308672	concatenate_7[0][0]
instance_normalization_19 (Inst	(None, 256, 256, 256 512	conv2d_19[0][0]
activation_11 (Activation)	(None, 256, 256, 256 0	instance_normalization_19[0][0]
conv2d_20 (Conv2D)	(None, 256, 256, 256 590080	activation_11[0][0]
instance_normalization_20 (Inst	(None, 256, 256, 256 512	conv2d_20[0][0]
concatenate_8 (Concatenate)	(None, 256, 256, 256 0	instance_normalization_20[0][0] concatenate_7[0][0]
conv2d_transpose (Conv2DTranspo	(None, 512, 512, 128 2949248	concatenate_8[0][0]
instance_normalization_21 (Inst	(None, 512, 512, 128 256	conv2d_transpose[0][0]
activation_12 (Activation)	(None, 512, 512, 128 0	instance_normalization_21[0][0]
conv2d_transpose_1 (Conv2DTrans	(None, 1024, 1024, 6 73792	activation_12[0][0]
instance_normalization_22 (Inst	(None, 1024, 1024, 6 128	conv2d_transpose_1[0][0]
activation_13 (Activation)	(None, 1024, 1024, 6 0	instance_normalization_22[0][0]
conv2d_21 (Conv2D)	(None, 1024, 1024, 3 9411	activation_13[0][0]
instance_normalization_23 (Inst	(None, 1024, 1024, 3 6	conv2d_21[0][0]
activation_14 (Activation)	(None, 1024, 1024, 3 0	instance_normalization_23[0][0]
=====		
Total params: 35,276,553		
Trainable params: 35,276,553		
Non-trainable params: 0		
=====		

Figure S4: ResNet generator architecture (9 ResNet blocks)

U-Net-ResNet generator model:

Layer (type)	Output Shape	Param #	Connected to
input_1 (InputLayer)	[(None, None, None, 3)]	0	[]
ResNetConv0_1 (Conv2D)	(None, None, None, 64)	1792	['input_1[0][0]']
instance_normalization_19 (InstanceNormalization)	(None, None, None, 64)	128	['ResNetConv0_1[0][0]']
activation (Activation)	(None, None, None, 64)	0	['instance_normalization_19[0][0]']
ResNetConv0_2 (Conv2D)	(None, None, None, 64)	36928	['activation[0][0]']
instance_normalization_20 (InstanceNormalization)	(None, None, None, 64)	128	['ResNetConv0_2[0][0]']
concatenate_1 (Concatenate)	(None, None, None, 67)	0	['instance_normalization_20[0][0]', 'input_1[0][0]']
sequential (Sequential)	(None, None, None, 64)	68608	['concatenate_1[0][0]']
sequential_1 (Sequential)	(None, None, None, 128)	131328	['sequential[0][0]']
ResNetConv1_1 (Conv2D)	(None, None, None, 256)	295168	['sequential_1[0][0]']
instance_normalization_21 (InstanceNormalization)	(None, None, None, 256)	512	['ResNetConv1_1[0][0]']
activation_1 (Activation)	(None, None, None, 256)	0	['instance_normalization_21[0][0]']
ResNetConv1_2 (Conv2D)	(None, None, None, 256)	590080	['activation_1[0][0]']
instance_normalization_22 (InstanceNormalization)	(None, None, None, 256)	512	['ResNetConv1_2[0][0]']
concatenate_2 (Concatenate)	(None, None, None, 384)	0	['instance_normalization_22[0][0]', 'sequential_1[0][0]']
sequential_2 (Sequential)	(None, None, None, 256)	1573376	['concatenate_2[0][0]']
sequential_3 (Sequential)	(None, None, None, 512)	2098176	['sequential_2[0][0]']
ResNetConv2_1 (Conv2D)	(None, None, None, 512)	2359808	['sequential_3[0][0]']
instance_normalization_23 (InstanceNormalization)	(None, None, None, 512)	1024	['ResNetConv2_1[0][0]']
activation_2 (Activation)	(None, None, None, 512)	0	['instance_normalization_23[0][0]']
ResNetConv2_2 (Conv2D)	(None, None, None, 512)	2359808	['activation_2[0][0]']
instance_normalization_24 (InstanceNormalization)	(None, None, None, 512)	1024	['ResNetConv2_2[0][0]']
concatenate_3 (Concatenate)	(None, None, None, 1024)	0	['instance_normalization_24[0][0]', 'sequential_3[0][0]']
sequential_4 (Sequential)	(None, None, None, 512)	8389632	['concatenate_3[0][0]']
sequential_5 (Sequential)	(None, None, None, 1024)	8390656	['sequential_4[0][0]']
ResNetConv3_1 (Conv2D)	(None, None, None, 1024)	9438208	['sequential_5[0][0]']
instance_normalization_25 (InstanceNormalization)	(None, None, None, 1024)	2048	['ResNetConv3_1[0][0]']
activation_3 (Activation)	(None, None, None, 1024)	0	['instance_normalization_25[0][0]']
ResNetConv3_2 (Conv2D)	(None, None, None, 1024)	9438208	['activation_3[0][0]']
instance_normalization_26 (InstanceNormalization)	(None, None, None, 1024)	2048	['ResNetConv3_2[0][0]']
concatenate_4 (Concatenate)	(None, None, None, 2048)	0	['instance_normalization_26[0][0]', 'sequential_5[0][0]']
sequential_6 (Sequential)	(None, None, None, 1024)	33556480	['concatenate_4[0][0]']
sequential_7 (Sequential)	(None, None, None, 1024)	16779264	['sequential_6[0][0]']
ResNetConv4_1 (Conv2D)	(None, None, None, 1024)	9438208	['sequential_7[0][0]']
instance_normalization_27 (InstanceNormalization)	(None, None, None, 1024)	2048	['ResNetConv4_1[0][0]']
activation_4 (Activation)	(None, None, None, 1024)	0	['instance_normalization_27[0][0]']
ResNetConv4_2 (Conv2D)	(None, None, None, 9438208)	9438208	['activation_4[0][0]']

		1024)		
instance_normalization_28 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv4_2[0][0]']
concatenate_5 (Concatenate)	(None, None, None, 2048)	0		['instance_normalization_28[0][0]', 'sequential_7[0][0]']
sequential_8 (Sequential)	(None, None, None, 1024)	33556480		['concatenate_5[0][0]']
sequential_9 (Sequential)	(None, None, None, 1024)	16779264		['sequential_8[0][0]']
ResNetConv5_1 (Conv2D)	(None, None, None, 1024)	9438208		['sequential_9[0][0]']
instance_normalization_29 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv5_1[0][0]']
activation_5 (Activation)	(None, None, None, 1024)	0		['instance_normalization_29[0][0]']
ResNetConv5_2 (Conv2D)	(None, None, None, 1024)	9438208		['activation_5[0][0]']
instance_normalization_30 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv5_2[0][0]']
concatenate_6 (Concatenate)	(None, None, None, 2048)	0		['instance_normalization_30[0][0]', 'sequential_9[0][0]']
ResNetConv6_1 (Conv2D)	(None, None, None, 1024)	18875392		['concatenate_6[0][0]']
instance_normalization_31 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv6_1[0][0]']
activation_6 (Activation)	(None, None, None, 1024)	0		['instance_normalization_31[0][0]']
ResNetConv6_2 (Conv2D)	(None, None, None, 1024)	9438208		['activation_6[0][0]']
instance_normalization_32 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv6_2[0][0]']
concatenate_7 (Concatenate)	(None, None, None, 3072)	0		['instance_normalization_32[0][0]', 'concatenate_6[0][0]']
ResNetConv7_1 (Conv2D)	(None, None, None, 1024)	28312576		['concatenate_7[0][0]']
instance_normalization_33 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv7_1[0][0]']
activation_7 (Activation)	(None, None, None, 1024)	0		['instance_normalization_33[0][0]']
ResNetConv7_2 (Conv2D)	(None, None, None, 1024)	9438208		['activation_7[0][0]']
instance_normalization_34 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv7_2[0][0]']
concatenate_8 (Concatenate)	(None, None, None, 4096)	0		['instance_normalization_34[0][0]', 'concatenate_7[0][0]']
sequential_10 (Sequential)	(None, None, None, 1024)	67110912		['concatenate_8[0][0]']
concatenate (Concatenate)	multiple	0		['sequential_10[0][0]', 'sequential_8[0][0]', 'sequential_11[0][0]', 'sequential_7[0][0]', 'sequential_12[0][0]', 'sequential_6[0][0]', 'sequential_13[0][0]', 'sequential_5[0][0]', 'sequential_14[0][0]', 'sequential_4[0][0]', 'sequential_15[0][0]', 'sequential_3[0][0]', 'sequential_16[0][0]', 'sequential_2[0][0]', 'sequential_17[0][0]', 'sequential_1[0][0]', 'sequential_18[0][0]', 'sequential[0][0]']
sequential_11 (Sequential)	(None, None, None, 1024)	33556480		['concatenate[0][0]']
ResNetConv8_1 (Conv2D)	(None, None, None, 1024)	18875392		['concatenate[1][0]']
instance_normalization_35 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv8_1[0][0]']
activation_8 (Activation)	(None, None, None, 1024)	0		['instance_normalization_35[0][0]']
ResNetConv8_2 (Conv2D)	(None, None, None, 1024)	9438208		['activation_8[0][0]']
instance_normalization_36 (InstanceNormalization)	(None, None, None, 1024)	2048		['ResNetConv8_2[0][0]']
concatenate_9 (Concatenate)	(None, None, None, 3072)	0		['instance_normalization_36[0][0]', 'concatenate[1][0]']
sequential_12 (Sequential)	(None, None, None, 1024)	50333696		['concatenate_9[0][0]']


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1024)
sequential_13 (Sequential)      (None, None, None, 33556480 ['concatenate[2][0]']
1024)
ResNetConv9_1 (Conv2D)         (None, None, None, 18875392 ['concatenate[3][0]']
1024)
instance_normalization_37 (Ins (None, None, None, 2048 ['ResNetConv9_1[0][0]']
tanceNormalization)          1024)
activation_9 (Activation)      (None, None, None, 0 ['instance_normalization_37[0][0]']
1024)
ResNetConv9_2 (Conv2D)         (None, None, None, 9438208 ['activation_9[0][0]']
1024)
instance_normalization_38 (Ins (None, None, None, 2048 ['ResNetConv9_2[0][0]']
tanceNormalization)          1024)
concatenate_10 (Concatenate)  (None, None, None, 0 ['instance_normalization_38[0][0]']
3072)
sequential_14 (Sequential)      (None, None, None, 50333696 ['concatenate_10[0][0]']
1024)
sequential_15 (Sequential)      (None, None, None, 12583936 ['concatenate[4][0]']
512)
ResNetConv10_1 (Conv2D)        (None, None, None, 4719104 ['concatenate[5][0]']
512)
instance_normalization_39 (Ins (None, None, None, 1024 ['ResNetConv10_1[0][0]']
tanceNormalization)          512)
activation_10 (Activation)     (None, None, None, 0 ['instance_normalization_39[0][0]']
512)
ResNetConv10_2 (Conv2D)        (None, None, None, 2359808 ['activation_10[0][0]']
512)
instance_normalization_40 (Ins (None, None, None, 1024 ['ResNetConv10_2[0][0]']
tanceNormalization)          512)
concatenate_11 (Concatenate)  (None, None, None, 0 ['instance_normalization_40[0][0]']
1536)
sequential_16 (Sequential)      (None, None, None, 12583936 ['concatenate_11[0][0]']
512)
sequential_17 (Sequential)      (None, None, None, 3146240 ['concatenate[6][0]']
256)
ResNetConv11_1 (Conv2D)        (None, None, None, 442496 ['concatenate[7][0]']
128)
instance_normalization_41 (Ins (None, None, None, 256 ['ResNetConv11_1[0][0]']
tanceNormalization)          128)
activation_11 (Activation)     (None, None, None, 0 ['instance_normalization_41[0][0]']
128)
ResNetConv11_2 (Conv2D)        (None, None, None, 147584 ['activation_11[0][0]']
128)
instance_normalization_42 (Ins (None, None, None, 256 ['ResNetConv11_2[0][0]']
tanceNormalization)          128)
concatenate_12 (Concatenate)  (None, None, None, 0 ['instance_normalization_42[0][0]']
512)
sequential_18 (Sequential)      (None, None, None, 1048832 ['concatenate_12[0][0]']
128)
conv2d_transpose_10 (Conv2DTra (None, None, None, 9219 ['concatenate[8][0]']
nspose)                       3)
=====
Total params: 578,254,659
Trainable params: 578,254,659
Non-trainable params: 0
=====

```

Figure S5: U-Net-ResNet architecture used as a generator.

Discriminator model:

Layer (type)	Output Shape	Param #
input_6 (InputLayer)	[(None, 1024, 1024, 3)]	0
conv2d_46 (Conv2D)	(None, 512, 512, 64)	3136
leaky_re_lu_45 (LeakyReLU)	(None, 512, 512, 64)	0
conv2d_47 (Conv2D)	(None, 256, 256, 128)	131200
instance_normalization_80 (InstanceNormalization)	(None, 256, 256, 128)	256
leaky_re_lu_46 (LeakyReLU)	(None, 256, 256, 128)	0
conv2d_48 (Conv2D)	(None, 128, 128, 256)	524544
instance_normalization_81 (InstanceNormalization)	(None, 128, 128, 256)	512
leaky_re_lu_47 (LeakyReLU)	(None, 128, 128, 256)	0
conv2d_49 (Conv2D)	(None, 64, 64, 512)	2097664
instance_normalization_82 (InstanceNormalization)	(None, 64, 64, 512)	1024
leaky_re_lu_48 (LeakyReLU)	(None, 64, 64, 512)	0
conv2d_50 (Conv2D)	(None, 64, 64, 512)	4194816
instance_normalization_83 (InstanceNormalization)	(None, 64, 64, 512)	1024
leaky_re_lu_49 (LeakyReLU)	(None, 64, 64, 512)	0
conv2d_51 (Conv2D)	(None, 64, 64, 1)	8193

=====
Total params: 6,962,369
Trainable params: 6,962,369
Non-trainable params: 0
=====

Figure S6: Discriminator architecture used in the adversarial neural network.