```
!pip install torch_geometric
```

```
Collecting torch_geometric
  Downloading torch_geometric-2.6.1-py3-none-any.whl.metadata (63 kB)
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etric
Successfully installed torch_geometric-2.6.1
```

```python
import numpy as np
import torch
import torch_geometric
import h5py
import matplotlib.pyplot as plt

from torch_geometric.data import Data, Batch
from torch_geometric.loader import DataLoader
from sklearn.neighbors import kneighbors_graph
from sklearn.model_selection import train_test_split

import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

from torch_geometric.nn import global_mean_pool
from torch.nn import Linear

Data_Path = '/kaggle/input/paraquet-df/quark-gluon_data-
set_n139306.hdf5'
Data_Size = 40000
k = 8

import h5py
import numpy as np
import torch
from torch_geometric.data import Data
from sklearn.neighbors import kneighbors_graph

def load_data(k=8, max_nodes=800, activation_threshold=1e-3):
    # Adding coordinates to the featues.
    data = h5py.File(Data_Path, "r")
    images = data['X_jets'][0:Data_Size]
    coords = np.indices((125, 125))
    coords = np.moveaxis(coords, 1, -1).T
    coords = np.expand_dims(coords, axis=0)
    coords = coords.astype(np.float32) / 125.
    coords = np.repeat(coords, Data_Size, axis=0)

    # Surpressing smaller activations
    images[images < activation_threshold] = 0.0
    images_with_coords = np.concatenate((images, coords), axis=-1)

    del coords
    del images
```

```
    del data

    data = images_with_coords.reshape((-1, images_with_coords.shape[1]
* images_with_coords.shape[2], 5))
    node_list = []

    for i, x in enumerate(data):
        mask = np.any(x[..., :3] != [0., 0., 0.], axis=-1)
        filtered_nodes = x[mask]
        # canonical ordering of nodes.(sorted positions)
        sorted_nodes = filtered_nodes[np.lexsort((filtered_nodes[:,
4], filtered_nodes[:, 3]))]

        if sorted_nodes.shape[0] > max_nodes:
            sorted_nodes = sorted_nodes[:max_nodes]

        node_list.append(sorted_nodes)


    dataset = []
    for i, nodes in enumerate(node_list):
        edges = kneighbors_graph(nodes[..., 3:], k,
mode='connectivity', include_self=True)
        c = edges.tocoo()
        edge_list = torch.from_numpy(np.vstack((c.row,
c.col))).type(torch.long)
        edge_weight = torch.from_numpy(c.data.reshape(-1, 1))
        data = Data(x=torch.from_numpy(nodes), edge_index=edge_list,
edge_attr=edge_weight)
        dataset.append(data)

    return dataset

dataset = load_data()

train_loader = DataLoader(dataset[:36000], batch_size=64,
shuffle=True)
test_loader = DataLoader(dataset[36000:36004], batch_size=1,
shuffle=False)

from torch_geometric.nn import SAGEConv, GATConv


# Graph level latent Graph Auto Encoder
class GAE(torch.nn.Module):
  def __init__(self, input_embed_dim : int, latent_dim = None,
max_nodes : int = 800):
    super(GAE, self).__init__()

    self.node_dim = input_embed_dim
    if latent_dim is None:
```

```
      self.latent_dim = self.node_dim
    else:
      self.latent_dim = latent_dim
    self.max_nodes = max_nodes
    self.output_size = self.max_nodes * self.node_dim

    self.Conv1 = GATConv(self.node_dim, self.latent_dim, heads=1,
concat=False)
    self.Conv2 = GATConv(self.latent_dim, 2*self.latent_dim, heads=1,
concat=False)
    self.Conv3 = GATConv(2*self.latent_dim, 4*self.latent_dim,
heads=1, concat=False)
    self.Conv4 = GATConv(4*self.latent_dim, 8*self.latent_dim,
heads=1, concat=False)
    self.lin1 = torch.nn.Linear(8*self.latent_dim, 16*self.latent_dim)
    self.lin2 = torch.nn.Linear(16*self.latent_dim,
32*self.latent_dim)
    self.lin3 = torch.nn.Linear(32*self.latent_dim,
int(self.output_size / 2))
    self.lin4 = torch.nn.Linear(int(self.output_size / 2),
self.output_size)
    self.p5 = nn.Dropout(p=0.5)
    self.p3 = nn.Dropout(p=0.3)
    self.p1 = nn.Dropout(p=0.1)


  def forward(self, x, edge_index, batch):

    # Encoder.
    x = F.relu(self.Conv1(x, edge_index))
    x = F.relu(self.Conv2(x, edge_index))
    x = F.relu(self.Conv3(x, edge_index))
    x = F.relu(self.Conv4(x, edge_index))

    # mask generation and pooling.
    x, mask = torch_geometric.utils.to_dense_batch(x, batch,
fill_value=0)
    x = torch.mean(x, dim=1)

    # Decoder
    x = F.relu(self.lin1(x))
    x = self.p1(x)
    x = F.relu(self.lin2(x))
    x = self.p1(x)
    x = F.relu(self.lin3(x))
    x = self.lin4(x)
    x = torch.reshape(x, (-1, self.max_nodes, self.node_dim))
    new_mask = torch.zeros(mask.shape[0], self.max_nodes,
dtype=torch.bool)
    new_mask[:, :mask.shape[1]] = mask
```

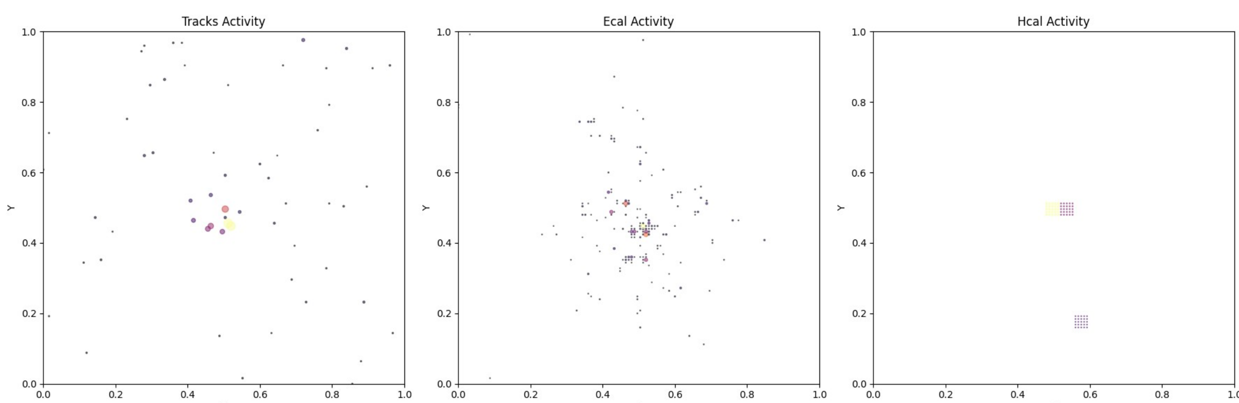
```
    mask = new_mask

    return x, mask

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

import torch
import torch.nn.functional as F
from torchvision import transforms
from torchvision.transforms import functional as TF
from torchmetrics.image import StructuralSimilarityIndexMeasure

ssim_metric = StructuralSimilarityIndexMeasure(data_range=1.0)

def reconstruct_image(features):
    x_coords = (features[:, -2] * 125).cpu().numpy().astype(int)
    y_coords = (features[:, -1] * 125).cpu().numpy().astype(int)
    tracks_act = features[:, 0].cpu().numpy()
    ecal_act = features[:, 1].cpu().numpy()
    hcal_act = features[:, 2].cpu().numpy()

    img_tracks = np.zeros((125, 125))
    img_ecal = np.zeros((125, 125))
    img_hcal = np.zeros((125, 125))

    for i in range(len(x_coords)):
        if 0 <= x_coords[i] < 125 and 0 <= y_coords[i] < 125:
            img_tracks[y_coords[i], x_coords[i]] = tracks_act[i]
            img_ecal[y_coords[i], x_coords[i]] = ecal_act[i]
            img_hcal[y_coords[i], x_coords[i]] = hcal_act[i]

    # Stack the channels to get a 3-channel image
    image = np.stack([img_tracks, img_ecal, img_hcal], axis=0)
    return torch.tensor(image, dtype=torch.float32).unsqueeze(0) /
np.max(image)

def calculate_ssim(data, x):
    original_image = reconstruct_image(data)
    reconstructed_image = reconstruct_image(x)

    # Ensure both images are in the correct format
    original_image = original_image.clamp(0, 1)
    reconstructed_image = reconstructed_image.clamp(0, 1)

    ssim_score = ssim_metric(reconstructed_image, original_image)
    return ssim_score.item()

# Graph features based reconstruction loss.
def weighted_mse_loss(output, target, mask):
    weights = torch.tensor([1.0, 1.0, 1.0], device=output.device)
    squared_error = (output - target) ** 2
```

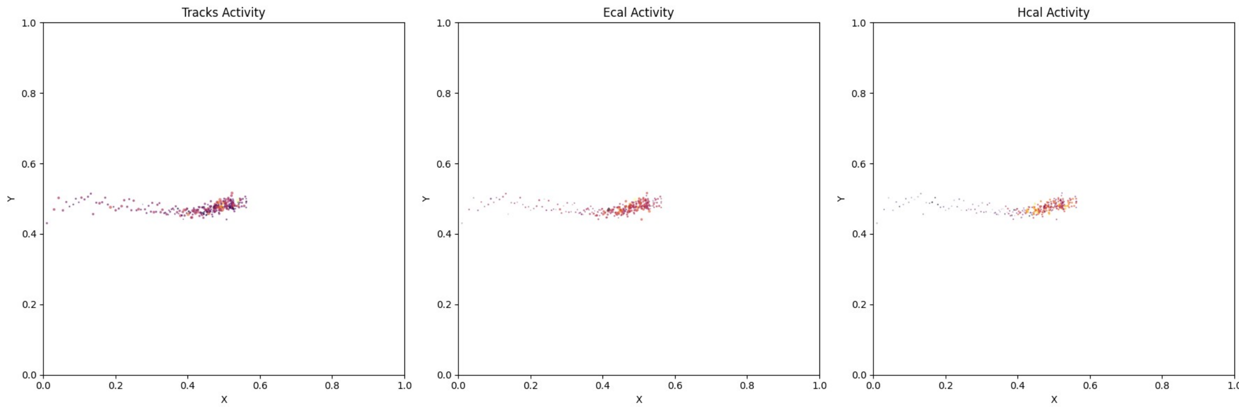
```
    for i in range(0, 3):
        squared_error[:,:,i] = squared_error[:,:,i] * weights[i]
    # Apply mask to the loss
    masked_error = squared_error * mask.unsqueeze(-1).to(device)
    loss = masked_error.sum() / (mask.sum() + 1e-8)  # Prevent
division by zero
    return loss

def visualize(data):
    x = data[:,3]
    y = data[:,4]
    tracks_act = data[:,0]
    hcal_act = data[:,2]
    ecal_act = data[:,1]
    fig, axs = plt.subplots(1, 3, figsize=(18, 6))
    axs[0].set_xlim(0, 1)  # Force x-axis to show 0-1 range
    axs[0].set_ylim(0, 1)
    # Plot tracks_act
    axs[0].scatter(x, y, c=tracks_act, s= torch.abs(tracks_act) * 500,
cmap='inferno', alpha=0.5)
    axs[0].set_title('Tracks Activity')
    axs[0].set_xlabel('X')
    axs[0].set_ylabel('Y')

    axs[1].set_xlim(0, 1)  # Force x-axis to show 0-1 range
    axs[1].set_ylim(0, 1)
    # Plot ecal_act
    axs[1].scatter(x, y,  c=ecal_act, s= torch.abs(ecal_act) * 500,
cmap='inferno', alpha=0.5)
    axs[1].set_title('Ecal Activity')
    axs[1].set_xlabel('X')
    axs[1].set_ylabel('Y')

    axs[2].set_xlim(0, 1)  # Force x-axis to show 0-1 range
    axs[2].set_ylim(0, 1)
    # Plot hcal_act
    axs[2].scatter(x, y, c=hcal_act, s= torch.abs(hcal_act) * 500,
cmap='inferno', alpha=0.5)
    axs[2].set_title('Hcal Activity')
    axs[2].set_xlabel('X')
    axs[2].set_ylabel('Y')


    plt.tight_layout()
    plt.show()

from tqdm import tqdm

def train():
    model.train()
```

```
    total_loss = 0

    with tqdm(train_loader, desc="Training", leave=False) as t:
        for data in t:
            data = data.to(device)
            out, mask = model(data.x, data.edge_index, data.batch)
            x,_ = torch_geometric.utils.to_dense_batch(data.x,
data.batch, fill_value=0)
            pad_size = model.max_nodes - x.shape[1]
            if (pad_size > 0):
                x = F.pad(x, (0, 0, 0, pad_size, 0, 0))
            loss = weighted_mse_loss(out, x, mask)
            loss.backward()
            optimizer.step()
            optimizer.zero_grad()
            total_loss += loss.item()
            t.set_postfix(loss=loss.item())
        return total_loss / 64.

def inference(model, data_loader, device):
    model.eval()
    all_outputs = []

    with torch.no_grad():
        with tqdm(data_loader, desc="Inference", leave=False) as t:
            for data in t:
                data = data.to(device)
                out, mask = model(data.x, data.edge_index, data.batch)
                # Convert input to dense and pad if necessary
                x, _ = torch_geometric.utils.to_dense_batch(data.x,
data.batch, fill_value=0)
                visualize(x[0].cpu())
                visualize(out[0][:data.x.shape[0]].cpu())
                ssim_score = calculate_ssim(data.x, out[0]
[:data.x.shape[0]])
                print(f"SSIM Score: {ssim_score}")
                # Save output and mask for further analysis
                all_outputs.append((out.cpu(), mask.cpu()))

    return all_outputs

model = GAE(5, 32)
#model = nn.DataParallel(model)
model.to(device)
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

for epoch in range(50):
    loss = train()
    if (epoch + 1) % 10  == 0:
```

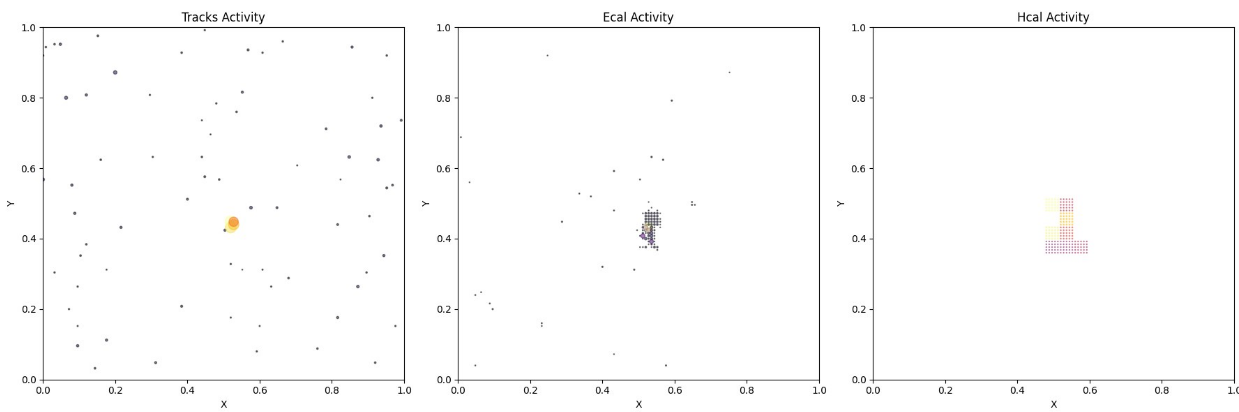
```
        inference(model, test_loader, device)
    print("Epoch : ", epoch + 1, " Loss : ", loss)
```

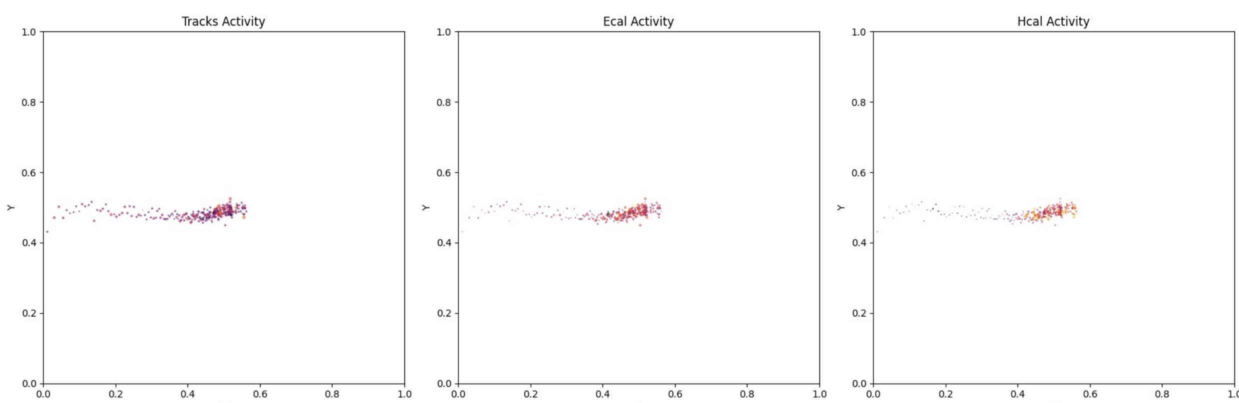
```
Epoch :  1  Loss :  0.4885169903864153

Epoch :  2  Loss :  0.4273867362062447

Epoch :  3  Loss :  0.41587010002695024

Epoch :  4  Loss :  0.41350331372814253

Epoch :  5  Loss :  0.406645750394091

Epoch :  6  Loss :  0.4042461492936127

Epoch :  7  Loss :  0.3997525214217603

Epoch :  8  Loss :  0.3953606700524688

Epoch :  9  Loss :  0.3950712438672781
Inference:   0%|          | 0/4 [00:00<?, ?it/s]
```



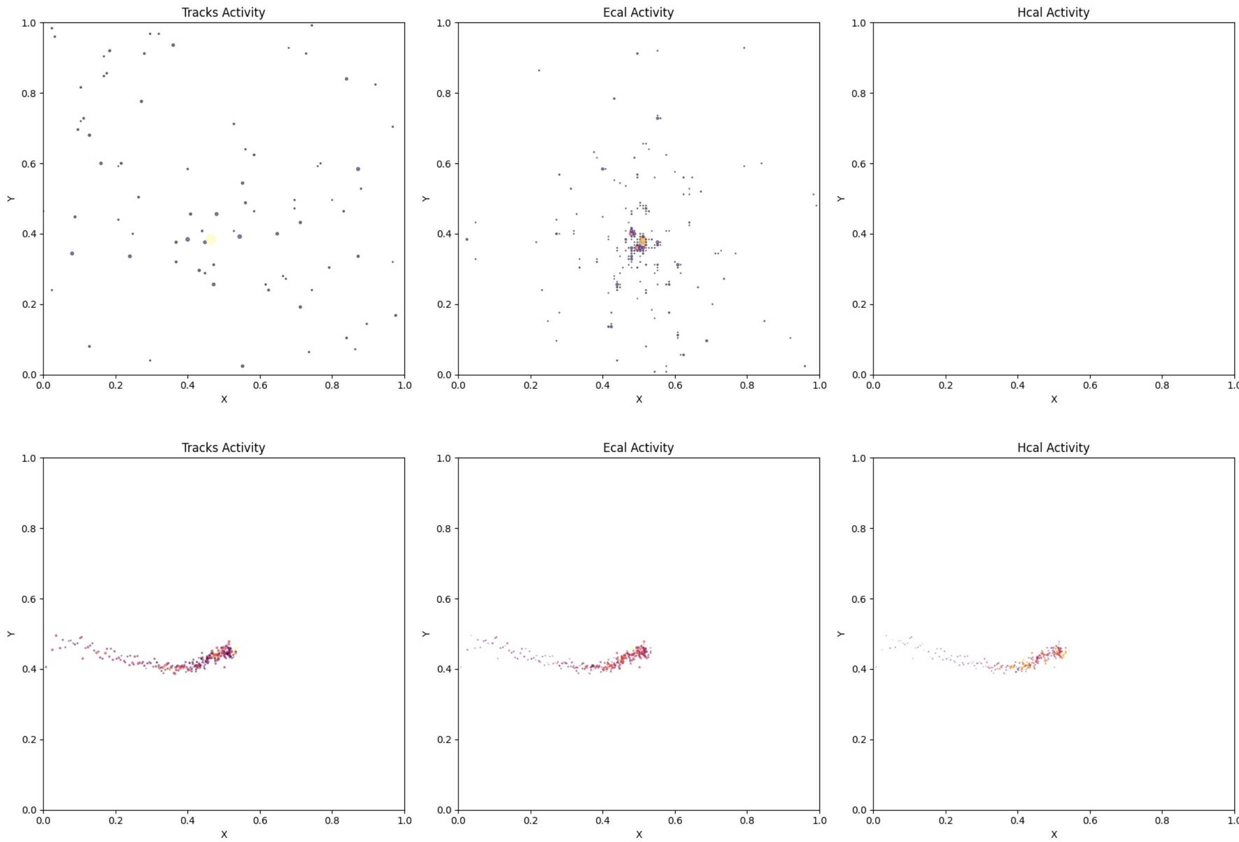



```
Inference:  25%|██▌       | 1/4 [00:01<00:03,  1.12s/it]

SSIM Score: 0.9650533199310303
```

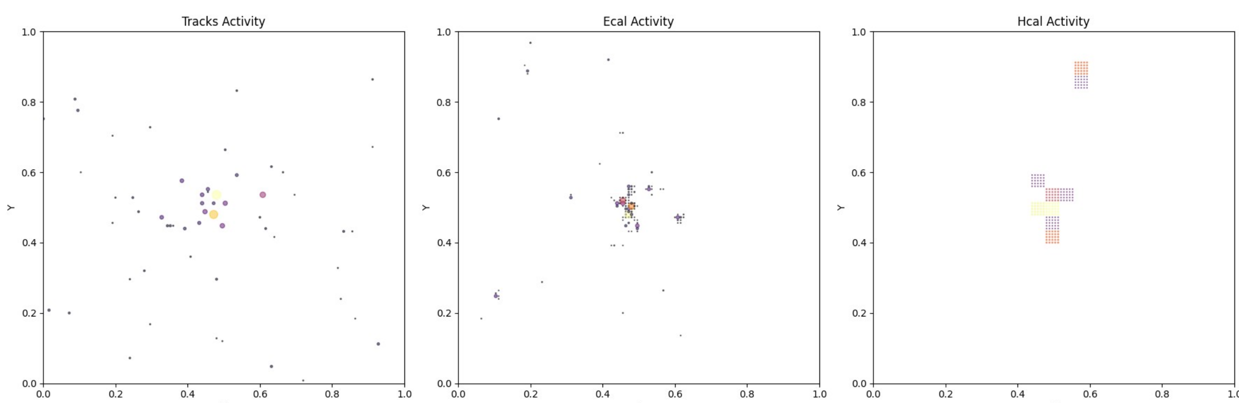


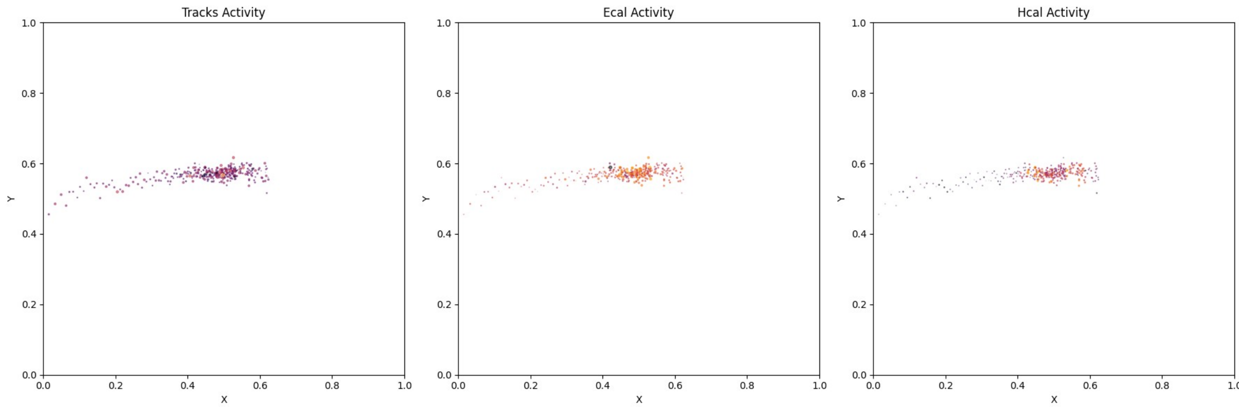



```
Inference:  50%|█████     | 2/4 [00:02<00:02,  1.10s/it]

SSIM Score: 0.9667884707450867
```

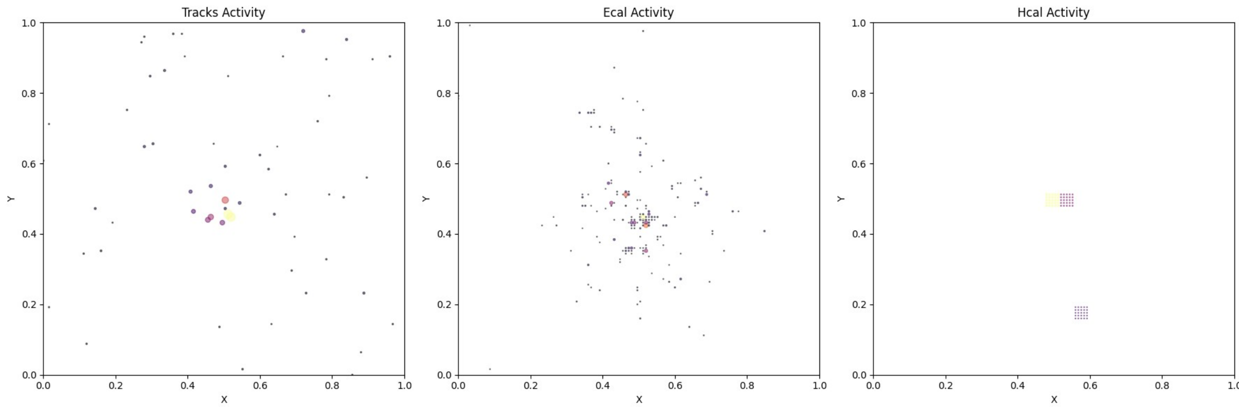


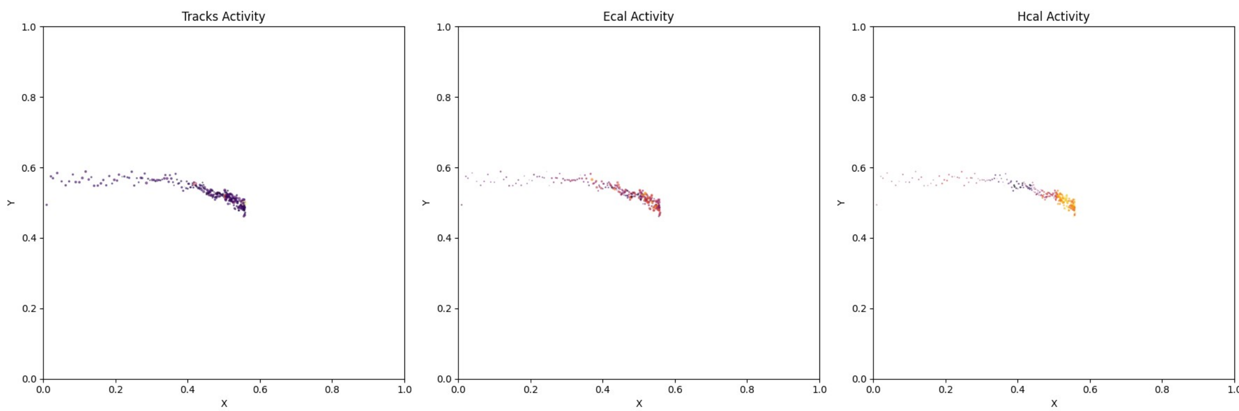

```
Inference:  75%|███████▌  | 3/4 [00:03<00:01,  1.09s/it]

SSIM Score: 0.9605690836906433
```



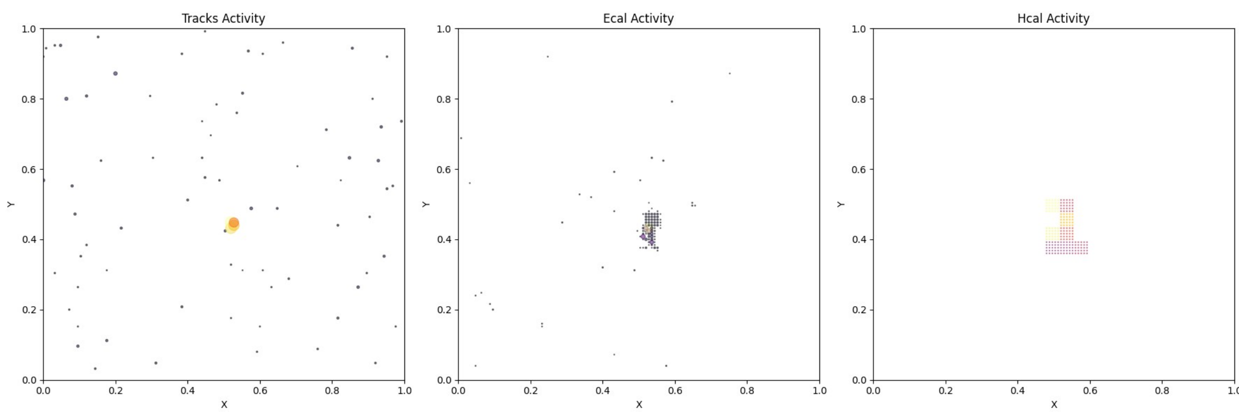


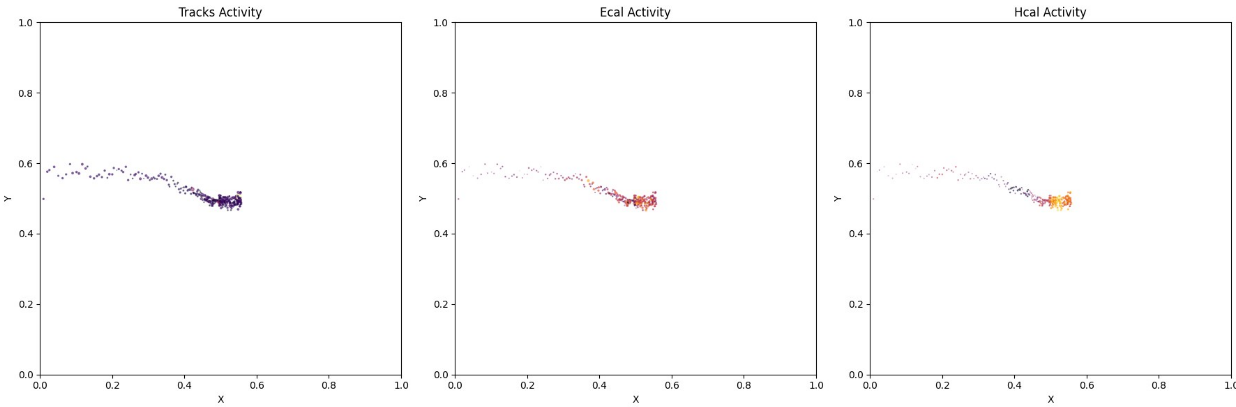

```
SSIM Score: 0.9466950297355652
Epoch :  10  Loss :  0.3924267978873104

Epoch :  11  Loss :  0.3910132232122123

Epoch :  12  Loss :  0.39108332118485123

Epoch :  13  Loss :  0.3865274336421862

Epoch :  14  Loss :  0.38521769584622234

Epoch :  15  Loss :  0.3847420209203847

Epoch :  16  Loss :  0.3834813795401715

Epoch :  17  Loss :  0.3829147926880978

Epoch :  18  Loss :  0.38055123237427324

Epoch :  19  Loss :  0.37853219045791775
Inference:   0%|          | 0/4 [00:00<?, ?it/s]
```



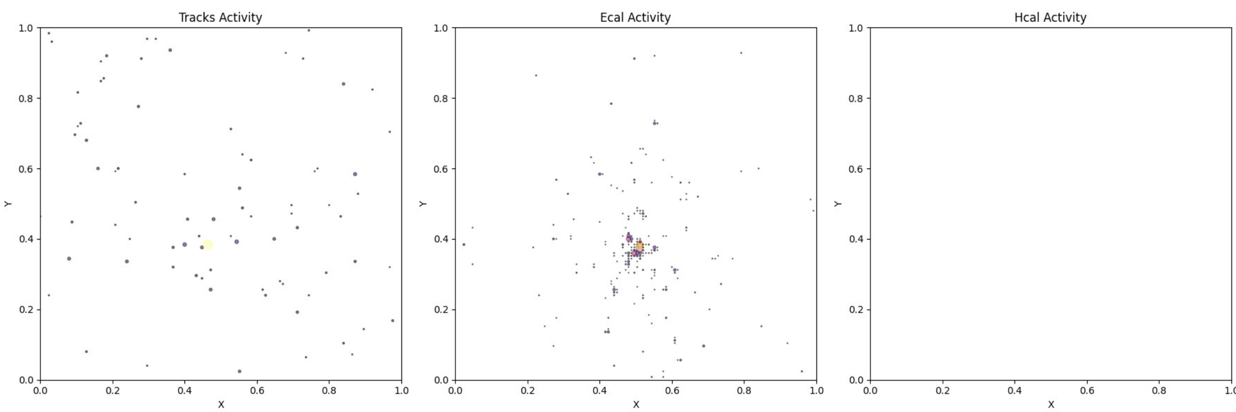


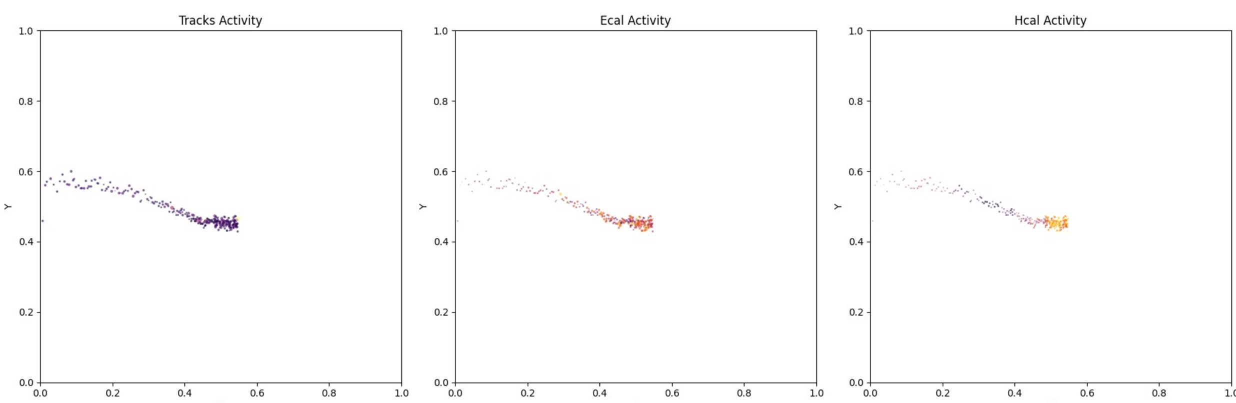

```
Inference:  25%|██▌       | 1/4 [00:01<00:03,  1.19s/it]

SSIM Score: 0.9642724990844727
```



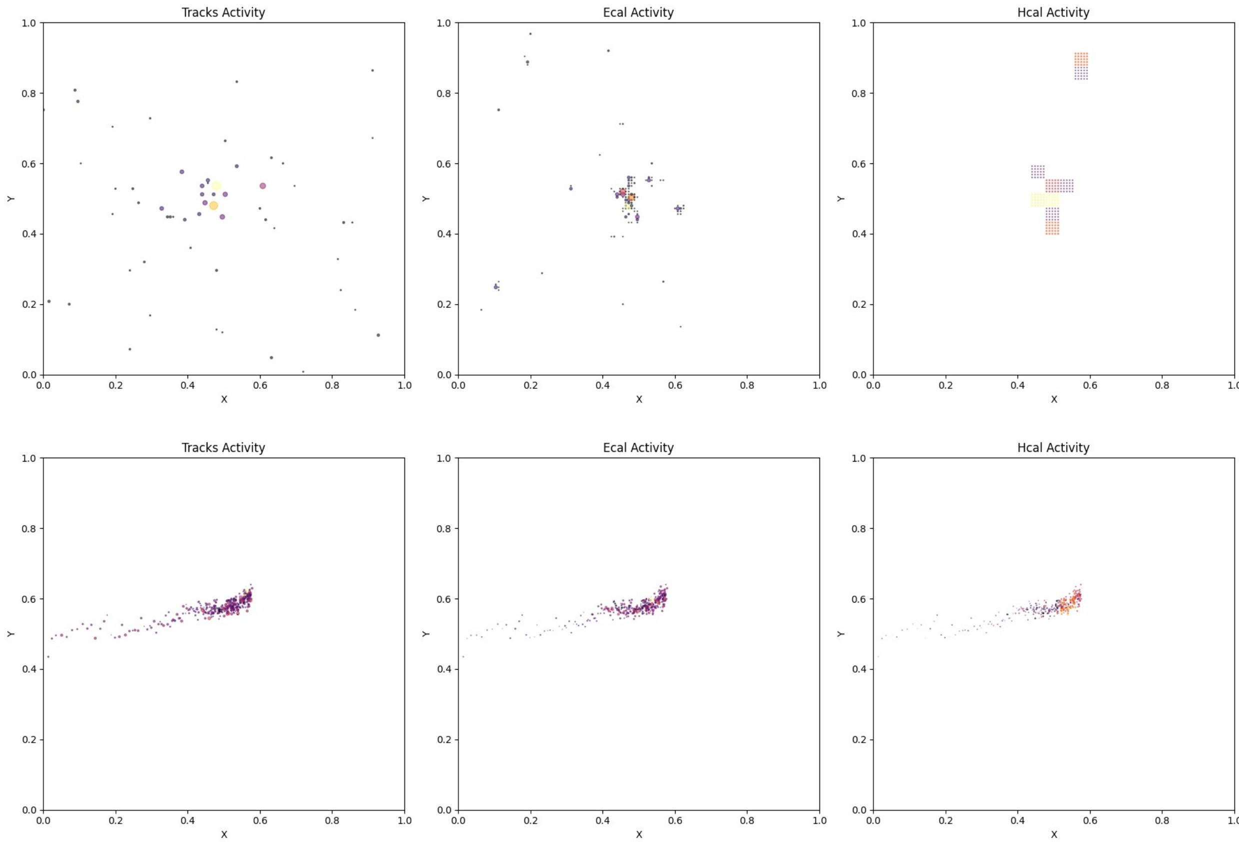



```
Inference:  50%|█████     | 2/4 [00:02<00:02,  1.46s/it]
SSIM Score: 0.9665165543556213
```



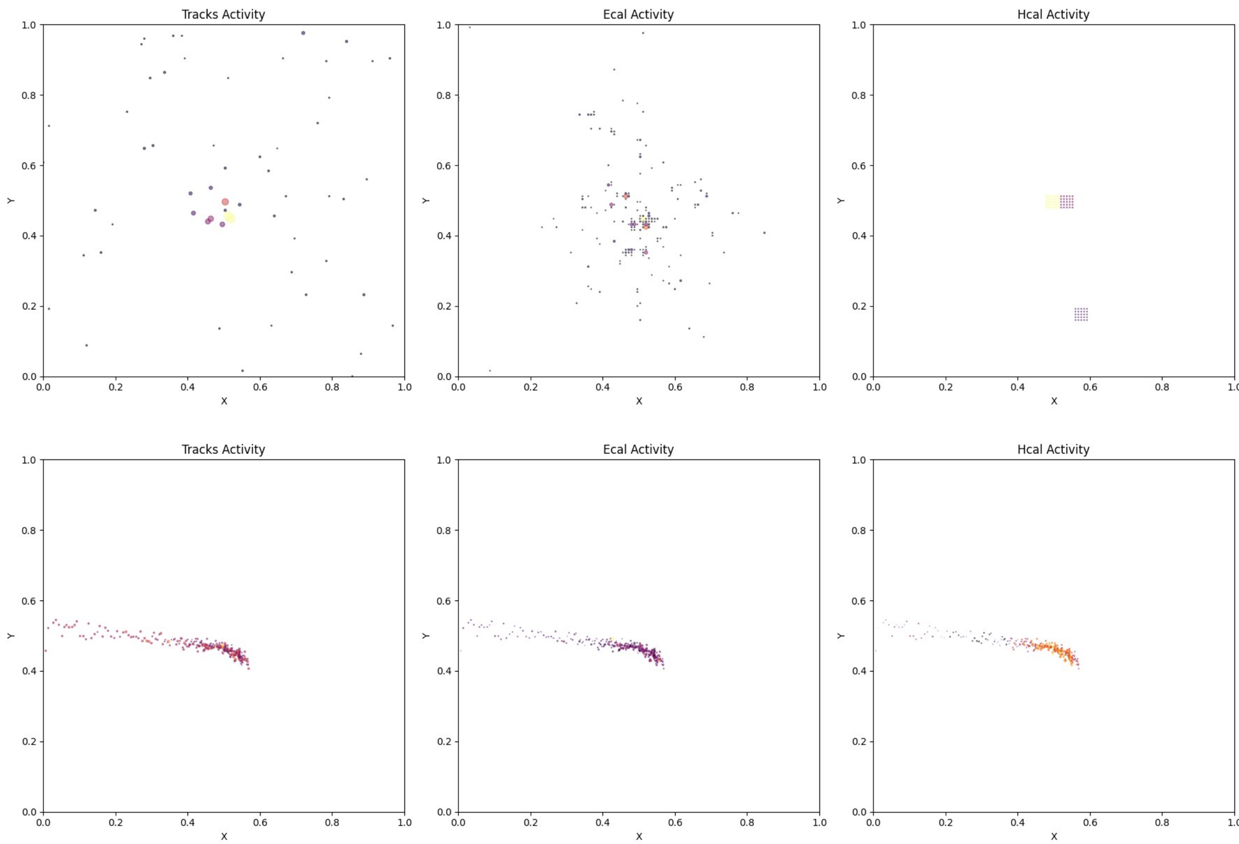



```
Inference:  75%|███████▌  | 3/4 [00:03<00:01,  1.31s/it]
SSIM Score: 0.9693546891212463
```

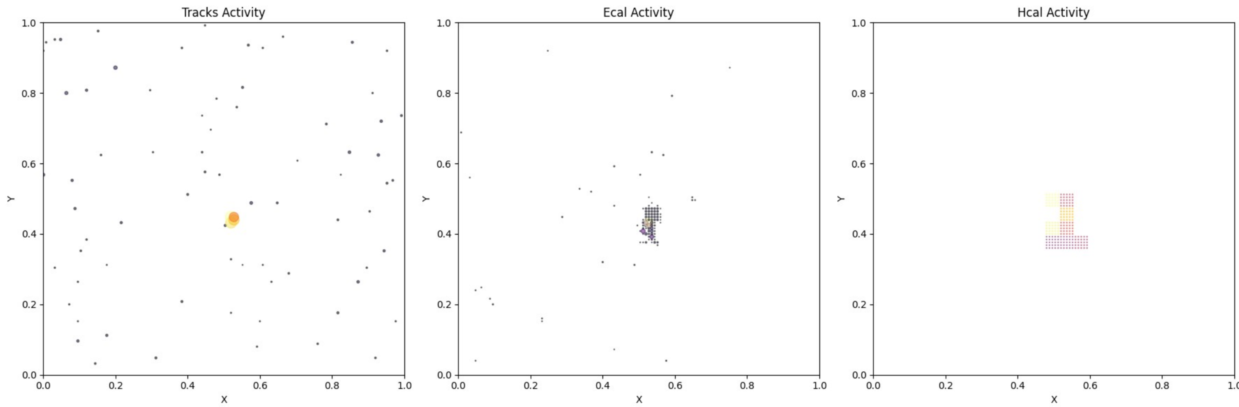


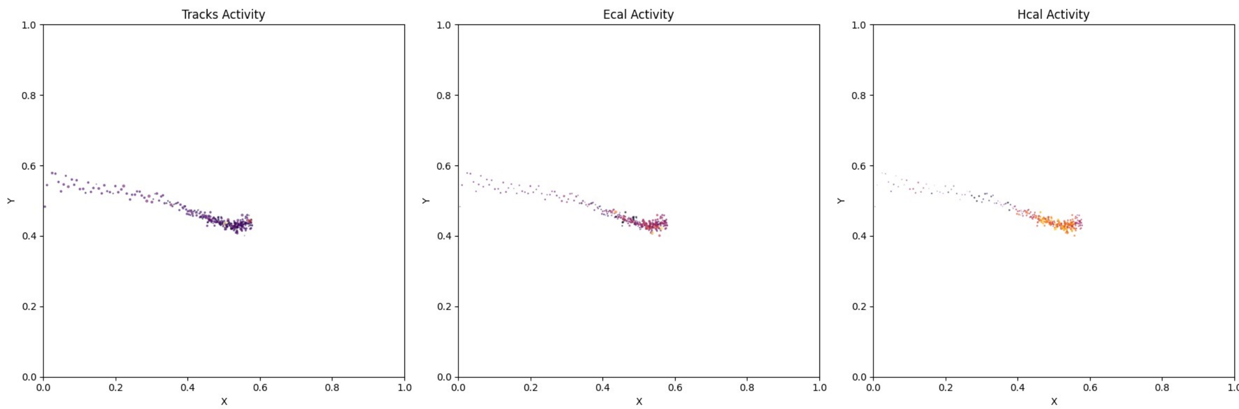

```
SSIM Score: 0.9679346084594727
Epoch :  20  Loss :  0.37936603714479133

Epoch :  21  Loss :  0.3773382002254948

Epoch :  22  Loss :  0.3752671583206393

Epoch :  23  Loss :  0.37536795635242015

Epoch :  24  Loss :  0.37367189454380423

Epoch :  25  Loss :  0.37270672514569014
```

```
Epoch :  26  Loss :  0.37280520843341947


Epoch :  27  Loss :  0.37045288959052414


Epoch :  28  Loss :  0.3714130853768438


Epoch :  29  Loss :  0.3689171593869105
Inference:   0%|          | 0/4 [00:00<?, ?it/s]
```

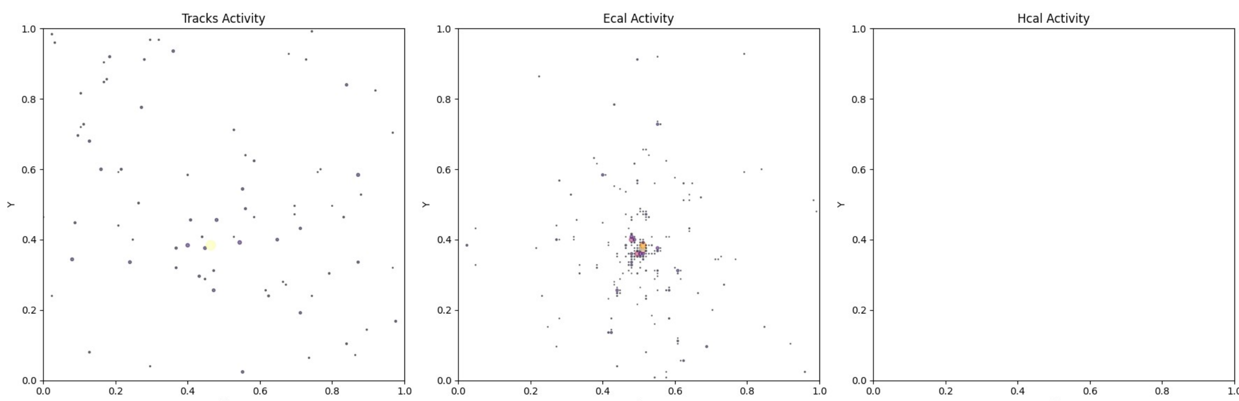


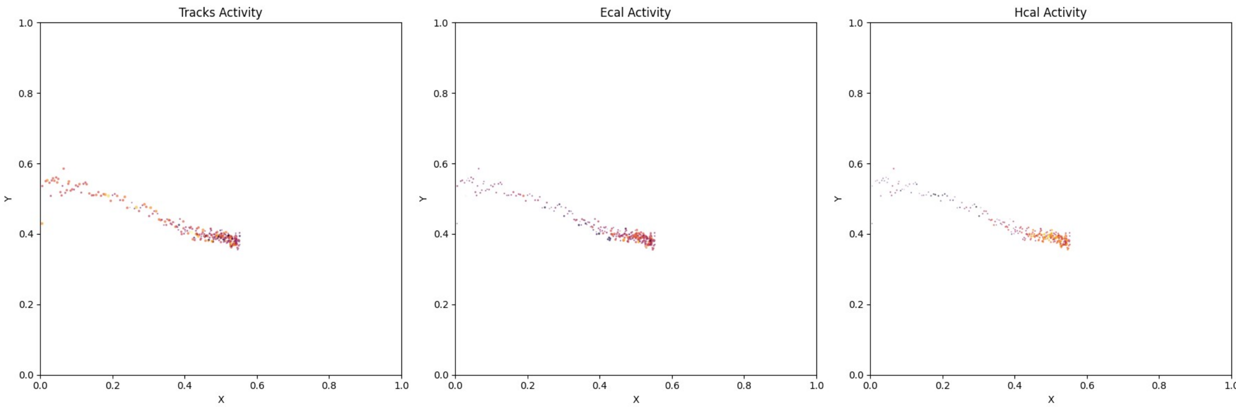

```
Inference:  25%|██        | 1/4 [00:01<00:03,  1.10s/it]
SSIM Score: 0.9636886119842529
```



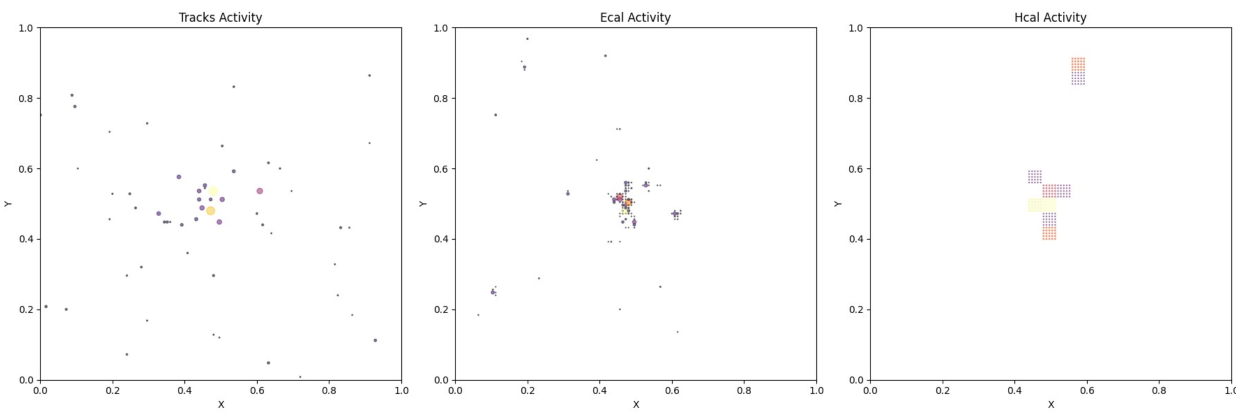


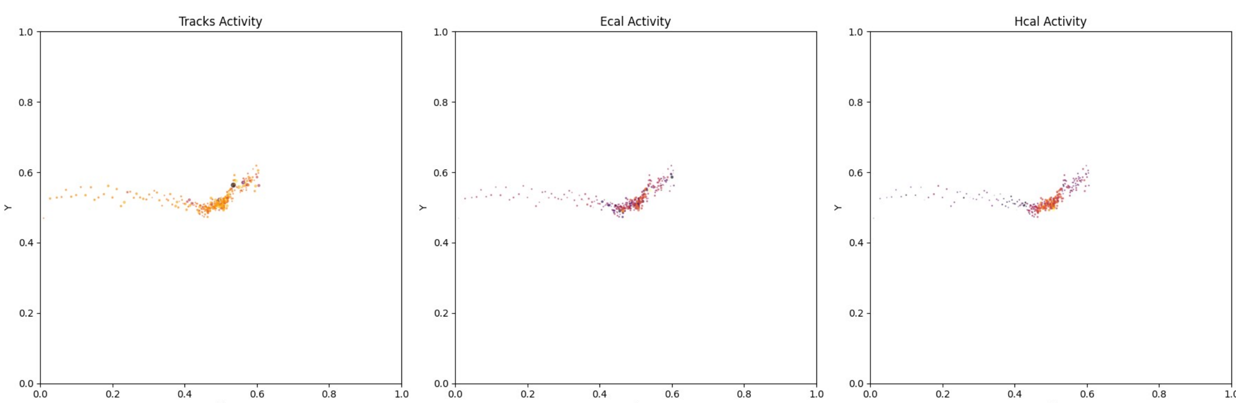

```
Inference:  50%|█████     | 2/4 [00:02<00:02,  1.13s/it]

SSIM Score: 0.9673603177070618
```





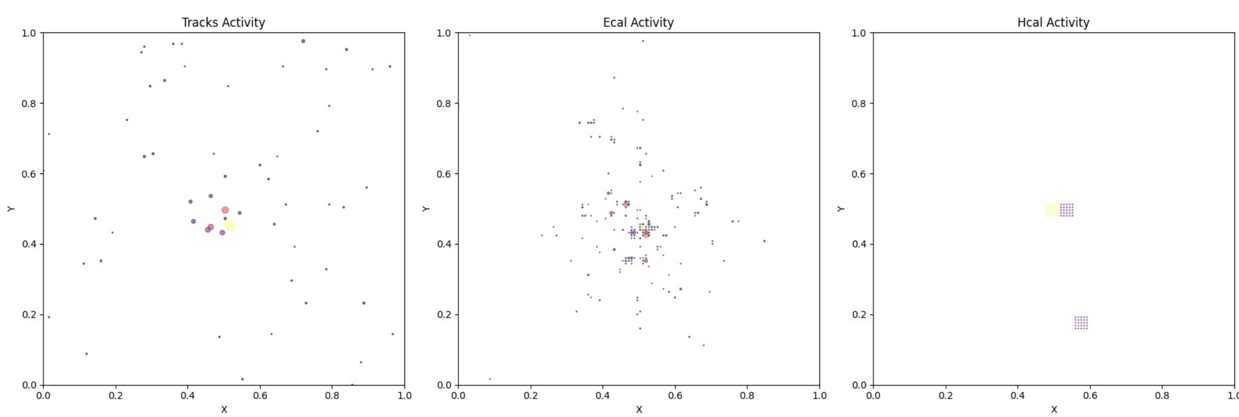

```
Inference:  75%|███████▌  | 3/4 [00:03<00:01,  1.13s/it]

SSIM Score: 0.9540446400642395
```

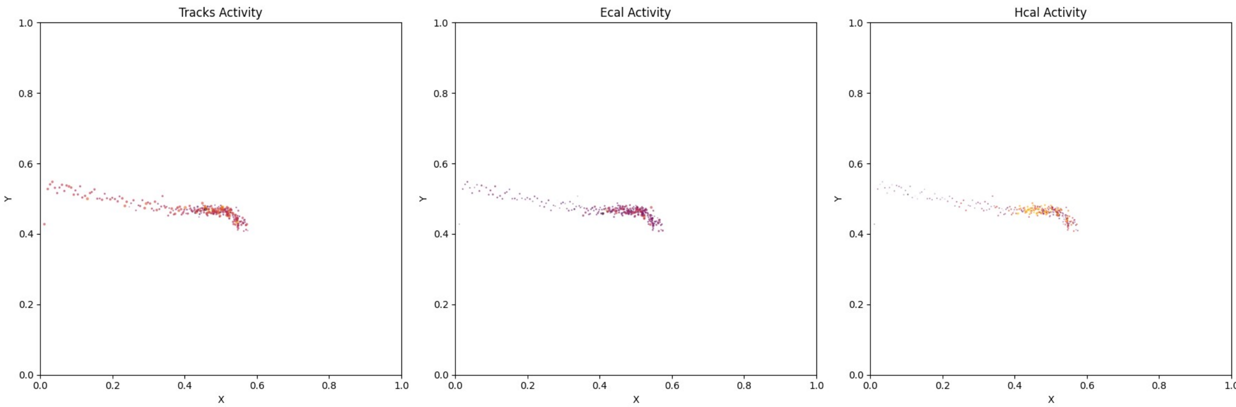




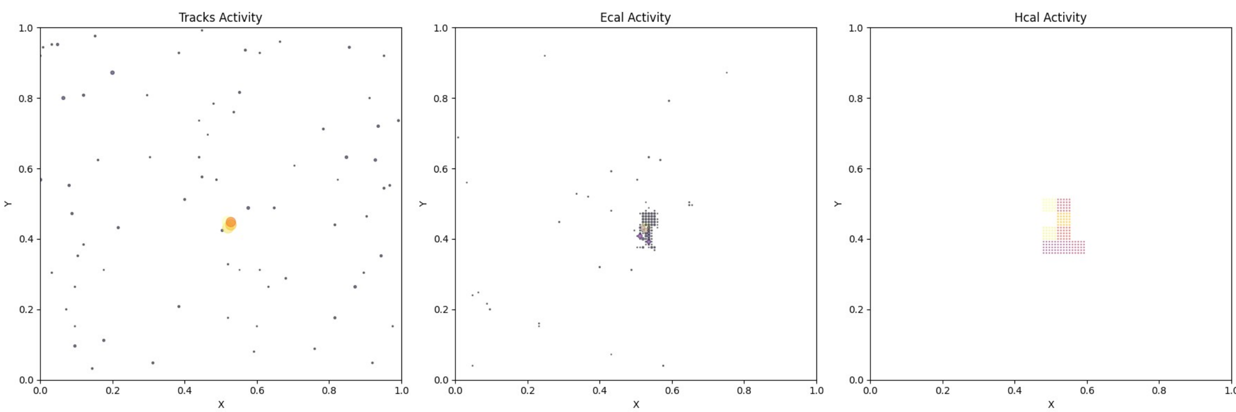

```
SSIM Score: 0.9546252489089966
Epoch :  30  Loss :  0.36720014380989596
```

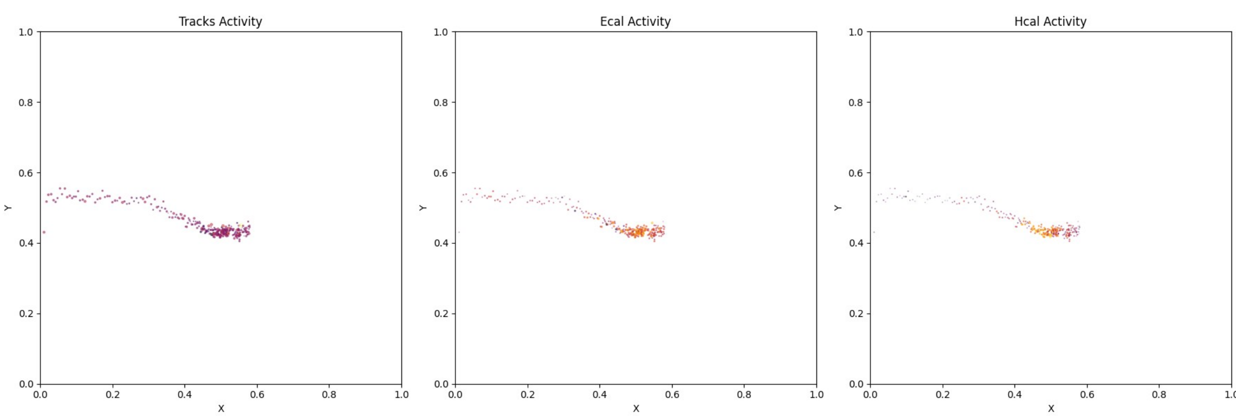
```
Epoch :  31  Loss :  0.36754182865843177


Epoch :  32  Loss :  0.36744653148343787


Epoch :  33  Loss :  0.36526265839347616


Epoch :  34  Loss :  0.3657751535065472


Epoch :  35  Loss :  0.3649989479454234


Epoch :  36  Loss :  0.36272374010877684


Epoch :  37  Loss :  0.36301920824917033


Epoch :  38  Loss :  0.3631019930471666


Epoch :  39  Loss :  0.3620968206669204
Inference:   0%|          | 0/4 [00:00<?, ?it/s]
```



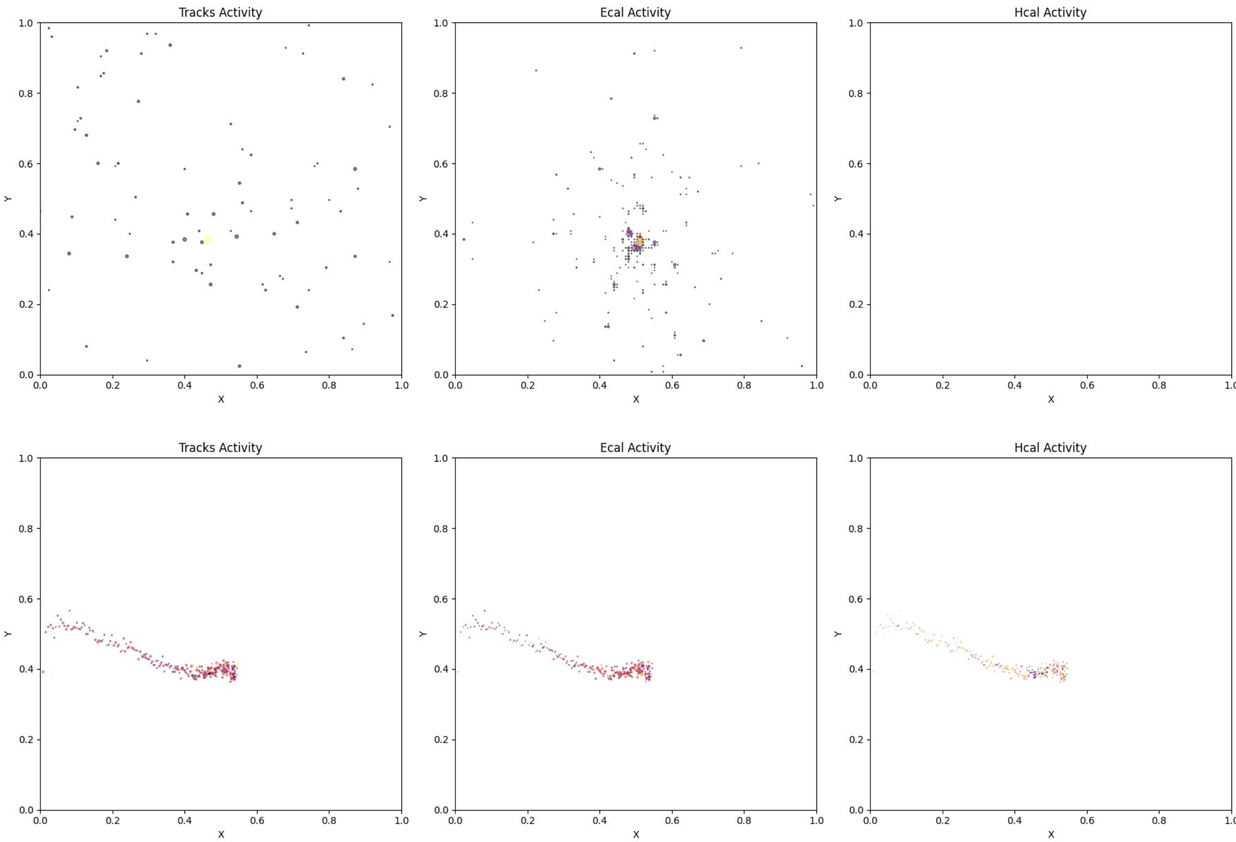



```
Inference:  25%|██        | 1/4 [00:01<00:03,  1.05s/it]
SSIM Score: 0.9604158401489258
```

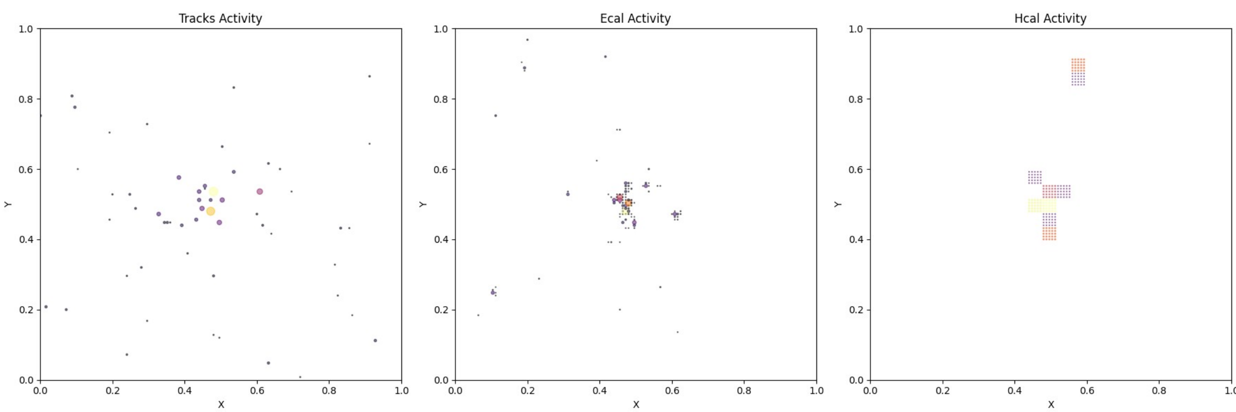


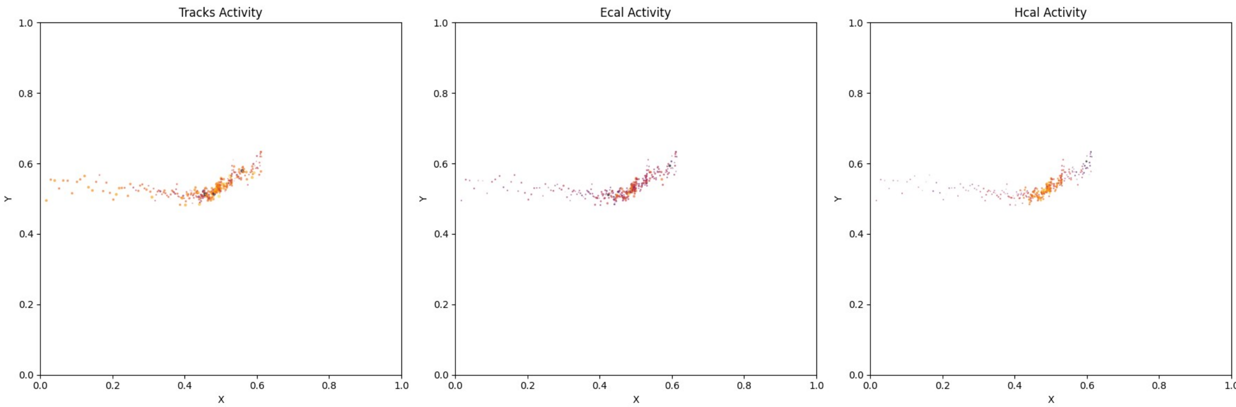



```
Inference:  50%|█████     | 2/4 [00:02<00:02,  1.04s/it]
SSIM Score: 0.9698946475982666
```

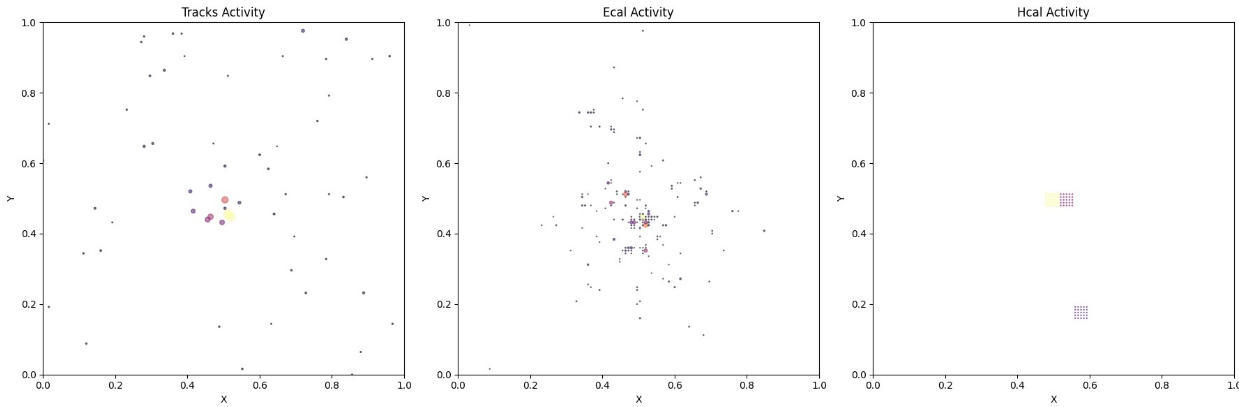


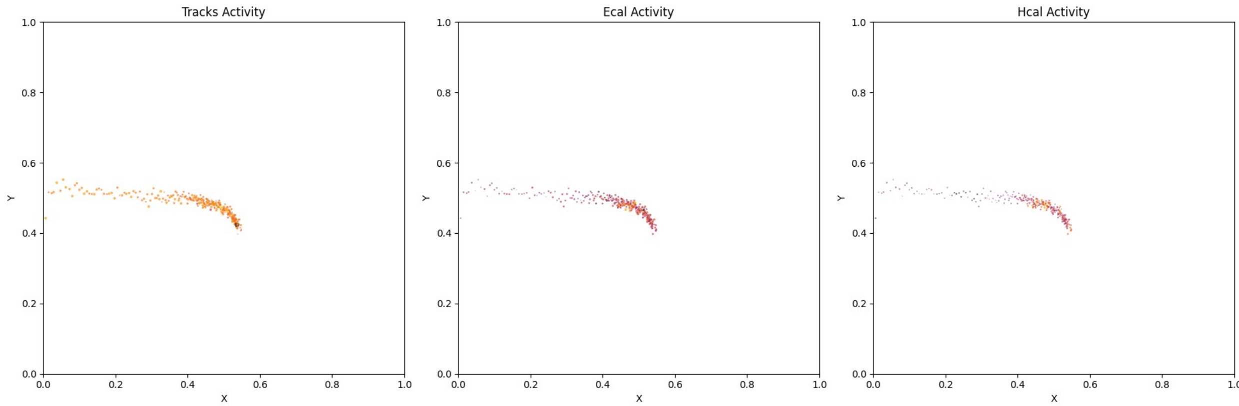

```
Inference:  75%|███████▌  | 3/4 [00:03<00:01,  1.04s/it]

SSIM Score: 0.962800145149231
```



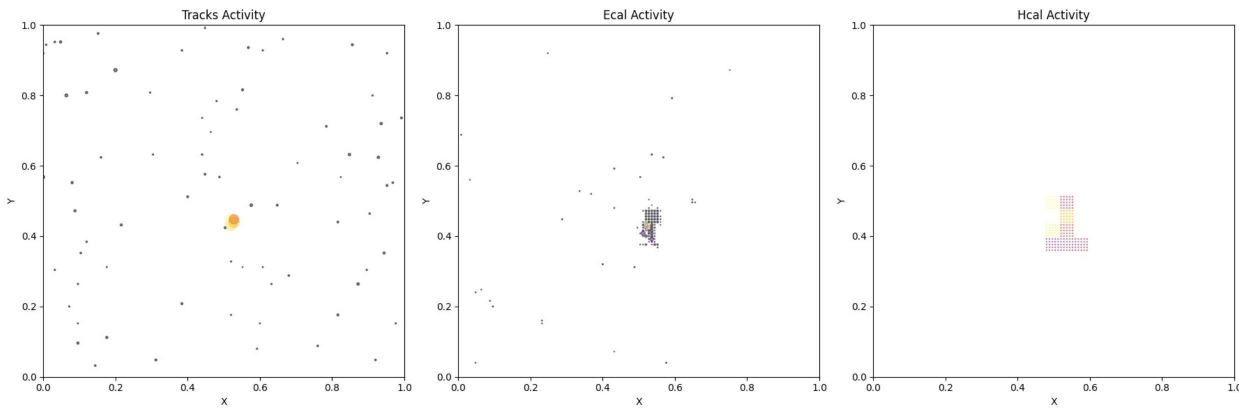


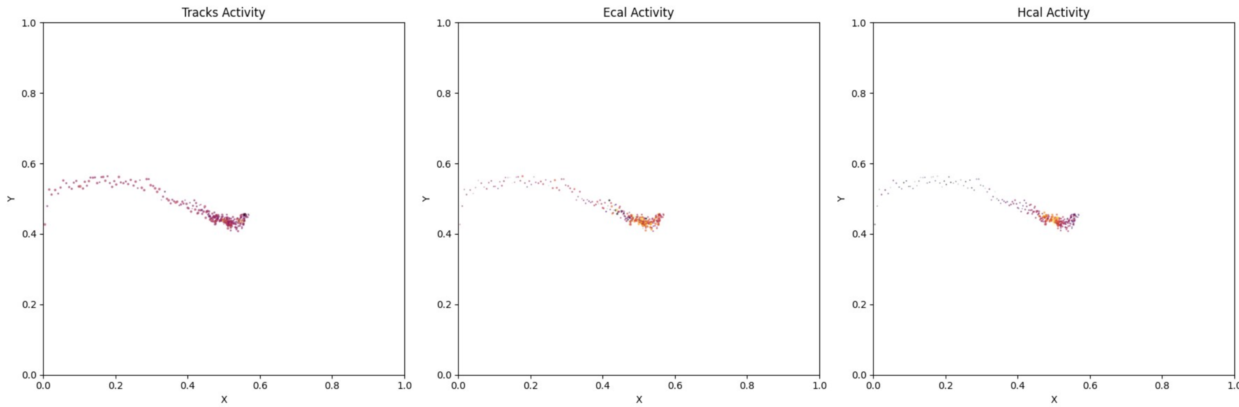

```
SSIM Score: 0.9509390592575073
Epoch :  40  Loss :  0.36183792422525585


Epoch :  41  Loss :  0.36205158807570115


Epoch :  42  Loss :  0.36113130825106055


Epoch :  43  Loss :  0.3591077043674886


Epoch :  44  Loss :  0.35901512764394283


Epoch :  45  Loss :  0.3582064629881643


Epoch :  46  Loss :  0.3587997148861177


Epoch :  47  Loss :  0.3599551059305668


Epoch :  48  Loss :  0.3572996624279767


Epoch :  49  Loss :  0.3567603591363877

Inference:   0%|          | 0/4 [00:00<?, ?it/s]
```



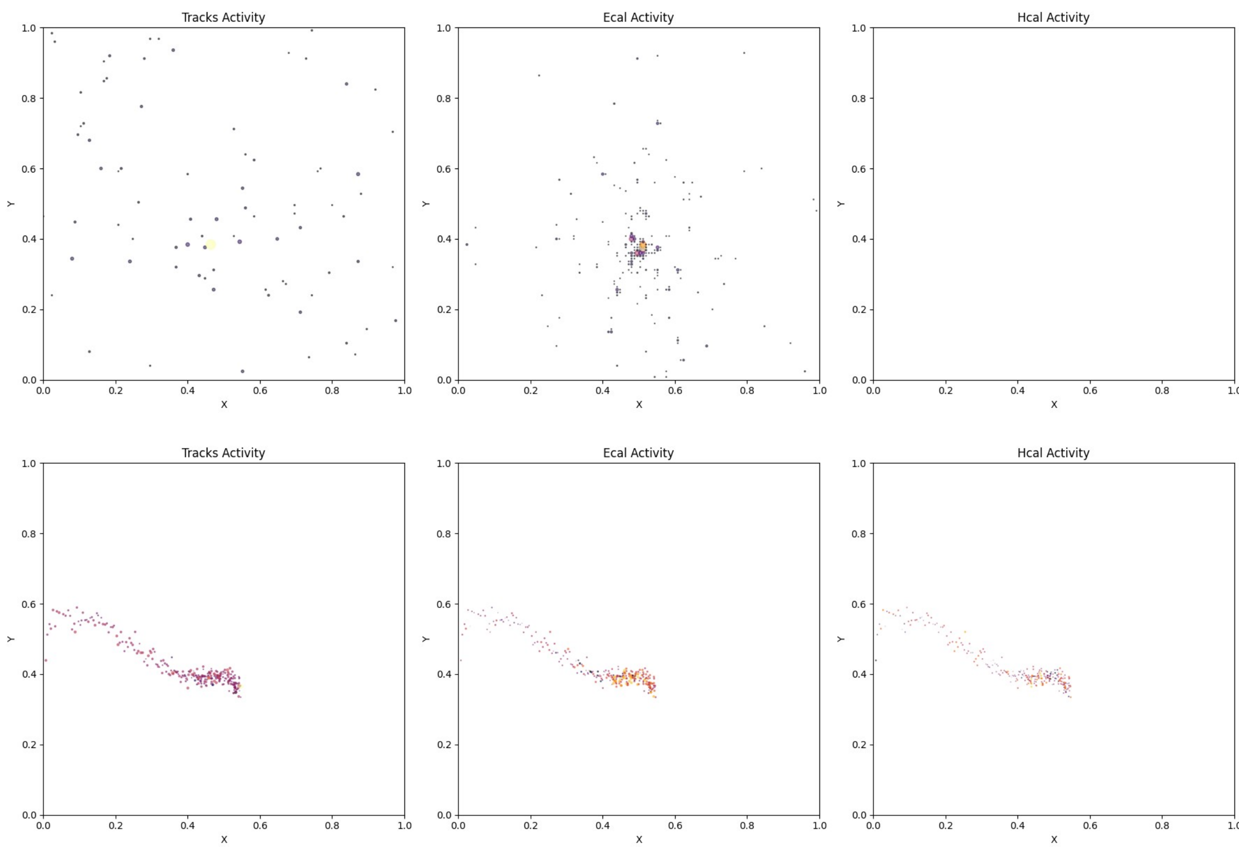



```
Inference:  25%|██        | 1/4 [00:01<00:03,  1.06s/it]

SSIM Score: 0.9613601565361023
```

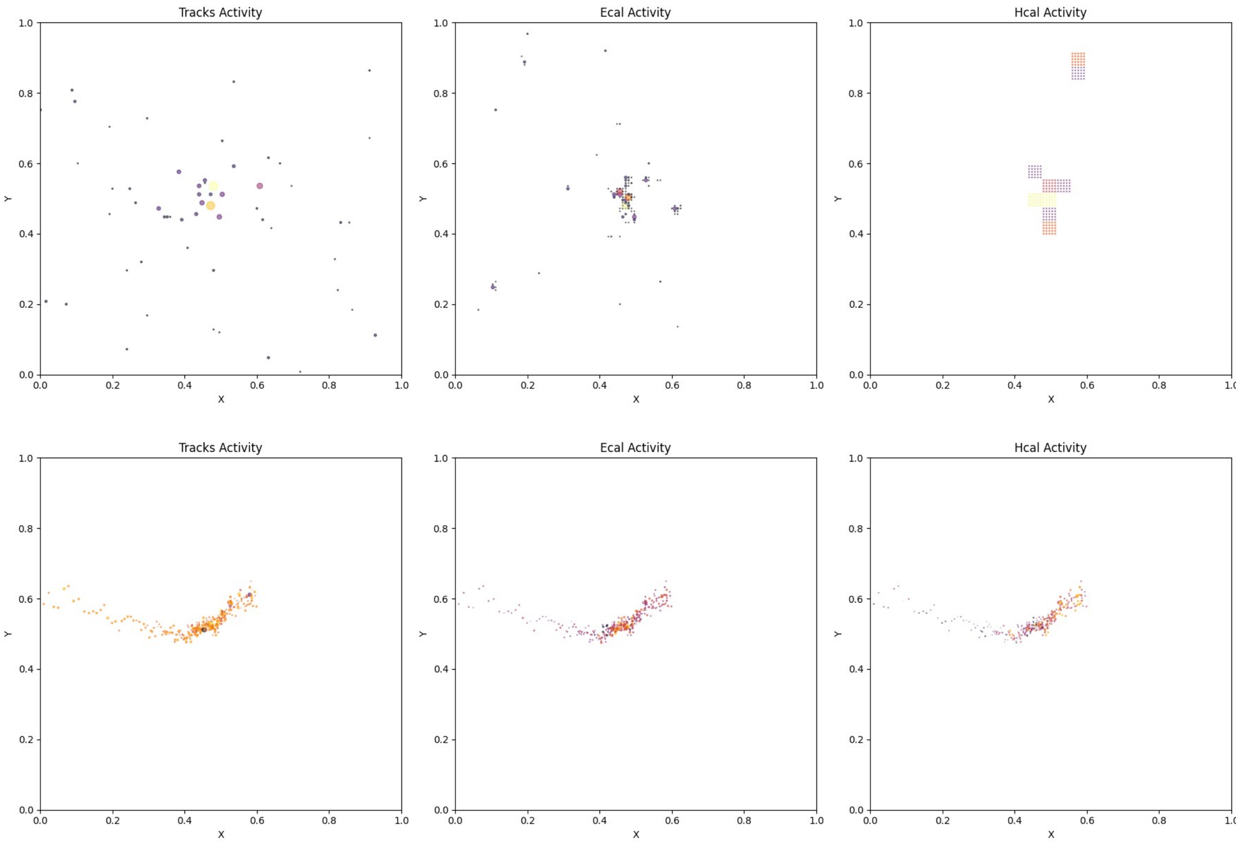





```
Inference:  50%|█████     | 2/4 [00:02<00:02,  1.37s/it]
SSIM Score: 0.9571297764778137
```




```
Inference:  75%|███████▌  | 3/4 [00:03<00:01,  1.23s/it]
SSIM Score: 0.9593967795372009
```




```
SSIM Score: 0.9552584886550903
Epoch :  50  Loss :  0.35717338463291526
```

```python
torch.save(model, "task_3_GAE.pth")

del train_loader
del test_loader
del val_loader
```

Observations and Inferences

1. The model faced challenges in accurately reconstructing node features for graphs with varying node counts.

2. Increasing the k value improved reconstruction quality by providing more context for each node, but this also led to denser graphs, making learning more complex.

3. Coordinate-based sorting effectively simplified the loss calculation since a graph matching algorithm was not needed.

4. Masking-based loss contributed to stable training across graphs with different sizes by focusing on the most relevant nodes.

5. However, the canonical ordering introduced artifacts, notably a horizontal line of points. This occurred because the model learned the sorted ordering, and the mask consistently selected the first (n) nodes.
6. Varying the layers or the individual channels weights in the loss calculations used did not cause any significant changes to the reconstructions
7. Structural Similarity Index Measure (SSIM) was used as the evaluation metric to assess the reconstruction quality, providing insight into how well the spatial structures were preserved.