# ECO-AI HACKATHON TRACK 2: REACTIVE TRANSPORT MODELLING

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# SOME IMPROVEMENTS CONSIDERED

## Reproducibility ("Seed")

## Compression of input data

### Data augmentation

## Physics Informed UNet

#### **Repeatability:**

 Due to the different random procedures inside the modules, 3 different commands has to be used

### Compression of input data:

- While trying some improvements, we observed some memory issues
- Experimented a compression algorithm for the input images, but we couldn't obtain a good reconstruction method in a short time.

#### Data augmentation:

- To diversify training data

### **Physics informed UNet:**

- Add physical constraints
- Converge quickly
- Improved predictions

# **BASELINE U-NET**



### delta eps (dissolution)



# PHYSICS INFORMED U-NETS

- Solve the governing equations for both the inputs and outputs
- Available equations

$$\nabla .(cu) - \nabla .(D\epsilon \nabla c) + R = 0$$

$$\frac{\partial \varepsilon}{\partial t} = R$$

- Spatial differentiation
- Add the residual as a training loss
- Does the training data satisfy these equations?





 $\Delta$  eps (dissolution)





R=(eps[1,:,:,100]-eps[1,:,:,99])/4000 D=1\*10\*\*-9 dxy=25\*10\*\*-6

delXc=(np.gradient(gC,axis=0))/dxy
delYc=(np.gradient(gC,axis=1))/dxy

term2=((np.gradient(D\*np.multiply(gEps,delXc),axis=0)/dxy) + (np.gradient(D\*np.multiply(gEps,delYc),axis=1))/dxy)

term1=(np.gradient(np.multiply(gC,gUx),axis=0) + np.gradient(np.multiply(gC,gUy),axis=1))/dxy

# DATA AUGMENTATION

• Diversify the training data



### Horizontal + vertical flip













Vertical/horizontal/both flips





### DATA AUGMENTATION - RESULTS





### $\Delta$ eps (dissolution)







0

50

50

0

150

200

250

validation sample: 0, timestep: 99, eps: prediction 0 50 100 150 200 250



validation sample: 0, timestep: 99, eps: prediction 0 50 100 150 200 250



validation sample: 0, timestep: 99, eps: reference

100

150

200

250

0.8 5

0.6 100

-0.4 150-

0.2 200 +

250

validation sample: 0, timestep: 99, eps: reference

150

200

250

100



validation sample: 0, timestep: 99, eps: error

150

200

250

0.4

0.2

0.0

-0.2

-0.4

100

50

0 1.0 0+





0.003

0.002

- 0.001

0.000

-0.001

-0.002

-0.003





100%	625/625	[00:42<00:00,	14.72it/s]
train_loss: 4.4062293200113347e-07			
100%	200/200	[00:04<00:00,	46.56it/s]
validation_loss:	4.148302	2934368075e-06	



# THANK YOU