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Context & Motivation

Multi-Fidelity Tools



Numerical Methods



Machine Learning (cGAN)





 Preliminary Design
 Detailed Design
 Scan processing

 Image: Detailed Design
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Damage identification



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Conditional Generative Adversarial Networks (cGAN):

What is a cGAN

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- Neural network used for generating realistic text, audio, images or video
- Consists of two neural networks generator and discriminator

Training process

- 1. Train generator and discriminator using a 'real' dataset
- 2. Generator creates item
- 3. Discriminator decides if it is a 'real' item, or made by the generator
- 4. Generator and discriminator learn from the outcome and adjust model
- Eng tool developed in MATLAB by the University of Southampton
- The encoded images** produced by the encoder are fed into the cGAN

** The IP described on this slide is protected by patent.



 cGANs thus offer an alternative to expensive simulations, with a prediction accuracy R² of up to 97%

encodings



Conditional Generative Adversarial Networks (cGAN*):

Benefits over conventional workflows

* Andy J. Keane and Ivan I. Voutchkov, Embedded Parameter Information in Conditional Generative Adversarial Networks for Compressor Airfoil Design, AIAA, 4 Aug 2022.

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A set of possible geometries that fall within the performance parameter of interest range (i.e. Loss Coefficient).



Methodology



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System prototype within Rolls-Royce:

Encoding



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- Encoding Images: Method used to embed a set of specific input/output parameters chosen by the user into an image.
- Utilises 'real' design images with design parameters to then encode these into the image in contrasting bar charts

| Image Enc | oder & Decod | er Set-up | | | |
|--|--------------|-----------|-----------------------------------|----------------|------------|
| Encoder Image Decoder | | | Histogram and Glyphs Definition I | Parameters | |
| Encoding Parameters File: | | | Histograms Image PrefixName | | - |
| | | Browse | Glyphs Image PrefixName | | - |
| Images to Encode: | | | Number of Splits | | - |
| | | Browse | | Configure | |
| Location to save encoded image: | | | Taper Angle | | |
| | | Browse | Maximum Pixel Height Value | | _ |
| J | | | Width of each bar in the Bar Plot | | - |
| Location to sure instograms and gryphs | • | | Distance Between Each Bar | | _ Output |
| | | Browse | Minimum Value Pixel Ratio | | |
| Image Definition Param | neters | | Histogram Images Scaling Factor | | – paralite |
| Image Name | | | Encoded Image PrefixName | | encodi |
| Top Left corner Point | х, у | | Encoded Image Format | e.g. jpeg, png | - |
| Top Right Corner Point | х, у | | Input Parameters to Encode | Select | |
| Bottom Left Corner Point | х, у | | Output Parameters to encode | Select | |
| Bottom Right Corner Point | х, у | | | Encode | |



System prototype within Rolls-Royce: Prediction extraction

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User inputs









Use cases: Fuel Spray Nozzle design



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High Cone Angle



Use cases: Multi-stage fan design use case







Use cases: Cantilever Beam

Key challenges:

- Higher-GPU resources
- Scalability (fidelity &dimensionality)
- Configuration (hyperparameters)
- Computational time Vs costs





Example of encoded image

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Cloud capabilities

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Cloud capabilities





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Cloud Advantages

- At least 1 Order of Magnitude reduction in comp time
- Hyperparameters optimisation
- Parallelisation
- Costs
- Scalability
- Traceability (MLFlow)
- Access Control
- Data [pre/post] processing automation

Design of Experiment: CPU vs GPU and Desktop vs Cloud

| Exp (~ | Do ~ | Cloud Miflov ~ | Valid ~ | Environm | Hostname | Cloud | GPU/C ~ | Sin | Computat ~ | package 🗸 | Package Name | File Name | version | architectu | Data | Encoder/~ | Image Siz ~ | Learning Ri |
|---------|------|----------------|---|----------|----------------|-------------|---------|------|--------------|--------------|-----------------|---------------------------|----------------|--------------|------------------------|-----------|-------------|-------------|
| | ? | Exp ID | on | t | | Runtime | | Node | n Spec | | reference | | | 1 - | | coder | | |
| | | | done? | | | | | ? | | | (Orginal) | | | | | | | |
| 1 | LΥ | | Y | Desktop | GBA-E105039872 | N/A | GPU | Y | NVIDIA Quad | d Matlab | Matlab | | R2021B | NGAN | matlabbeam_98K | Python | 128X128 | 0.0002G/0 |
| 2 | 2 Y | | | Desktop | GBA-E105039870 | N/A | GPU | Y | NVIDIA Quad | d Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_98K | Python | 128X128 | 0.0 |
| 3 | 8 Y | | Y | Desktop | GBA-E105039872 | N/A | GPU | Y | NVIDIA Quad | d Matlab | Matlab | | R2021B | NGAN | matlabbeam_63K | Python | 128X128 | 0.0002G/0 |
| 4 | Y | | | Desktop | GBA-E105039870 | N/A | GPU | Y | NVIDIA Quad | d Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_63K_matlabe | Matlab | 128X128 | 0.0 |
| 5 | 5 Y | | | Desktop | GBA-E105055523 | N/A | CPU | Y | i9-10980XE 3 | 3 Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 6 | δY | | | Desktop | GBA-E105055523 | N/A | CPU | Y | i9-10980XE 3 | 3 Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 7 | 7 Y | PyTorch_cantil | e/ | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | CGAN with Pytorch | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 8 | 8 N | | 1 | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Tensorflow | Tensorflow | | 2.14.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 9 | 9 N | | | laptop | | N/A | GPU | Y | NVIDIA T120 | (Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X129 | 0.0 |
| 10 | N | | | laptop | | N/A | CPU | Y | 11Gen Intel | C Pytorch | Pytorch | | 1.10.2 | Conv Layer | matlabbeam_63K | Python | 128X130 | 0.0 |
| 11 | N | | | laptop | | N/A | CPU | Y | 11Gen Intel | C Tensorflow | Tensorflow | | 2.5.0 | Conv Layer | matlabbeam_63K | Python | 128X131 | 0.0 |
| 12 | 2 N | | 1 | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | | 2.0.1+cu118 | linear Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 13 | 8 Y | PyTorch_cantil | eΥ | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | CGAN with Pytorch | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 14 | I Y | PyTorch_cantil | e/ | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | CGAN with Pytorch | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 15 | 5 Y | | | Desktop | GBA-E105055523 | N/A | GPU | Y | i9-10980XE 3 | 3 Pytorch | Pytorch | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 16 | 5 N | | 1 | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch_CKPTS | | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0 |
| 17 | 7 N | | 1 | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch_CKPTS | | 2.0.1+cu118 | Conv Layer | matlabbeam_63K_matlabe | Matlab | 128X128 | 0.0 |
| 18 | 8 Y | PyTorch_cantil | eΥ | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | cgan pytorch 128x128 v1 | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0002G/0 |
| 19 | γ | PyTorch cantil | eΥ | Cloud | | 14.3 LTS ML | GPU | Y | NC6 sv3, 16 | C Pytorch | Pytorch | cgan pytorch 128x128 v1 | 2.0.1+cu118 | Conv Layer | matlabbeam 63K | Python | 128X128 | 0.0002G/0 |
| 20 | Y | PyTorch_cantil | e/ | Cloud | | 14.3 LTS ML | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch | cgan_pytorch_128x128_v1 | 2.0.1+cu118 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0002G/0 |
| 21 | ΙY | PyTorch cantil | e/ | Cloud | | 14.3 LTS ML | GPU | Y | NC6 sv3, 16 | C Pytorch | Pytorch | cgan pytorch 128x128 v1 | 2.0.1+cu118 | Conv Layer | matlabbeam 63K | Python | 128X128 | 0.0002G/0 |
| 22 | 2 Y | PyTorch cantil | e/ | Cloud | | 14.3 LTS ML | GPU | Y | NC6 sv3, 16 | C Pytorch | Pytorch | cgan pytorch 128x128 v1 n | ne 2.0.1+cu118 | Conv Layer | matlabbeam 63K matlabe | Matlab | 128X128 | 0.0002G/0 |
| 23 | 3 Y | PyTorch cantil | e N | Cloud | | 14.3 LTS ML | GPU | Y | NC6 sv3. 16 | C Pytorch | Pytorch updated | cgan pytorch 128x128 Upd | at 2.0.1+cu118 | Conv Laver | matlabbeam 63K | Python | 128X128 | 0.00026/0 |
| 24 | Y | PyTorch cantil | e/ | Cloud | | 14.3 ITS MI | GPU | Y | NC6_sv3, 16 | C Pytorch | Pytorch updated | cgan pytorch 128x128 Upd | at 2.0.1+cu118 | Conv Laver | matlabbeam_63K | Python | 128X128 | 0.0002G/0 |
| 25 | Y | PyTorch64/per | </td <td>Cloud</td> <td></td> <td>14.3 ITS MI</td> <td>GPU</td> <td>Y</td> <td>NC6 sv3 16</td> <td>Pytorch</td> <td>Pytorch 64x64</td> <td>cgan pytorch 64x64 (CGAN)</td> <td>vi 2.0.1+cu118</td> <td>Conv Laver</td> <td>matlabbeam_63K</td> <td>Python</td> <td>64X64</td> <td>0.00026/0</td> | Cloud | | 14.3 ITS MI | GPU | Y | NC6 sv3 16 | Pytorch | Pytorch 64x64 | cgan pytorch 64x64 (CGAN) | vi 2.0.1+cu118 | Conv Laver | matlabbeam_63K | Python | 64X64 | 0.00026/0 |
| | | · · · | 1, | ol 1 | | 1.0.170.141 | | 2 | | | | | | o i | 111 690 | | 10004 | |



Cloud Compute Strategies



databricks

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- 1. Number of images < .5M
 - Single Node GPU
- 2. Number of images > .5M
 - Single Node multiple GPU
 parallelization or

• N

O C

- Multi Node cluster for Distributed computation
- 3. Hyperparameter optimisation
 - Multi Node cluster for Distributed computation

Databricks Single GPU config example

| w | Compute > | | |
|-----------------|---|------------|-----------|
| orkspace | Databricks Single Node GPU 🖉 | | |
| cents | Policy ① | | UI JSON |
| talog | cpu_all_purpose_sn_policy_cgan | | |
| mpute | Multi node 💿 Single node 🛇 | | |
| | Access mode ① Single user access ① | | |
| Editor | Single user | | |
| eries | Performance | | |
| shboards | Databricks runtime version ⁽¹⁾ | | |
| rts | Runtime: 14.3 LTS ML (GPU, Scala 2.12, Spark 3.5.0) VID | IA EULA () | |
| ery History | | | |
| L Warehouses | Use Photon Acceleration | | |
| | Node type ① | | |
| Runs | Standard_NC6s_v3 [V100] 112 GB Memory, 1 GPU V | | |
| ta Ingestion | | | |
| Ita Live Tables | 0 | | |
| e Learning | Tags 0 | | |
| yground | Additaon | | |
| periments | Kay | | Add |
| itures | toute | | Huu |
| odels | > Automatically added tags | | |
| ving | Advanced options | | |
| rketplace | | | |



Results: Training data







Experiment3 Epoch160 bin3

3 y_act

y_act

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Results: CPU Vs GPU



| xp ID | Done | Cloud Miflow | Validati | Environmen | Hostname | Cloud | GPU/CPU | Single | Computatio packag | ge Package Na | me | File Name | version | architecture | Data | Encoder/D | e Image Size | Learning Rate | Batch | Numb | Number |
|-------|------|--------------|----------|------------|----------------|---------|---------|--------|---------------------|---------------|----|-----------|---------|--------------|----------------|-----------|--------------|---------------|-------|---------|-----------|
| | ? | Exp ID | on | t | | Runtime | | Node | n Spec | reference | | | | | | coder | | | Size | er of | of Latent |
| - | - | - | don 🔻 | - | - | - | - | ? 👻 | - | | - | · | | · · | - | | • | - | - | filte 🔻 | Dimen 🔻 |
| 6 | Y | | | Desktop | GBA-E105055523 | N/A | CPU | Y | i9-10980XE 3 Pytoro | ch Pytorch | | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0002 | 50 | 64 | 1 100 |
| 15 | Y | | | Desktop | GBA-E105055523 | N/A | GPU | Y | i9-10980XE 3 Pytoro | ch Pytorch | | | 1.12.1 | Conv Layer | matlabbeam_63K | Python | 128X128 | 0.0002 | 50 | 64 | 1 100 |



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Results: Current Challenges & WIP

& PCUIBCI Discriminator loss Configuration UseGPU = False BatchSize = 50 shuffle = True learningrate = 0.0002 onvergence Generator loss classes = 7 embeddingdimension = 50 NoOfFilters = 64 **Discriminator Structure** labels Architecture

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Future work



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- Short term:
 - Continue investigation and definition of best practices for the setup of settings
 - Dimensionality limits shift to fully 3D NN processing



- Longer term:
 - How to exploit knowledge from unsuccessful/unconverged simulations
 - How to address studies with multiple (conflicting) objectives and design metrics

