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Fast Prediction of Indoor Airflow Distribution Inspired by Synthetic Image Generation Artificial Intelligence

Abstract

Prediction of indoor airflow distribution often relies on high-fidelity, computationally intensive Computational Fluid Dynamics (CFD) simulations. Artificial intelligence (AI) models trained by CFD data can be used for fast and accurate prediction of indoor airflow, but current methods have limitations, such as only predicting limited outputs rather than the entire flow field. Furthermore, conventional AI models are not always designed to predict different outputs based on a continuous input range, and instead make predictions for one or a few discrete inputs. This work addresses these gaps using a Conditional Generative Adversarial Network (CGAN) model approach, which is inspired by current state-of-the-art AI for synthetic image generation. We create a new Boundary Condition CGAN (BC-CGAN) model by extending the original CGAN model to generate 2D airflow distribution images based on a continuous input parameter, such as a boundary condition. Additionally, we design a novel feature-driven algorithm to strategically generate training data, with the goal

of minimizing the amount of computationally expensive data while ensuring training quality of the AI model. The BC-CGAN model is evaluated for two benchmark airflow cases: an isothermal lid-driven cavity flow and a non-isothermal mixed convection flow with a heated box. We also investigate the performance of the BC-CGAN models when training is stopped based on different levels of validation error criteria. The results show that the trained BC-CGAN model can predict the 2D distribution of velocity and temperature with less than 5% relative error and up to about 75,000 times faster when compared to reference CFD simulations. The proposed feature-driven algorithm shows potential for reducing the amount of data and epochs required to train the AI models while maintaining prediction accuracy, particularly when the flow changes non-linearly with respect to an input.

Keywords: artificial intelligence, indoor airflow, conditional generative adversarial network, computational fluid dynamics.

¹ 1. Introduction

² Simulation of indoor airflow distribution can be used for understanding
³ indoor air quality, thermal comfort, and building energy efficiency. Computational
⁴ Fluid Dynamics (CFD) methods are a popular approach for indoor airflow
⁵ simulation [1] that numerically solve the governing equations of fluid flow,

6 such as conservation of mass, momentum, and energy. For example, Han
7 et al. [2] used a CFD approach to simulate data center cooling scenarios to
8 provide guidance for reducing energy consumption while meeting thermal
9 requirements. Researchers have also used CFD methods to study the impact
10 of ventilation strategies on thermal comfort [3, 4, 5], evaluate dispersion of
11 airborne pollutants [6, 7, 8], and more. While these methods have been
12 useful in many applications related to indoor airflow, they are still limited in
13 a number of ways. First, CFD simulations are computationally expensive [9]
14 and may be too slow for applications such as long-term evaluations (e.g.,
15 annual simulations) or optimization problems requiring thousands of realizations.
16 Additionally, it is often infeasible to perform real-time or faster simulations
17 using CFD, which can be required for emergency management scenarios [10].
18 Therefore, there is a need for computationally efficient methods of indoor
19 airflow distribution prediction.
20 Modifications to traditional CFD methods have been proposed to accelerate
21 these numerical simulations, such as Fast Fluid Dynamics methods [11, 12].
22 While these methods can be used for real-time or faster flow simulations,
23 they may sacrifice some accuracy compared to traditional CFD methods.
24 They are also unable to perform real-time simulations for more complex

25 airflow scenarios. Data-driven regression methods, such as in situ adaptive
26 tabulation [13, 14], can quickly predict key flow information, such as the
27 occupied zone temperature. However, these methods are often used to predict
28 a few key outputs rather than the entire flow distribution.

29 Artificial intelligence (AI) methods have emerged as a popular approach
30 to address some of the limitations of indoor airflow prediction. Zhou and
31 Ooka [15] analyzed using deep neural networks for isothermal airflow distribution
32 prediction in an ofice room and found the trained networks could accurately
33 predict the velocity distribution 1.9 million times faster than reference CFD
34 simulations. Generative Adversarial Network (GAN) [16] models have become
35 a popular AI approach, particularly for generating synthetic images [17,
36 18]. Variations of the original GAN model have been introduced, such as
37 Conditional Generative Adversarial Network (CGAN) [19] models, which
38 generate synthetic data based on categorical labels. In [19], the categorical
39 labels include different single digit numbers and the CGAN model generates
40 synthetic hand-drawn images for each specified digit. These models have
41 been used for generating synthetic images of faces at different ages [20],
42 producing power demand profiles for different types of buildings [21], and
43 predicting wireless networking environments [22]. CGAN models trained by

44 CFD simulations have been used for flow prediction, for example Chen et
45 al. [23] predicted airflow over different airfoil shapes and Wang et al. [24]
46 predicted the temperature distribution of different vortex generator designs
47 for film cooling.

48 While significant advances have been made to use AI for indoor airflow
49 prediction, some limitations still exist. First, many AI models are designed to
50 predict one or a few critical outputs in the airflow (e.g., average temperature
51 in the occupied zone or temperature values at a few sensor locations) rather
52 than the entire airflow distribution, which is necessary for many modeling
53 applications. GAN and CGAN models have shown significant potential for
54 image generation, including prediction of flow distribution, and are thus
55 worthy of further research for indoor airflow prediction. However, they are
56 often designed to make predictions based on discrete categorical inputs, for
57 example different specific designs or geometries. However, in many scenarios
58 it is useful to be able to make predictions based on continuous input parameters.
59 For example, boundary conditions, such as supply airflow rate in indoor
60 airflow simulations, may be optimized based on a continuous design space.
61 This is because the supply airflow rate can be optimized to be any possible
62 value within a defined range, rather than being limited to a few select values.

63 Finally, generating training data for AI models using CFD simulations can be
64 time consuming, and it is not always clear how much data should be included
65 to train the models.

66 To address the limitations discussed, we create a new Boundary Condition
67 CGAN (BC-CGAN) model for predicting indoor airflow distribution based on
68 a continuous input parameter, such as a boundary condition. Furthermore,
69 we design a novel feature-driven algorithm for efficiently generating training
70 data. The algorithm minimizes the amount of generated data while ensuring
71 a diverse set of training data for AI models by selecting data points based on
72 significant changes in the flow output. The feature-driven algorithm and
73 BC-CGAN model are evaluated for two benchmark airflow cases: 1) an
74 isothermal lid-driven cavity flow and 2) a non-isothermal mixed convection
75 flow with a heated box. CFD simulations are used to generate the training,
76 validation, and test data for both cases. Using the dimensionless Reynolds
77 number as an input, the BC-CGAN model predicts the velocity magnitude
78 distribution for the lid-driven cavity case. For the mixed convection flow with
79 heated box case, the BC-CGAN model predicts the velocity magnitude and
80 temperature distributions based on the heat flux of the box. The model is
81 also designed to reproduce the existence of an obstruction in the flow, in this

82 case the box within the flow. Finally, noise is added to some of the boundary
83 conditions in the CFD simulations for this case to mimic uncertainty in
84 experimental conditions.

85 Our specific scientific contributions include: 1) creating a new BC-CGAN
86 model by extending the traditional CGAN model to generate images of flow
87 distribution using a continuous input parameter (e.g., a boundary condition);
88 2) designing a novel feature-driven algorithm to strategically reduce the
89 amount of required training data while ensuring training quality for AI
90 models; and 3) demonstrating the BC-CGAN model framework for two
91 benchmark flow cases and showing the trained model can predict airflow
92 distribution with less than 5% relative error and up to about 75,000 times
93 faster when compared to reference CFD simulations.

94 The rest of this paper is organized as follows. The BC-CGAN model
95 is introduced in Section 2. We then detail the feature-driven algorithm for
96 generating training data in Section 3. Next, Section 4 outlines the entire
97 workflow including generation of training data, model training, and model
98 evaluation. After that, Section 5 presents the results for the isothermal
99 lid-driven cavity flow case and Section 6 shows the results for the non-isothermal
100 mixed convection flow with heated box case. Finally, conclusions are drawn

₁₀₁ in Section 7.

₁₀₂ 2. New Boundary Condition Conditional Generative Adversarial
₁₀₃ Network (BC-CGAN) Model

₁₀₄ In this section, we first provide an overview of the original GAN and
₁₀₅ CGAN models, then detail our new BC-CGAN model.

₁₀₆ 2.1. Original GAN and CGAN Models

₁₀₇ The CGAN model used to develop BC-CGAN is based on the original
₁₀₈ GAN model [16], but modified to generate images based on different classes.
₁₀₉ GAN-based models are selected for this study because of their strength in
₁₁₀ image generation [25], which is useful for applying to prediction of indoor
₁₁₁ airflow distribution. Furthermore, they have been extended for 3D image
₁₁₂ generation applications [26, 27, 28], which can be beneficial for 3D airflow
₁₁₃ prediction. As shown in Figure 1 (left), the original GAN model consists
₁₁₄ of two competing neural networks: a generator (G) and discriminator (D).
₁₁₅ The generator receives a vector containing randomly generated noise (z)
₁₁₆ as an input and attempts to output an image accordingly ($G(z)$). The
₁₁₇ discriminator receives a mixture of real images (x) randomly selected from
₁₁₈ the training data and synthetic or “fake” images produced by the generator.

119 The discriminator then attempts to correctly classify each image as real or
120 fake, and the output of the discriminator ($D(G(z)|x)$) is compared with the
121 correct classification of real or fake. Based on this final outcome, the weights
122 of the generator (θ_G) and discriminator (θ_D) networks are updated and the
123 process repeats, starting with new batches of training images and new noise
124 inputs. Early in the training process, the generator has not learned how
125 to output realistic images, so the discriminator is able to easily classify the
126 images and the generator performs poorly. As the generator is trained over
127 many iterations, it learns how to produce more realistic images and is able to
128 fool the discriminator. Eventually, the generator produces images that are
129 so realistic that the discriminator can no longer distinguish between the real
130 and fake images. Ideally, the training process would reach a quasi-equilibrium
131 state where the discriminator has a 50-50 guess at whether images are real
132 or fake, and the training process can stop. Once the model is trained, the
133 discriminator is no longer needed and synthetic images can be generated
134 by providing a noise input to the generator. Although GAN models can
135 be difficult to train [29], in part because they involve two neural networks,
136 they have demonstrated advantages in image prediction over other types of
137 models [29].

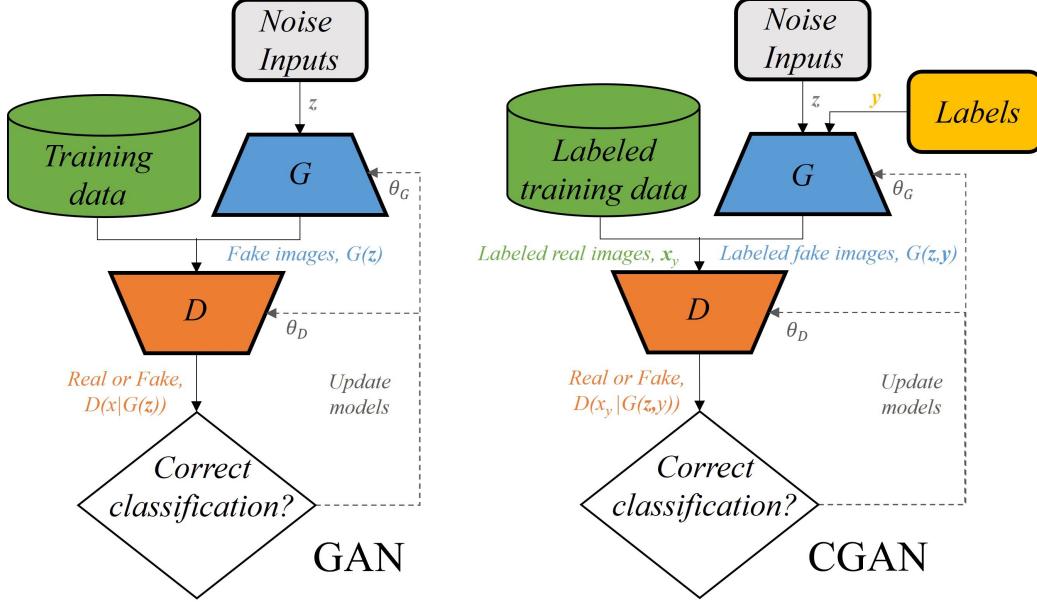


Figure 1: GAN training architecture (left) and CGAN training architecture (right).

138 What differentiates the CGAN model from the original GAN model is
 139 the addition of labels, as shown in Figure 1 (right). The generator receives
 140 a label (y) as an input in addition to the noise input and attempts to
 141 produce an image based on this label ($G(z, y)$), for example an image of
 142 a specific digit in [19]. The discriminator then instead receives labeled
 143 real images (x_y) mixed with labeled images produced by the generator, and
 144 determines whether an image is real or fake considering the received label.
 145 After training, synthetic images can be generated for a specific category by
 146 providing the generator with a label and noise input. The use of labels

147 is convenient for generation of images based on specific categories, which
148 is accomplished by assigning unique labels to the training data from each
149 category. Since the original GAN model generates images based on the
150 aggregated, non-categorized training data, the CGAN model is adopted in
151 this work to utilize labels for categorizing training data. This can mean
152 predicting airflow patterns for different labeled building designs, as in [30].
153 The use of labels, however, also adds complexity to training the model,
154 because the model needs to be trained to generate images for multiple categories.

155 2.2. BC-CGAN Model

156 We extend the previously described CGAN model to create a new BC-CGAN
157 model in this work that generates images using continuous inputs, rather
158 than a few discrete input classes. An example of using discrete input classes
159 would be prediction of airflow distribution in different rooms, where each
160 specific room configuration would be the discrete input class determining the
161 output airflow. Indoor airflow simulations often involve input parameters
162 that can be considered continuous rather than discrete, such as a boundary
163 condition like the supply airflow rate. This can be considered as a continuous
164 parameter because it can have any possible value within a defined range (e.g.,
165 any value between 1-5 kg/s), rather than only a few possible values (e.g., a

₁₆₆ few potential room configurations). The change in output airflow distribution
₁₆₇ can then be studied by varying the input parameter continuously within its
₁₆₈ range.

₁₆₉ Modifying the existing CGAN model to make predictions based on continuous
₁₇₀ input variables poses a challenge, since the original CGAN model is designed
₁₇₁ to make predictions based on discrete integer labels. Although a continuous
₁₇₂ input range can be discretized to assign labels for a CGAN model to many
₁₇₃ possible values within that range, this cannot cover every possible value, and
₁₇₄ a simpler method can be adopted. Thus, the structure of the CGAN models
₁₇₅ needs to be changed to address this challenge. First, the we want the trained
₁₇₆ CGAN model to receive an input that represents a specific continuous input
₁₇₇ value. Additionally, it is convenient during the training process to assign
₁₇₈ discrete labels to the training data, but a method is needed to convert these
₁₇₉ labels to the actual values of the continuous input for the model.

₁₈₀ The new BC-CGAN model is shown in Figure 2. The difference in this
₁₈₁ model is the input to the generator, where the noise inputs are replaced with
₁₈₂ inputs defined specifically by labels, using a translator. A noise input is used
₁₈₃ in the previous CGAN models to generate a distribution of images within a
₁₈₄ category, for example different handwriting styles for a specific digit in [19].

185 In this work, we want to generate a specific output given a specific input,
 186 rather than some distribution of outputs for a given input. Thus, the noise
 187 aspect is removed, since a single output for each input is desired rather than
 188 a distribution of outputs for each input. It should be noted Zheng et al. [31]
 189 proposed an alternative CGAN approach considering continuous inputs with
 190 the noise aspect included to produce a distribution of outputs.

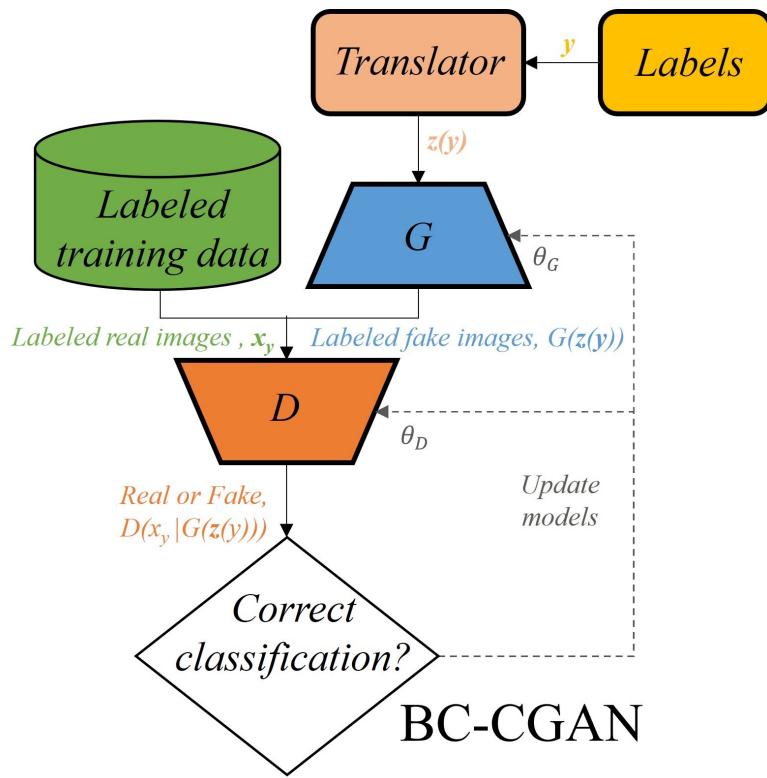


Figure 2: BC-CGAN training architecture.

191 The BC-CGAN model uses labels during the training process as a convenient

192 method for categorizing training data using an integer value. For generating
193 images after the model is trained, we want to provide the model specific input
194 parameter values directly instead of labels. The translator is thus needed
195 during the training process to convert the received integer label to a specific
196 input parameter value for the generator. This allows for: 1) the convenient
197 use of labels during the training process and 2) the ability for the generator
198 to learn to produce images based on an input parameter value, therefore
199 removing the need for labels and a translator after the model is trained.
200 Since the discriminator is only used during the training process, a simple
201 integer value label can be provided to the discriminator and a translator is
202 not needed to convert the label to its parameter value.

203 The goal of the translator is to map the received labels to the associated
204 input parameter values. Consider a scenario where the input boundary
205 condition for a given flow is a characteristic velocity U_0 . For this case, a
206 training label (y) is assigned to each training data image defined by their
207 different U_0 values. The purpose of the translator is then to map y to
208 its corresponding U_0 value. The function the translator uses to map these
209 values, $U_0(y)$, is dependent on the training data distribution. Assume a
210 uniformly distributed training dataset where each data point is chosen based

₂₁₁ on a change in U_0 of ΔU_0 , calculated as:

$$\Delta U_0 = (U_{0,\max} - U_{0,\min})/n_{\text{train}}, \quad (1)$$

₂₁₂ where $U_{0,\max}$ and $U_{0,\min}$ are the minimum and maximum U_0 values in the
₂₁₃ training dataset, respectively, and n_{train} is the total number of training
₂₁₄ data points in the dataset. The function for the translator to map y to
₂₁₅ a corresponding U_0 would then be:

$$U_0(y) = \Delta U_0 \cdot y + U_{0,\min}. \quad (2)$$

₂₁₆ Finally, interpolation is used so the input to the generator, $z(y)$, is a value
₂₁₇ between zero and one:

$$z(y) = [U_0(y) - U_{0,\min}]/[U_{0,\max} - U_{0,\min}], \quad (3)$$

₂₁₈ After training, images can be generated for a specific U_0 value by replacing
₂₁₉ $U_0(y)$ in Equation 3 with the desired U_0 value. allows for prediction of
₂₂₀ images using the continuous input value directly and without the need for
₂₂₁ a label or translator. Furthermore, the BC-CGAN model can be trained to
₂₂₂ make predictions considering multiple boundary conditions by using a vector
₂₂₃ containing multiple labels. The translator would then output a vector based

224 on the input label vector (i.e., $z(y)$). As a starting point, this paper considers
225 one varying input parameter for each case.

226 **3. Novel Feature-driven Algorithm for Generation of Training Data**

227 Although trained AI models can produce results quickly, generation of
228 training data for the AI models can be time consuming (e.g., by using CFD).

229 Using uniformly distributed inputs for training data generation is a simple
230 approach, but this may include more training data than an AI model actually
231 needs. For an indoor airflow prediction AI model, training data may be
232 generated by varying the supply airflow rate by a constant step of $\Delta \dot{m}$ in
233 each CFD simulation. This may pose a problem when the outputs vary
234 non-linearly with the inputs, for example if the airflow distribution varies
235 non-linearly with the supply airflow rate. If the resolution of generated
236 training data is not sufficiently high, a uniformly distributed training dataset
237 may exclude crucial points in regions where the gradient of the outputs with
238 respect to the inputs ($\partial_x f$) is high. This may exclude crucial data points
239 that capture the non-linear trends between inputs and outputs. On the other
240 hand, in regions where $\partial_x f$ is low, a high resolution of generated training
241 data may result in many redundant data points and excessive time required

242 to produce the training data. When generation of training data is costly,
243 a non-uniformly distributed training dataset can be beneficial for training
244 AI models, since redundant training data points can be avoided while still
245 including sufficient training data for the AI models.

246 To address this problem, we propose a novel feature-driven algorithm to
247 create non-uniformly distributed training datasets that minimize the amount
248 of generated training data for AI models. The algorithm strategically selects
249 training data points based on significant changes in the outputs with respect
250 to the inputs. In its strategic selection, the algorithm includes more data
251 points in regions where $\nabla_x f$ is high and excludes redundant data points in
252 regions where $\nabla_x f$ is low. The feature-driven algorithm can be used for
253 multiple inputs (e.g., multiple varying boundary conditions). However, we
254 focus on a single varying input parameter in this paper and explain the
255 algorithm in detail assuming one varying input.

256 The feature-driven algorithm flowchart is detailed in Figure 3. First,
257 initial grid points for the training dataset are included to provide a few
258 baseline points, as well as to create a defined range for the training data. The
259 grid points for the training data are defined by their different values of inputs,
260 represented by x . The algorithm begins by computing the changes in critical

261 outputs between neighboring grid points, for example between x_1 and x_2 . For
262 each pair of neighboring grid points, if the change in critical outputs (e.g.,
263 $|f(x_2) - f(x_1)|$) is greater than the defined threshold, ϵ , a new grid point is
264 added between those two points (e.g., at $(x_2+x_1)/2$). In this case, a new CFD
265 simulation is performed based on the input parameter defined by the new grid
266 point, and the simulation output is added to the training data. The results
267 from comparing neighboring grid points are cached to avoid performing the
268 same comparison redundantly during the process. If the change in critical
269 outputs does not exceed ϵ , then no new grid point is added between those
270 two points and a CFD simulation is not performed. After completing this
271 for each pair of neighboring grid points, the algorithm checks if any new
272 grid points were added in the most recent iteration. If no new points were
273 added, then the process ends since further iterations will not add any new
274 grid points. If there were new grid points added in the most recent iteration,
275 then the algorithm checks if a maximum resolution has been reached. The
276 initial resolution is the difference between values of the initial neighboring
277 grid points, e.g., $x_2 - x_1$. A defined maximum resolution can be useful to
278 prevent excessive training data from being generated with neighboring inputs
279 very close together. The process ends if the maximum resolution has been

280 reached. If the maximum resolution has not been reached, then the resolution
281 increases by a factor of two (e.g., $(x_2 - x_1)/2$). After increasing the resolution,
282 the set of grid points are reset with the newly added grid points. The process
283 repeats by computing the change in critical outputs between neighboring grid
284 points, now with the newly added grid points. The process ends once either
285 no new grid points are added in an iteration or once the maximum resolution
286 is reached.

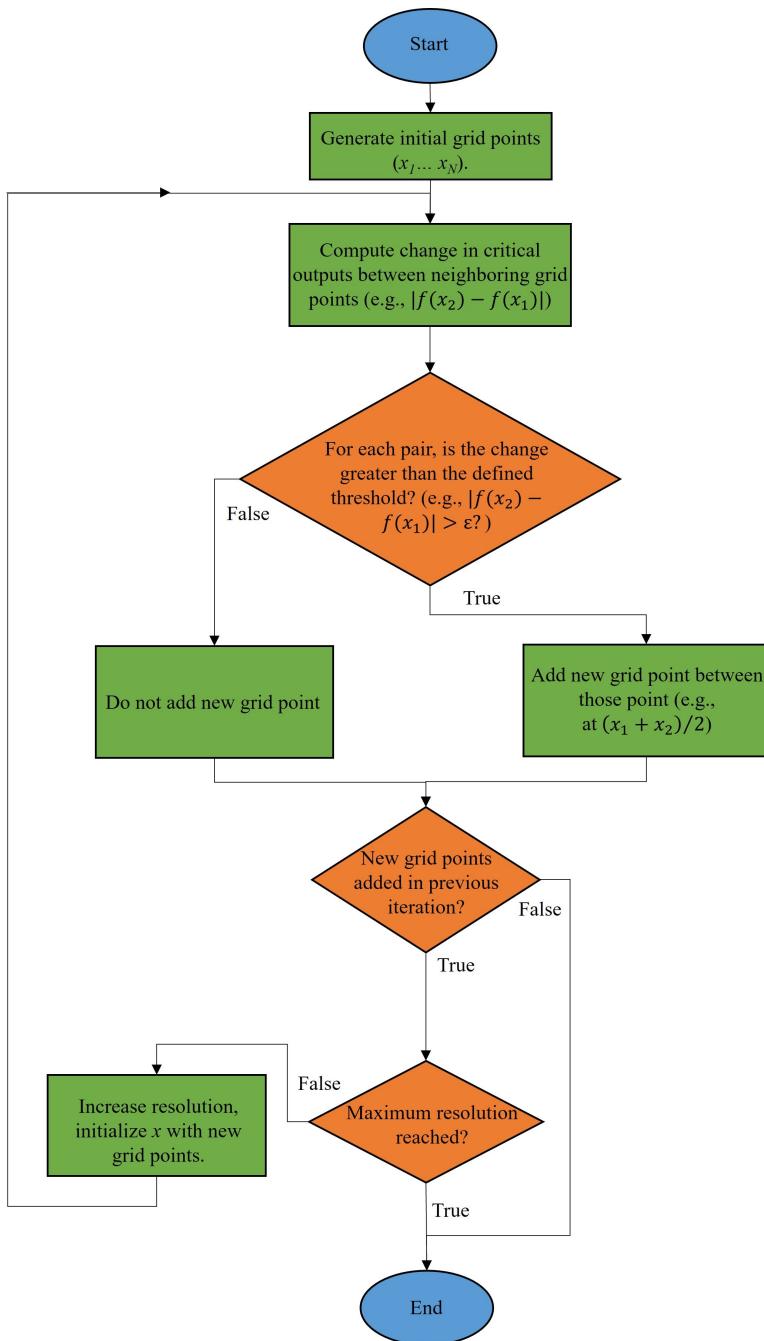


Figure 3: Flowchart of the feature-driven algorithm.

287 4. Description of Workflow

288 The description of the entire workflow including generation of training
289 data, model training process, and model evaluation is shown in Figure 4 and
290 described in this section.

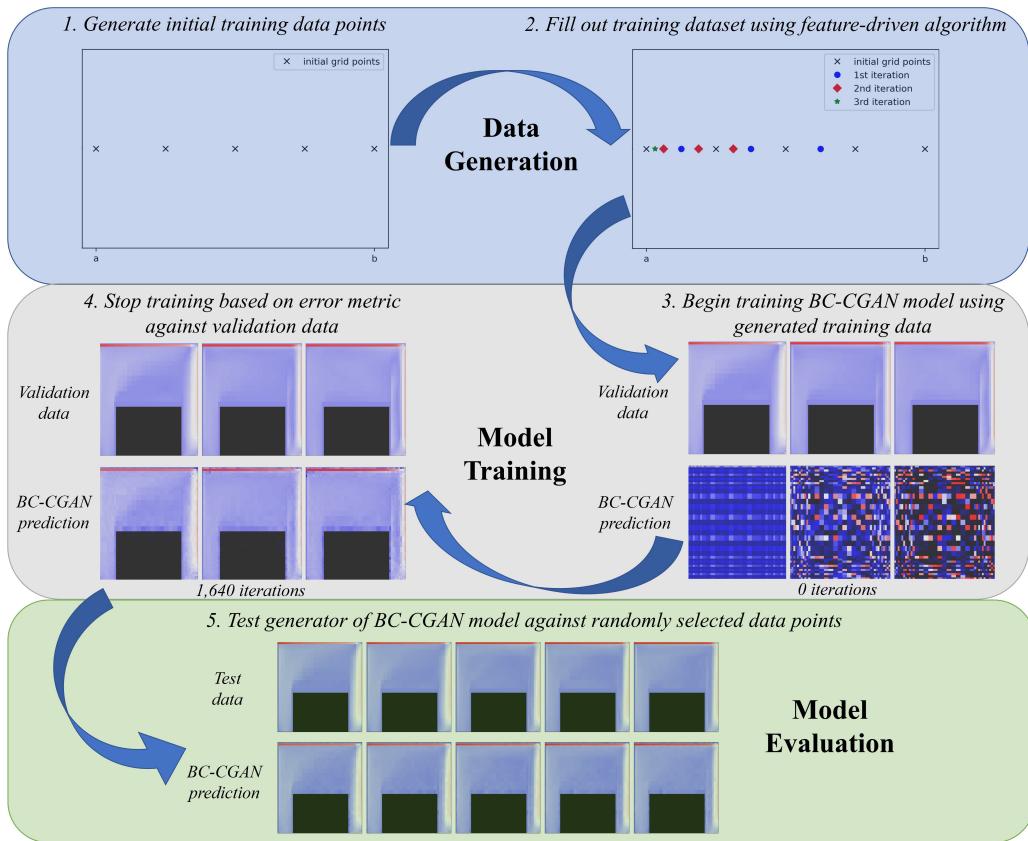


Figure 4: Description of entire workflow including generation of training data, model training, and model evaluation.

291 The workflow begins with the data generation process. Initial training

292 data points are first generated to provide baseline points for the feature-driven
293 algorithm and to define a range for the training data. In this case, a few
294 CFD simulations are performed to generate these initial points. Using too
295 many initial points can potentially include redundant training data, so fewer
296 initial points should be used to allow the algorithm to determine what data is
297 necessary to be included. For the cases studied in this paper, we find that, for
298 a given ϵ , the feature-driven algorithm only becomes sensitive to the initial
299 data points when a large amount of initial data is included. This is because
300 using a large amount of initial data may include redundant data points that
301 the algorithm would not include. Using fewer initial data points often results
302 in very similar training data sets, because the algorithm is designed to find
303 the necessary data points within the input range, which are similar regardless
304 of the initial data points. Thus, we use only about ten initial data points for
305 the cases in this paper, which uniformly span the range of the studied input
306 parameters.

307 Next, the feature-driven algorithm is used to select what input parameter
308 values should be used for the additional CFD simulations to generate the rest
309 of the training data. In this paper, a few training datasets are generated with
310 different settings of the feature-driven algorithm for each case. Additionally,

311 uniformly distributed training datasets are generated for comparison against
312 the training datasets produced by the feature-driven algorithm. BC-CGAN
313 models are then trained using the different training datasets, where the
314 initial settings of each BC-CGAN model are identical. We then compare the
315 training speed and prediction performance for the BC-CGAN models trained
316 by the different datasets. Since the training process is inherently stochastic,
317 we train ten BC-CGAN models for each training dataset to understand their
318 training and prediction performance over several runs.

319 To train the BC-CGAN models, one unique label is assigned to each
320 training data image within its dataset. Additionally, a few reference data
321 points are generated using CFD simulations for validation of the BC-CGAN
322 models during training. Periodically during the training process, the BC-CGAN
323 model produces flow distribution outputs based on the validation data input
324 values. Its outputs are then compared against the validation data points
325 and a relative error metric is computed for each output. The error metric
326 is calculated based on error between the flow outputs (e.g., velocity and/or
327 temperature) at each point in the flow. If the error metric between the
328 BC-CGAN prediction and validation data is below a defined threshold for all
329 the validation data points, then the model is considered to be sufficiently

330 trained and the training stops. Otherwise, training continues until this
331 criteria is satisfied. In this paper, we save the trained BC-CGAN models
332 at different error metric thresholds to compare the tradeoff between training
333 speed and prediction performance for different error thresholds.

334 Finally, the trained BC-CGAN models are evaluated against test data
335 points that were not selected from the training or validation data. The test
336 data is selected by using a bin sampling technique to produce ten random
337 input values that span the defined input range. CFD simulations are then
338 performed to generate the test data based on the ten input values. The
339 BC-CGAN models are evaluated by generating their flow distribution outputs
340 based on the test input values and computing their relative error against
341 the test data. The BC-CGAN models are trained to predict 2D airflow
342 distribution in this paper, but can be extended for 3D airflow prediction in
343 future research.

344 5. Isothermal Case: Lid-driven Cavity Flow

345 The first case studied in this paper is an isothermal lid-driven cavity
346 flow. We begin with a description of the setup for this flow case. Next, we
347 show the settings used for the BC-CGAN model and the generated training

348 datasets for the BC-CGAN models in this case. Finally, the training and
349 evaluation results for the BC-CGAN models trained by the different datasets
350 are detailed.

351 5.1. Case Description

352 The setup of the isothermal lid-driven cavity flow case is shown in Figure
353 5. This is a meaningful case because, despite having a simple configuration,
354 the flow pattern changes significantly depending on the initial conditions
355 and boundary conditions. Because of this, it is a benchmark flow case that is
356 frequently studied in the literature using both physical experiments [32, 33]
357 and numerical simulations [34, 35, 36, 37]. This flow is contained in a box of
358 length L on all sides. The left, right, and bottom walls are stationary, while
359 the lid moves at a constant velocity of U_0 to the right. The motion of the lid
360 causes a circulation pattern of the flow within the box. The flow is modeled
361 as 2D, steady, incompressible, and isothermal in this study.

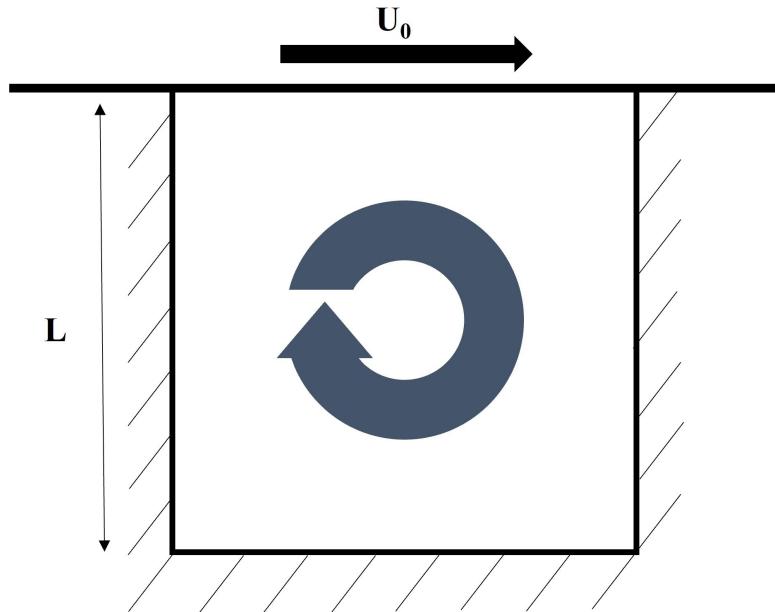


Figure 5: Diagram of the lid-driven cavity flow.

362 The lid-driven cavity flow is often defined by its Reynolds number (Re)
 363 in the literature [38, 39], which characterizes the ratio of inertial to viscous
 364 forces in the flow. Thus, we use Re as the input parameter for the flow in
 365 this study. For this case, Re is calculated as:

$$Re = U_0 L / \nu, \quad (4)$$

366 where U_0 is the constant velocity of the lid, L is the length of each side of
 367 the box, and ν is the kinematic viscosity of the flow.

368 We define the range of Re values to be from 100 to 10,000. We hold U_0

369 and L constant while changing v to vary the Reynolds number for the CFD
370 simulations in this paper. All the other simulations settings and boundary
371 conditions remain the same for each simulation, so the BC-CGAN models
372 only receive Re as an input. The flow output we study for this case is the
373 steady-state distribution of velocity magnitude. This means the training data
374 produced by CFD simulations is comprised of velocity magnitude distribution
375 data based on the input Re . The BC-CGAN models are then trained to
376 output the velocity magnitude distribution based on the input Re . The
377 CFD simulations used to generate the training, validation, and test data
378 for this case are performed using the Fast Fluid Dynamics method [11, 12]
379 on an AMD RadeonTM Pro WX 7100 GPU. The CFD simulations use a
380 64×64 non-uniform, structured grid, which is translated to a 36×36
381 uniform structured grid for the model training and evaluation to simplify
382 the predictions while providing sufficient resolution of the flow data. This
383 prediction resolution was selected to balance the tradeoff of training time and
384 resolution. The BC-CGAN model can be trained to predict a more resolved
385 flow output, but this may increase the training time and require re-tuning of
386 the model hyperparameters.

387 5.2. BC-CGAN Model Settings

388 The BC-CGAN model settings including neural network architectures and
389 hyperparameters are described in this section. First, the architectures of the
390 generator and discriminator are shown in Table 1 and Table 2, respectively.
391 The generator uses a deconvolutional neural network [40] and the discriminator
392 uses a convolutional neural network [41]. The generator receives an input
393 defined by Re (which is the only varying parameter), as described in Section
394 2.2, and outputs a 36×36 image representing the velocity magnitude distribution.
395 The discriminator receives a 36×36 image input as well as a label input
396 corresponding to a Re value. The label input uses one-hot encoding to give
397 the label of the image within the training dataset, with total number of
398 training data points of n_{train} . The discriminator produces an output of zero
399 or one, where zero corresponds to a classification of a “fake” image produced
400 by the generator and one corresponds to a classification of a “real” image
401 from the training dataset. The number of convolutional/deconvolutional
402 layers and filter sizes for these layers impact the training performance of
403 the generator and discriminator. For example, reducing the number of
404 layers in these neural networks can speed up each training step, but can
405 also negatively affect the training performance and result in more overall

406 iterations to successfully train the models. We selected these architectures
407 for the generator and discriminator to have reasonable training speed and
408 consistent convergence of the models.

Table 1: Summary of generator architecture.

Layer	Shape	Activation function
Input	200	N/A
Reshape	$9 \times 9 \times 128$	N/A
Deconvolution	$18 \times 18 \times 128$	ReLU
Deconvolution	$36 \times 36 \times 64$	ReLU
Deconvolution	$36 \times 36 \times 32$	ReLU
Deconvolution (output)	$36 \times 36 \times 1$	Sigmoid

Table 2: Summary of discriminator architecture.

Layer	Shape	Activation function
Label input	n_{train}	N/A
Image input	$36 \times 36 \times 1$	N/A
Reshape	$36 \times 36 \times 2$	N/A
Convolution	$18 \times 18 \times 32$	LeakyReLU
Convolution	$9 \times 9 \times 64$	LeakyReLU
Convolution	$5 \times 5 \times 128$	LeakyReLU
Convolution	$5 \times 5 \times 256$	LeakyReLU
Flatten	6400	N/A
Output	1	Sigmoid

⁴⁰⁹ The hyperparameters for the BC-CGAN models were tuned carefully for
⁴¹⁰ this case. Certain hyperparameters, such as the learning rate, can significantly
⁴¹¹ impact model training time and convergence or lead to overfitting [42]. For
⁴¹² this case we used the Adam optimizer [43] with learning rate of 0.0002 and
⁴¹³ decay rate of 0.5. A batch size of 32 was used for training the models as well.

414 5.3. Training Datasets

415 Four training datasets are generated using the novel feature-driven algorithm
416 and are compared against four uniformly generated datasets. A summary of
417 all the training datasets is included in Table 3. The uniformly distributed
418 datasets are defined by their uniform step (ΔRe), which describes the difference
419 in Re for which training data is generated. These datasets include training
420 data points from $Re = 100$ up to $Re = 10,000$ by step of ΔRe . Thus,
421 a higher ΔRe results in fewer training data points that are further apart
422 within the defined Re range, while a lower ΔRe results in more training
423 data. The selected values of ΔRe are chosen to be factors of the input Re
424 range, which is 9,900 in this case, as well as to include similar n_{train} values
425 as the non-uniform datasets.

426 The non-uniform datasets are defined by their ϵ threshold, which is the
427 threshold to decide whether a training data point is needed based on the
428 change in outputs between neighboring data points, as described in Section
429 3. In this case, ϵ is dimensionless and is described by the change in velocity
430 magnitude ($\Delta|U|$) at any of the critical output locations between neighboring
431 Re data points, normalized by the velocity of the moving lid (U_0). A lower
432 ϵ results in higher n_{train} , since it defines a smaller change in outputs to

433 determine that additional training data points are needed. The ϵ values in
434 this case were chosen to provide datasets with a wide range of data points and
435 study the impact of training data size on the model training and evaluation.

436 The locations of the critical outputs used for the feature-driven algorithm in
437 this case are the center points of each cell when dividing the flow domain into
438 a 4×4 grid, resulting in 16 locations. These locations were chosen to include
439 a range of possible locations where the flow can change, but the critical
440 locations can be narrowed based on the studied flow in future research.

Table 3: Summary of training datasets.

Uniform/	Uniform	step	ϵ threshold	n_{train}
Non-uniform	$(\Delta \text{ Re})$	$(\Delta U /U_0)$		
Uniform	25		N/A	397
Uniform	50		N/A	199
Uniform	100		N/A	100
Uniform	275		N/A	37
Non-uniform	N/A		0.001	378
Non-uniform	N/A		0.005	120
Non-uniform	N/A		0.01	67
Non-uniform	N/A		0.05	19

⁴⁴¹ Histograms of the non-uniform training datasets are shown in Figure 6.
⁴⁴² The results show a clear trend: the lid-driven cavity flow changes more
⁴⁴³ significantly at lower Re values, especially between 100 and 1,000. The
⁴⁴⁴ $\epsilon = 0.05$ dataset includes less than 5% of the training data points compared
⁴⁴⁵ to the $\epsilon = 0.001$ dataset, but still includes more of its training data between
⁴⁴⁶ Re values of 100 and 1,000. This is unsurprising as the lid-driven cavity flow

⁴⁴⁷ transitions from laminar to turbulent in this region of Re. In particular,
⁴⁴⁸ the boundary layer near the lid and circulation pattern along the right wall
⁴⁴⁹ change more significantly in this region of Re.

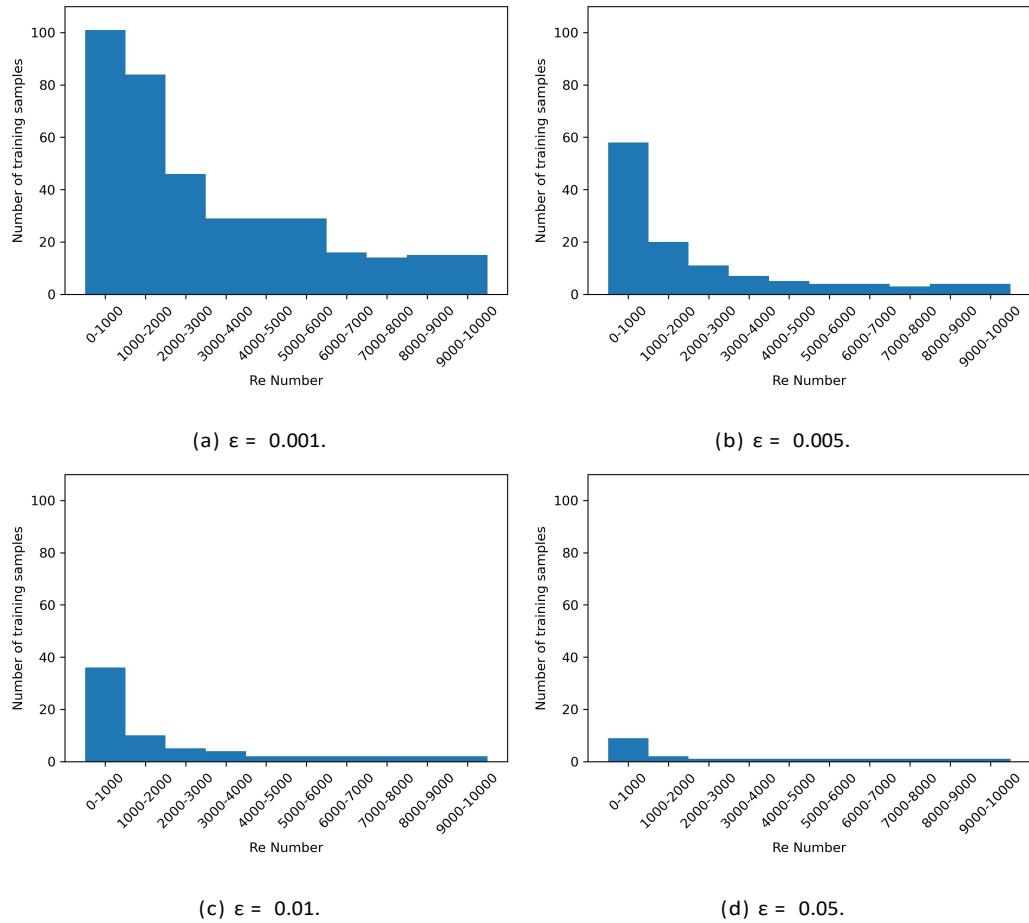


Figure 6: Histograms of training datasets generated using the feature-driven algorithm with different ϵ thresholds.

450 5.4. Training Results

451 We select five data points as validation data for this case using Re values
452 of 100, 500, 1,000, 5,000, and 10,000. These points span the range of
453 Re for this study, as well as include more points in the lower Re regime,
454 since we found this is the regime where the flow changes more significantly.
455 Sample validation results of the BC-CGAN model are shown in Figure 7.
456 The top row shows the validation data from the CFD simulations, while the
457 remaining rows show the BC-CGAN predictions at different error thresholds.
458 For example, the BC-CGAN prediction results at the 40% error threshold
459 are the saved validation results from when the BC-CGAN predictions were
460 first below the error metric of 40% for all five validation data points. The
461 error metric in this case is computed by weighting two error calculations:
462 55% root mean squared error (RMSE) and 45% maximum error. Rather
463 than simply using RMSE, we include maximum error in this case to prevent
464 points of large error in the predictions. The errors are also both normalized
465 by U_0 . The RMSE is calculated by considering the mean squared normalized
466 error in velocity magnitudes at each location in the 36×36 2D flow domain.
467 The maximum error is then the highest normalized error within the 36×36
468 domain. Initially during the training process, we saved the validation results

469 for different error metric thresholds of 5%, 10%, 15%, 25%, and 40%. Based
470 on the qualitative results, we can see the BC-CGAN prediction at an error
471 metric of 40% does not match well with the validation data. However, the
472 BC-CGAN prediction seems to capture the trends of the validation data for
473 error metrics of 15% and below. Consequently, for the remainder of this
474 paper we save the trained BC-CGAN model and their validation results for
475 error metric values of 5%, 10%, and 15%.

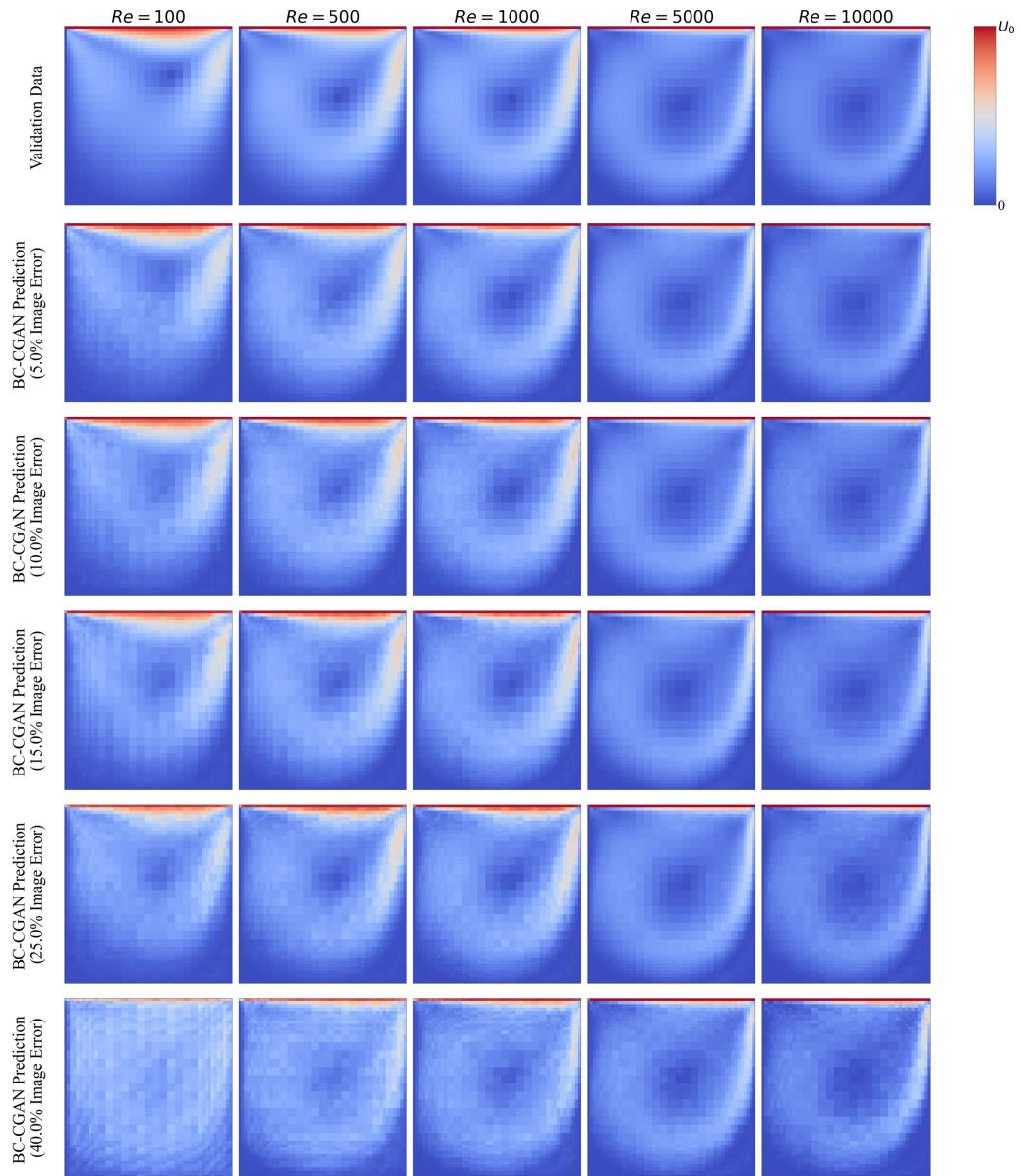


Figure 7: Sample validation results of the BC-CGAN prediction for different error metric thresholds.

476 The training results of the BC-CGAN models with different training

477 datasets and at different error metrics are shown in Figure 8. The training
478 process is performed ten times for each training dataset since the training
479 process is inherently stochastic. During each training process, the model
480 is saved once the validation results satisfy error metric thresholds of 5%,
481 10%, and 15%. The number of training iterations or “epochs” required to
482 achieve these error thresholds is also recorded and plotted (on a log-scale) in
483 Figure 8. Each box plot shows the range of the number of epochs required
484 to satisfy the different error metric thresholds over the ten runs for each
485 training dataset. The training datasets are differentiated by the number of
486 training data points included in each dataset, as well as whether they are
487 non-uniformly or uniformly generated sets.

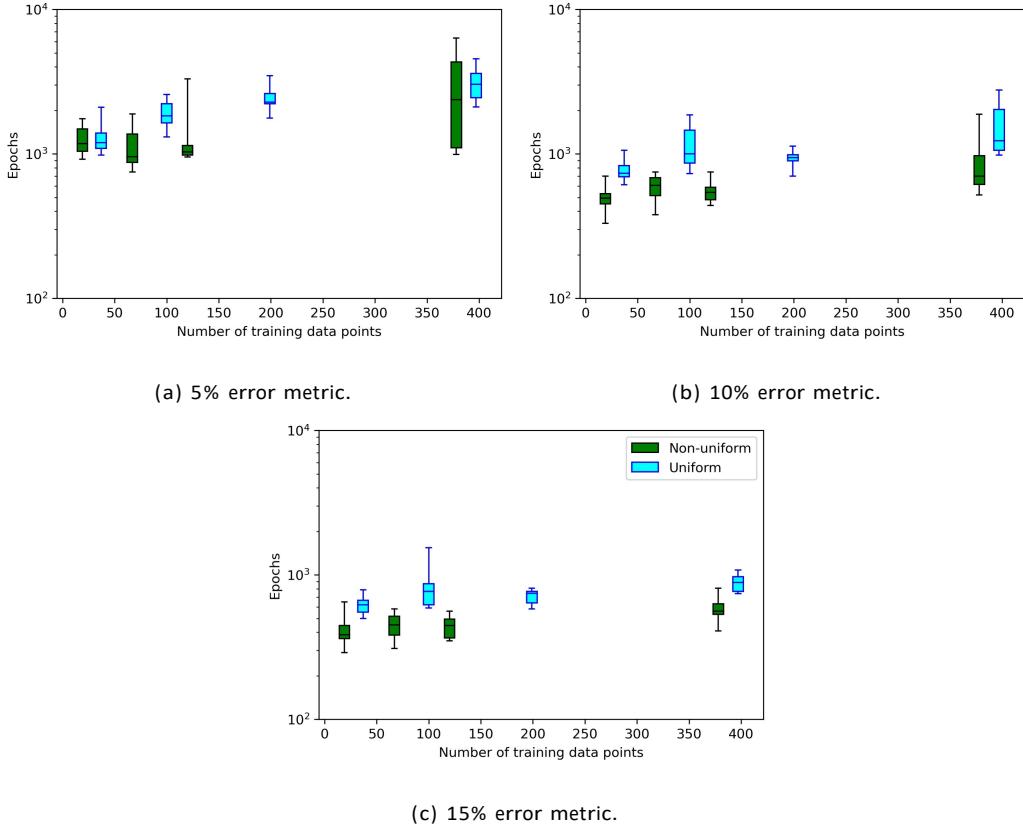


Figure 8: Box plots of the number of epochs required to train the BC-CGAN model for different training datasets and error metrics.

488 First, we see less epochs are required to train the models when the error
 489 metric is higher. This is because less training is required for a looser error
 490 threshold compared to a stricter one. We also see that the non-uniform
 491 training datasets often require less epochs, especially for the error thresholds
 492 of 10% and 15%. This can occur because the non-uniform datasets are more

493 capable of capturing the non-linear trends between the input Re and output
494 velocity distribution. For the 5% error metric, the non-uniform training
495 dataset with 378 training data points required a wide range of epochs to
496 converge. A wider range of epochs for model convergence often occurs for the
497 lower error metrics, because there is more variability of when the model is able
498 to satisfy the convergence criteria for stricter error metrics. This seems more
499 apparent for the non-uniform training datasets, especially the dataset with
500 378 data points. We found that the model often converged after around 1,000
501 epochs using this dataset, but when it took more epochs to converge it was
502 usually because of higher error for the validation data point of $Re = 10,000$.
503 The non-uniform datasets included less training data around this input value
504 since the flow changes less significantly in this range. This seems to have a
505 negative impact for a few training runs, especially when overfitting occurs
506 based on more data included in Re regions where the flow outputs change
507 more significantly. Finally, it seems that using less training data points
508 often leads to fewer epochs required to train the models, especially for the
509 uniform datasets. This can be a result of overfitting of the models when too
510 much training data is included. For the non-uniform datasets, decreasing
511 the amount of training data when there is less than about 150 data points

512 does not always reduce the number of epochs required to train the models.
513 There may be an optimal amount of training data points for the non-uniform
514 datasets around 50-150 data points.

515 **5.5. Evaluation Results**

516 Example evaluation results of the BC-CGAN model for the randomly
517 selected test data points are shown in Figure 9. The BC-CGAN predictions
518 match well with the test data based on a qualitative comparison, even at
519 higher error metrics. The BC-CGAN predictions also capture the change in
520 the lid-driven cavity flow pattern over the wide range of Re.

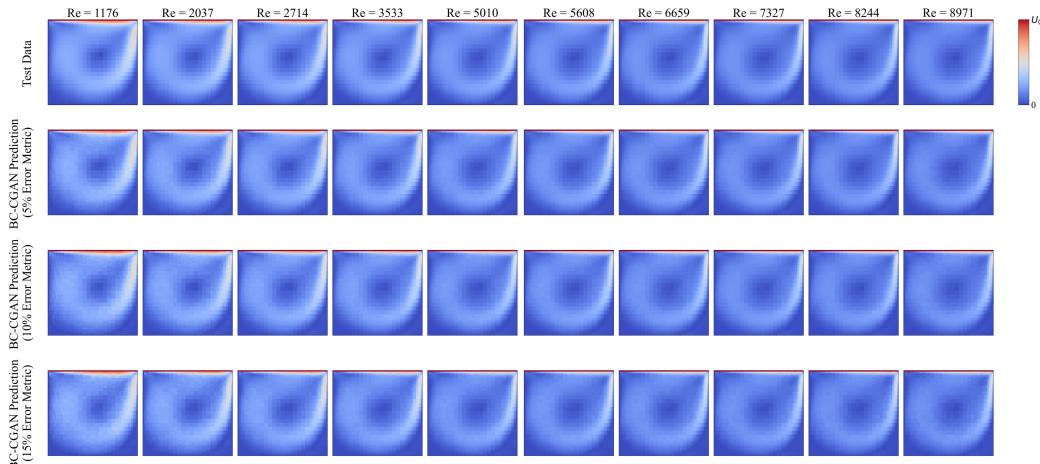


Figure 9: Example evaluation results for the trained BC-CGAN model with different error metrics.

521 A comprehensive quantitative evaluation for the BC-CGAN models trained

522 with different datasets and at different error metric thresholds is shown in
523 Figure 10. The box plots show the range of calculated RMSE (normalized by
524 U_0) for the trained BC-CGAN models against the test data. Similar to Figure
525 8, the BC-CGAN models trained by the different datasets are differentiated
526 by the number of training data points and whether they are non-uniform or
527 uniform datasets. The defined training error metric threshold is also included
528 in each plot for comparison.

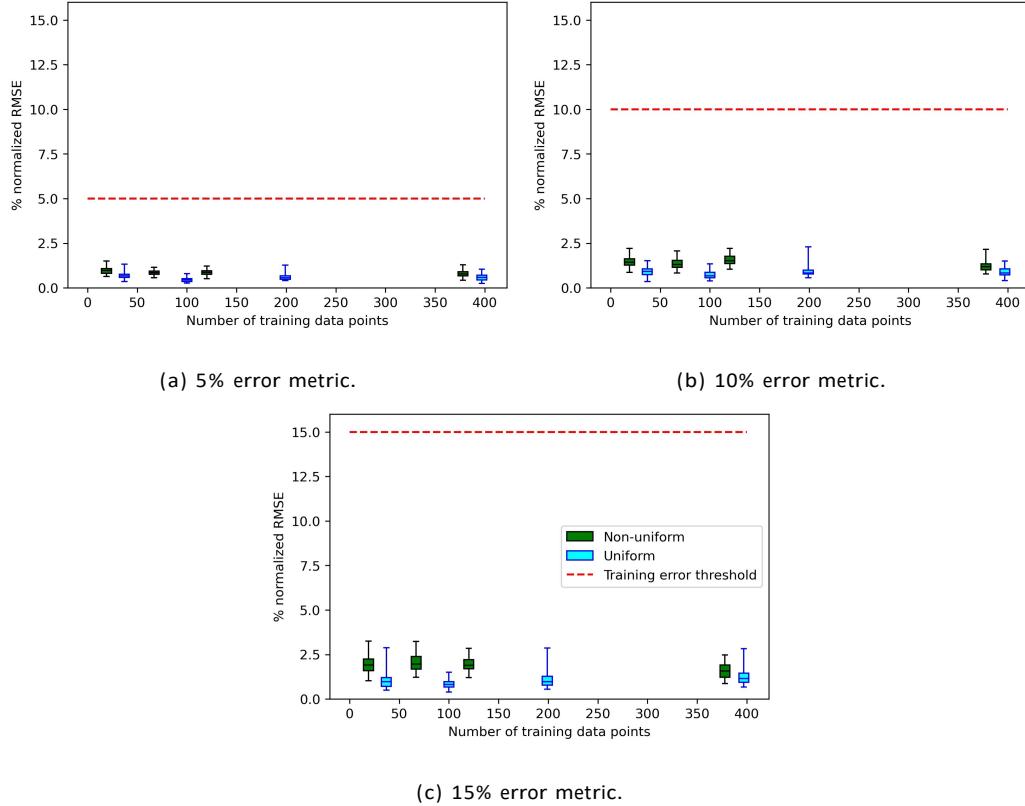


Figure 10: Box plots of the % normalized RMSE of the test predictions for the BC-CGAN models trained by different datasets and error metrics.

529 First, the prediction error is higher when the training error metric threshold
 530 is higher. However, even for the error metric of 15%, the prediction error
 531 is almost always lower than 5%. This is because the error metric in the
 532 training process is only satisfied once all the validation data points are below
 533 the metric, so it is possible one validation data point had much higher error

534 compared to others. Furthermore, the error metric used to train the models
535 included a combination of max error and RMSE to ensure predictions without
536 points of very high error. Since the evaluation results are shown in terms of
537 just RMSE for an easier understanding of the results, the prediction error is
538 much lower than the training error metric. Finally, we see the BC-CGAN
539 models trained by the uniform dataset often had lower prediction error
540 compared to those trained by the non-uniform datasets. This may occur
541 because the BC-CGAN models trained by the non-uniform datasets required
542 less training epochs to satisfy the error metric criteria. Thus, while their
543 predictions for the validation data may be similar to those of the models
544 trained by the uniform datasets, they seem to perform slightly worse against
545 the test data, perhaps due to less overall training. We also find that the
546 test error for the models trained by the non-uniform datasets tended to be
547 higher for the larger Re test values, which is the region of Re where the
548 non-uniform datasets included less data. Conversely, the models trained by
549 the uniform datasets often had higher error for the smaller Re test values,
550 which is the region of Re where the flow changes more non-linearly. However,
551 the prediction error is still well below the threshold for all the BC-CGAN
552 models. Additionally, the difference in error for the models trained by the

553 different datasets is almost negligible, especially for the stricter training error
554 metric thresholds. This is reasonable because the validation process to stop
555 the training of the models is the same regardless of the dataset. So while
556 the models trained by the different datasets may take different paths in their
557 training processes, the final trained models should be similar in performance.

558 Once trained, the BC-CGAN models can generate predictions with an
559 average speed of 7 ms per prediction. For this case, a CFD simulation took
560 an average of 56 s, which means the trained BC-CGAN prediction was on
561 average about 7,900 times faster than a CFD simulation. However, the time
562 to generate data and train the BC-CGAN models must be considered as
563 well. For all the training datasets considered in this case, it took an average
564 of 11.4 minutes to train the models to satisfy the 5% error metric. We found
565 that using less training data could often improve the training speed of the
566 models while maintaining sufficient accuracy, and the smallest tested training
567 dataset required about 17.7 minutes to generate the training data. If only a
568 few predictions are needed, then it would be faster to use CFD simulations
569 because of the time required to generate data and train the BC-CGAN
570 model. On the other hand, the time savings when using the BC-CGAN model
571 increases as the number of required predictions increases. After accounting

572 for the time to generate data and train the BC-CGAN model, it becomes
573 beneficial to use the BC-CGAN model over CFD simulations when more
574 than 31 predictions are required for this case.

575 6. Non-isothermal Case: Mixed Convection Flow with Heated Box

576 The next case we study is a mixed convection flow with heated box. This
577 case is chosen as a more complex flow compared to the lid-driven cavity flow,
578 since it is non-isothermal, 3D, and includes an obstacle in the flow. It has also
579 been used for indoor airflow simulation studies in the literature [44, 45]. We
580 first describe the case setup, then summarize the BC-CGAN model settings
581 and generated training datasets. Finally, the training and evaluation results
582 are detailed.

583 6.1. Case Description

584 The setup of this case is shown in Figure 11. The flow is contained in
585 a room with length of L in all dimensions. A heated box is in the center
586 of the room, with dimensions of $L/2$ in all dimensions. The box generates
587 heat with a uniform flux of Q_{box} . This is meant to represent an internal heat
588 load within a room, for example occupants. Cold air is supplied to the room
589 through the inlet along the top of the left wall with a velocity of U_{in} and

590 temperature of T_{in} . An outlet is located along the bottom of the right wall.

591 The ceiling, floor, and remaining walls have temperatures of T_{cei} , T_{flo} , and

592 T_{oth} , respectively. The flow is modeled as steady and incompressible in this

593 study.

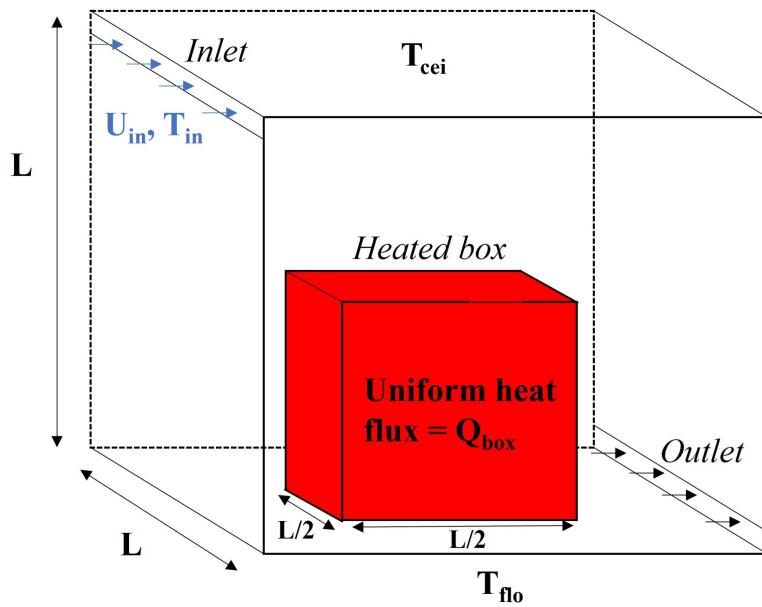


Figure 11: Diagram of the mixed convection flow with heated box case.

594 We select Q_{box} to be the input parameter for this case and vary this value

595 from 0 W/m^2 to 50 W/m^2 . Furthermore, we add noise to the boundary

596 conditions of U_{in} , T_{in} , T_{cei} , T_{flo} , and T_{oth} for all the CFD simulations used

597 to generate training, validation, and test data. Noise is added to U_{in} by

598 randomly increasing or decreasing this value by up to $\pm 5\%$ of its default

599 value of 1.36 m/s for each simulation. Similarly, the temperature boundary
600 conditions are randomly increased or decreased by up to \pm 0.5 $^{\circ}$ C of their
601 default values. The default values for T_{in} , T_{cei} , T_{flo} , and T_{oth} are 22.2 $^{\circ}$ C,
602 25.8 $^{\circ}$ C, 26.9 $^{\circ}$ C, and 27.4 $^{\circ}$ C. This added noise can represent uncertainty in
603 experimental conditions, for example. It also adds a potential challenge for
604 the BC-CGAN model, since the model is only given the value of Q_{box} as an
605 input. Since the BC-CGAN models assume the other boundary conditions
606 are unchanged, their values (including the added noise) are not given as an
607 input. Similarly, since the geometry (including locations of the box, inlet,
608 and outlet), is unchanged, these are not given as an input. Future research
609 can extend the BC-CGAN model to consider multiple varying boundary
610 conditions for this case. The CFD simulations use a $44 \times 44 \times 44$ non-uniform
611 grid, similar to in [44]. For this case, the BC-CGAN model outputs the 2D
612 airflow distribution at the mid-plane of the flow. It outputs both the velocity
613 and temperature distribution, since it is a non-isothermal flow. Thus, the
614 CFD data is translated to provide a 36×36 uniform grid of velocity and
615 temperature data at the mid-plane of the flow. The model also must generate
616 the box within the surrounding flow. This can be useful for when AI models
617 are needed to detect obstacles in the flow.

618 6.2. BC-CGAN Model Settings

619 The architectures for the generator and discriminator are shown in Table
620 4 and Table 5, respectively. While they are mostly similar to the architectures
621 used in the previous case described in Section 5.2, there are a few key
622 differences. First, the generator produces a 72×36 output and the discriminator
623 receives 72×36 image inputs. This is because the flow outputs in this
624 study are the 36×36 distribution of both velocity and temperature. The
625 other key difference is the output layer of the generator uses the Tanh
626 activation function rather than Sigmoid. The activation function in the
627 output layer outputs the value of velocity or temperature in the flow based
628 on the information received at that node within the layer. In the training
629 data for this case, a value of -1 is assigned to the points where the box
630 is located to differentiate it from the fluid flow (represented by normalized
631 velocity/temperature values from 0 to 1). Thus, the Tanh activation function
632 is chosen for the generator in this case, because it can output values from -1
633 to 1 while the Sigmoid activation function only outputs values from 0 to 1.
634 For this case, we used the Adam optimizer with learning rate of 0.0001 and
635 decay rate of 0.25, as well as a batch size of 32 for training the models.

Table 4: Summary of generator architecture.

Layer	Shape	Activation function
Input	200	N/A
Reshape	$18 \times 9 \times 128$	N/A
Deconvolution	$36 \times 18 \times 128$	ReLU
Deconvolution	$72 \times 36 \times 64$	ReLU
Deconvolution	$72 \times 36 \times 32$	ReLU
Deconvolution (output)	$72 \times 36 \times 1$	Tanh

Table 5: Summary of discriminator architecture.

Layer	Shape	Activation function
Label input	n_{train}	N/A
Image input	$72 \times 36 \times 1$	N/A
Reshape	$72 \times 36 \times 2$	N/A
Convolution	$36 \times 18 \times 32$	LeakyReLU
Convolution	$18 \times 9 \times 64$	LeakyReLU
Convolution	$9 \times 5 \times 128$	LeakyReLU
Convolution	$9 \times 5 \times 256$	LeakyReLU
Flatten	11520	N/A
Output	1	Sigmoid

636 6.3. Training Datasets

637 Two training datasets are generated using the feature-driven algorithm
 638 and are compared against three uniformly generated datasets, summarized
 639 in Table 6. The thresholds for the non-uniform datasets are dimensionless
 640 values of 0.05 and 0.10 and are chosen to provide two different sizes for the
 641 non-uniform datasets. These thresholds correspond to a relative change in

either velocity magnitude or temperature. If this threshold is exceeded for significant changes in either velocity or temperature at any of the critical output locations, a new point is added. The change in velocity magnitude is normalized by the maximum velocity for the case, which is the inlet velocity (U_{in}). The change in temperature is normalized by the difference between the maximum and minimum temperatures for the entire case ($T_{max} - T_{min}$), where T_{max} comes from the highest Q_{box} scenario and T_{min} is the cold inlet air temperature. The locations of the critical outputs are the center points of the cells when dividing the flow into a 5×5 grid, resulting in 25 locations.

Uniform steps of 0.5, 2, and 25 W/m^2 are chosen to produce three uniform datasets with very different amounts of training data. In the previous case in Section 5, we found that using less training data often reduced the number of epochs required to train the models. Thus, we include the training dataset with uniform step of 25 W/m^2 to observe the impact of using very few training data points on the training and prediction performance of the BC-CGAN models. Furthermore, the training data points in this dataset are identical to the validation data points for this case. This was done intentionally to observe the impact on the performance of the BC-CGAN models when the training data is more biased towards the validation data.

Table 6: Summary of training datasets.

Uniform/	Uniform	step	ϵ threshold	Total	number	of
Non-uniform	$(\Delta W/m^2)$			training data points		
Uniform	0.5		N/A	101		
Uniform	2		N/A	26		
Uniform	25		N/A	3		
Non-uniform	N/A		0.05	40		
Non-uniform	N/A		0.10	14		

661 Histograms of the two non-uniform training datasets generated by the
 662 feature-driven algorithm are shown in Figure 12. Unlike the lid-driven cavity
 663 case, there is not a clear trend in the non-linearity between the inputs and
 664 outputs. It seems that there are more changes in the flow between Q_{box}
 665 values of 25-40, as shown in Figure 12a. In this region, the flow pattern
 666 in the room transitions from being dominated by the cold supply airflow to
 667 being significantly impacted by the thermal plume from the heated box. We
 668 see more noticeable changes in the boundary layers around the box because
 669 of this effect in this region. However, these changes do not seem to be very

670 large, as shown by the more uniform training dataset in Figure 12b with the
 671 looser ϵ threshold.

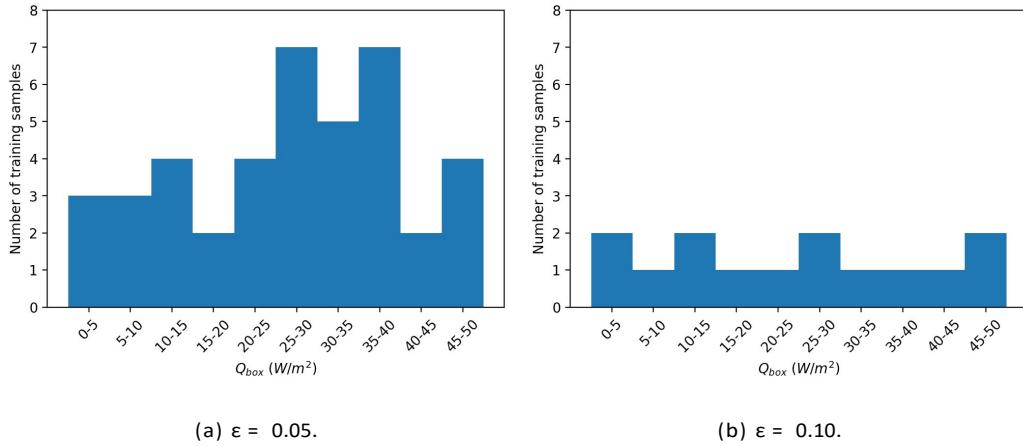


Figure 12: Histograms of training datasets generated using the feature-driven algorithm with different ϵ thresholds.

672 6.4. Training Results

673 Sample validation results of the BC-CGAN model are shown in Figure
 674 13. The validation data points selected for this case are Q_{box} values of 0, 25,
 675 and 50 W/m². The error metric is computed only using RMSE in this case,
 676 instead of a combination of RMSE and max error as in the previous case. This
 677 change was made because it was difficult for the model training to converge
 678 using a stricter error metric for this more complex flow case. Additionally,
 679 the error metric combines the error for both velocity and temperature by

680 scaling the ranges of both these values from 0 to 1. The RMSE is then
681 calculated by considering the mean squared error using the scaled errors
682 for both velocity and temperature at each location in the 36×36 2D flow
683 domain. Because of the change in error metric calculation for this case, the
684 BC-CGAN predictions are qualitatively more different than the reference
685 CFD simulations, especially for error metric thresholds of 10% and 15%.
686 The change in velocity magnitude is more subtle for this case, since the input
687 parameter is a heat flux rather than Re . The most noticeable difference in
688 velocity magnitude is between the right side of the box and the right wall.
689 The boundary layer along the right wall thins as Q_{box} increases. There is
690 also a more noticeable boundary layer along the right side of the box as
691 Q_{box} increases, because the heat of the box causes the surrounding air to
692 heat up and rise. The velocity magnitude just above the box also slightly
693 increases with Q_{box} because of this buoyant flow. The change in temperature
694 distribution for the different Q_{box} values is more apparent, since the increase
695 in Q_{box} creates a significant thermal boundary layer surrounding the box.

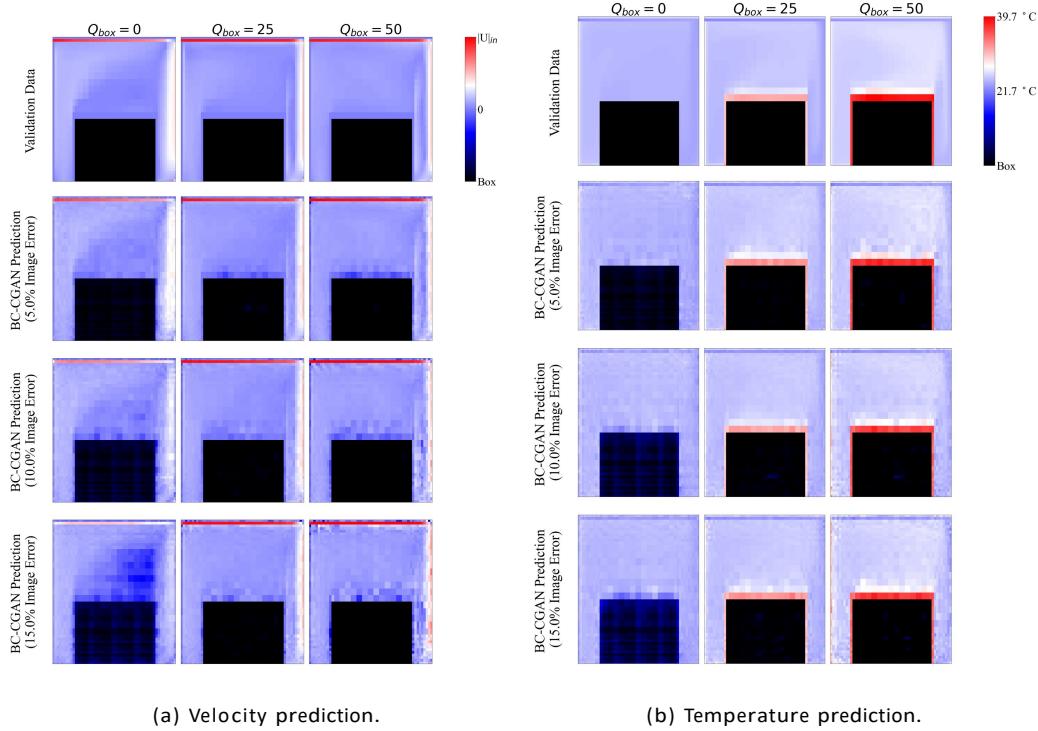


Figure 13: Validation results for velocity and temperature prediction with different error metrics.

696 The quantitative training results of the BC-CGAN model with different
 697 training datasets is shown in Figure 14. Similar to before, the higher error
 698 metric results in less epochs to train the models. Reducing the amount of
 699 training data seems to decrease the number of required epochs to train the
 700 models, until the uniform training dataset with only three data points. It
 701 seems that the training epochs can increase when the amount of training data
 702 is drastically reduced, especially for the looser error metric thresholds. The

703 non-uniform dataset with the least amount of training data typically requires
 704 the least number of epochs to train the models, while the non-uniform dataset
 705 with the most amount of training data often requires the most epochs to train
 706 the models. This discrepancy is likely because the outputs did not vary as
 707 non-linearly with the inputs for this case compared to the previous lid-driven
 708 cavity case.

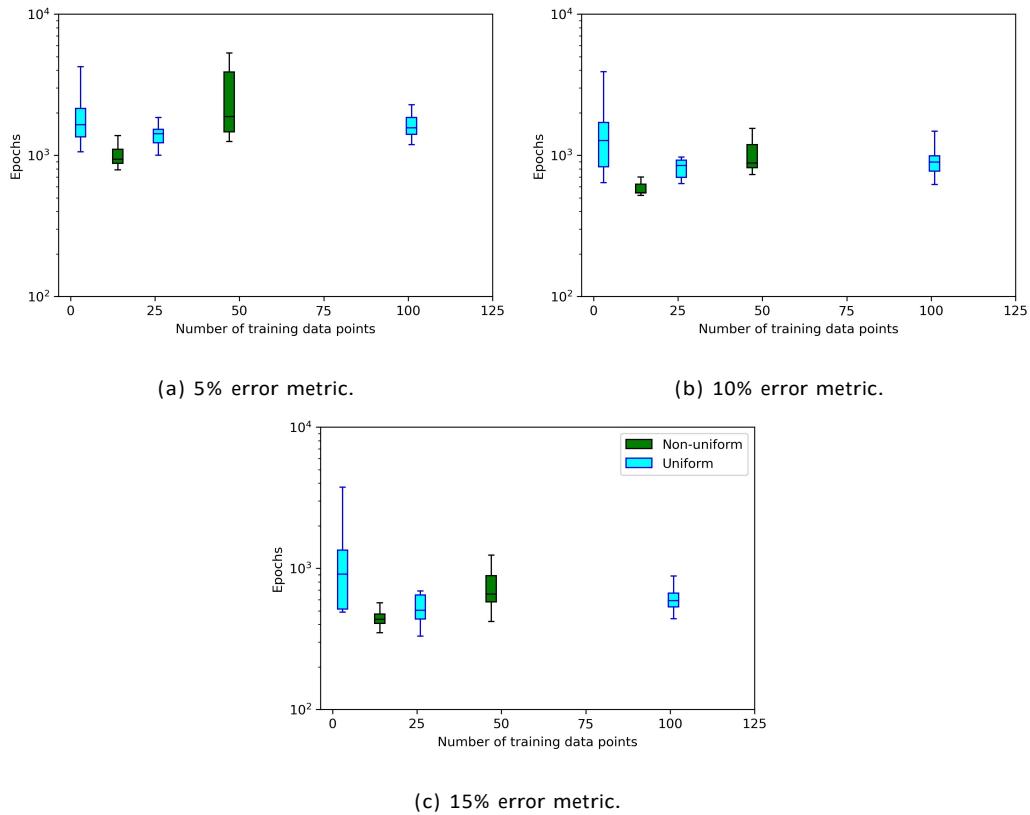


Figure 14: Box plots of the number of epochs required to train the BC-CGAN model for different training datasets and error metrics.

709 6.5. Evaluation Results

710 Example evaluation results of the BC-CGAN model for the randomly
711 selected test data points are shown in Figure 15. The BC-CGAN predictions
712 capture the main trends and features of the velocity and temperature distributions
713 at different Q_{box} values. However, the qualitative differences between the
714 BC-CGAN predictions and reference test data are more apparent for this
715 case compared to the previous. This is because the error metric is calculated
716 entirely based on RMSE for this case rather than a combination of RMSE
717 and max error, so locations with higher error may persist in these predictions.

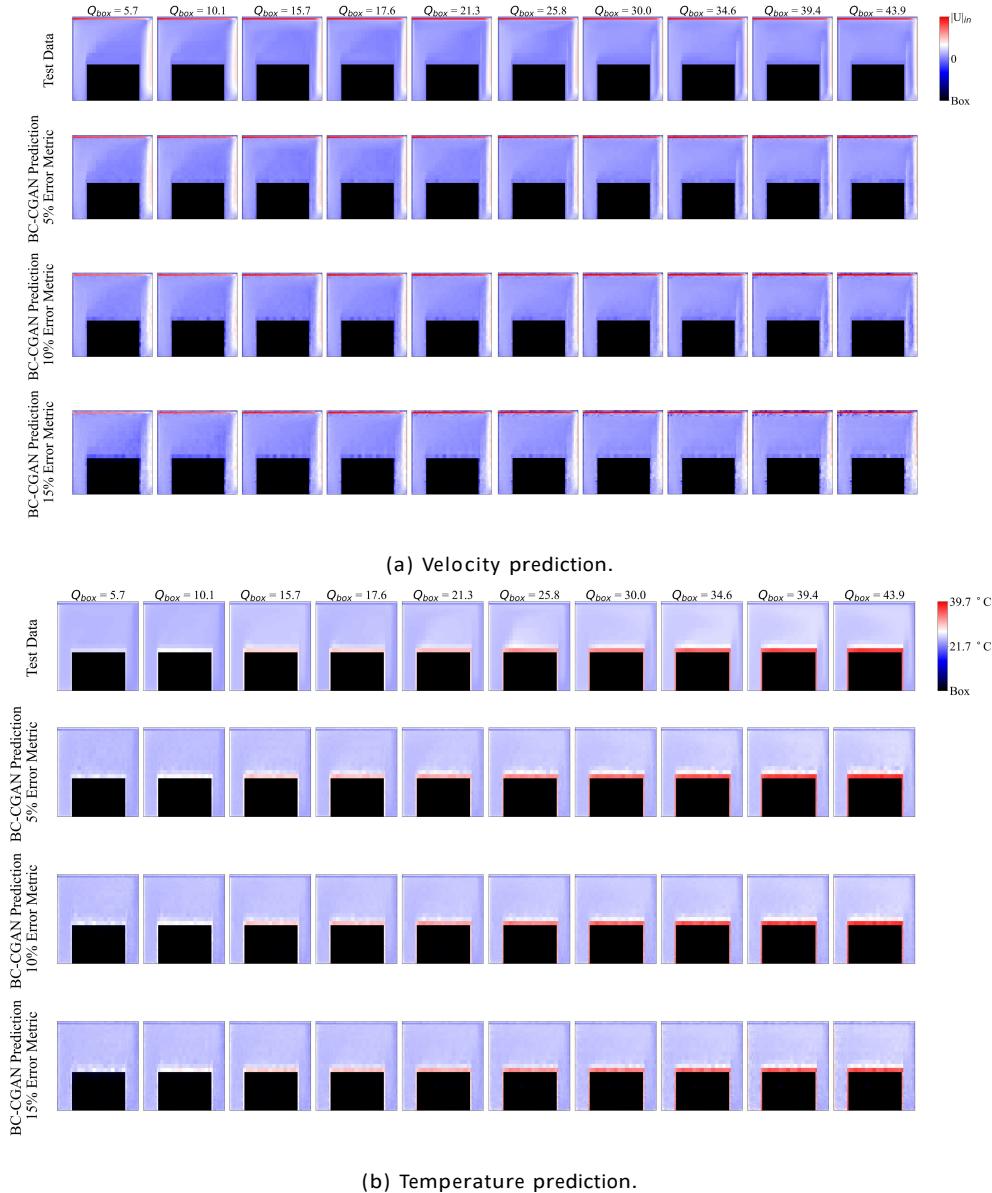


Figure 15: Evaluation results for velocity and temperature prediction for the trained BC-CGAN model with different error metric thresholds.

719 models trained with different datasets is shown in Figure 16. The results
720 show the error threshold is satisfied by the predictions from all the datasets
721 except the smallest training dataset with only three points. This shows the
722 consequences of drastically reducing the amount of training data, since it is
723 not able to capture the trends across the range of Q_{box} as well. Additionally,
724 the non-uniform training dataset with more training data points often performs
725 the best in terms of its predictions. This was also the training dataset that
726 typically required the most epochs to train the models. The results from this
727 case as well as the previous case appear to show a tradeoff between training
728 epochs and prediction performance. While some training datasets may take
729 more time to satisfy the validation criteria, they can perform better on a
730 wider range of test data, perhaps because of the additional training. The
731 difference in error is more apparent for the looser error metric thresholds
732 compared to the 5% error threshold. The change in error among the models
733 trained by the different datasets is almost negligible for this strict error
734 threshold, except for the dataset with only three data points. Tuning either
735 the uniform step of the input parameter or ϵ for the training datasets may
736 help balance training time and evaluation performance.

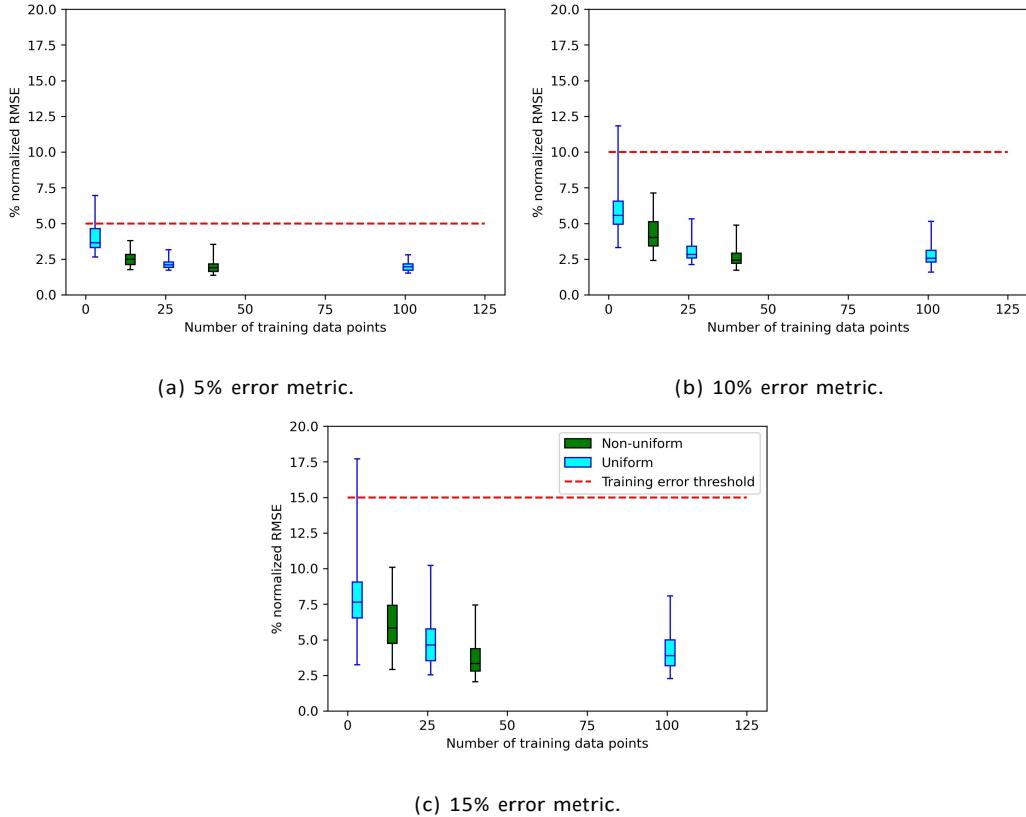


Figure 16: Box plots of the % normalized RMSE of the test predictions for the BC-CGAN models trained by different datasets and error metrics.

737 For this case, the BC-CGAN models can generate predictions with an
 738 average speed of 11 ms per prediction, while a CFD simulation took an
 739 average of 13.7 minutes. Both the BC-CGAN prediction and CFD simulation
 740 times are higher for this case because of the additional complexity compared
 741 to the lid-driven cavity flow, with the increase in CFD time being more

742 significant. The trained BC-CGAN prediction was on average about 75,680
743 times faster than a CFD simulation for this case. It took an average of 18
744 minutes to train the models to satisfy the 5% error metric, when considering
745 all the training datasets used in this case except for the one with only
746 three data points, which was found to have poor evaluation performance.
747 When excluding that dataset, it took a minimum of 3.2 hr to generate
748 training data. After accounting for the time to generate data and train
749 the BC-CGAN models, it becomes beneficial to use the BC-CGAN approach
750 over CFD simulations when more than 15 predictions are required for this
751 case. The results for this case show the significant potential of this model for
752 accelerating flow prediction with more complex cases.

753 7. Conclusion

754 In this paper, we proposed a new BC-CGAN model for fast prediction
755 of indoor airflow distribution. We extended the original CGAN model to
756 make predictions based on a continuous input parameter, such as a boundary
757 condition, rather than a discrete parameter, like a specific design. We also
758 designed a novel feature-driven algorithm for generating training data for
759 AI models. The algorithm includes training data points based on significant

760 changes between the flow outputs and inputs, with the goal of minimizing
761 the amount of generated training data while ensuring training quality. The
762 new BC-CGAN model and feature-driven algorithm are evaluated for two
763 benchmark flow cases: an isothermal lid-driven cavity flow and non-isothermal
764 mixed convection flow with a heated box.

765 The results show the trained model can predict velocity and temperature
766 distribution with less than 5% normalized RMSE and up to 75,000 times
767 faster than reference CFD simulations. For the lid-driven cavity case, the
768 trained models were able to make predictions for the test data with much less
769 than 5% normalized RMSE, even for the higher error metric threshold cases.

770 This is because we could use a stricter error metric that combined RMSE
771 and max error during the training process, which allowed for the predictions
772 to produce images without points of very high error. For the more complex
773 mixed convection flow with heated box case, this type of training error metric
774 could not be used, since it was difficult for the models to converge during
775 training with this method. Despite this, the trained BC-CGAN models for
776 this case make predictions below their error threshold for the test data,
777 except for the models trained by the dataset with only three data points.
778 While reducing the amount of training data often reduces the training time

779 in this paper, drastically reducing the amount of training data caused the
780 BC-CGAN models to perform poorly against the test data.

781 Use of the feature-driven algorithm often reduces the epochs required to
782 train the BC-CGAN models for the lid-driven cavity flow case, since it was
783 able to capture the non-linear trend between the change in flow outputs and
784 inputs. However, the feature-driven algorithm did not always produce this
785 same effect for the mixed convection flow with heated box case, perhaps
786 because there was not a clear non-linear trend between the flow outputs
787 and inputs. For both cases, there is an apparent tradeoff between training
788 time and test performance. The BC-CGAN models that took longer to train
789 often performed better on the test data compared to the BC-CGAN models
790 that were trained quicker. For the lid-driven cavity case, the increase in test
791 prediction error was very small for the models that were trained quicker,
792 particularly since all the models were very accurate because of the use of
793 max error in the training process. The change in error for the predictions on
794 the test data in the mixed convection flow with heated box case was more
795 significant when the error metric threshold was higher. A strict error metric
796 in this case resulted in small changes in test error among the models trained
797 by the different datasets, except for the dataset with only three data points,

798 which performed poorly for this case.

799 Future studies can be conducted based on the work in this paper. First,
800 more practical applications can be studied, for example data center airflow
801 scenarios. One input parameter was used for each of the studies in this paper,
802 but the BC-CGAN models and feature-driven algorithm can be evaluated for
803 applications with multiple input parameters. This is important for expanding
804 the BC-CGAN models to more applications, for example optimizing both
805 supply airflow rate and temperature considering the indoor environment.

806 Additionally, the models in this paper were trained to predict 2D airflow
807 distributions, but a 3D prediction may be necessary for certain applications.

808 The impacts of the additional complexity when considering multiple inputs
809 and 3D outputs on the model training and evaluation needs to be studied in
810 future research. Incremental training, by either expanding the training range
811 to new data or using “online” training when deploying the models [46, 47]
812 can be performed to improve the models over time with new data. Finally,
813 the trained BC-CGAN models can be used for a long-term evaluation or
814 optimization study that requires many realizations to show the computational
815 benefits of using this model over other numerical methods in these scenarios.
816 They can also provide real-time or faster predictions of airflow distribution,

817 which can be useful for emergency management scenarios.

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824 **References**

825 [1] Y. Li, P. V. Nielsen, CFD and ventilation research, *Indoor Air* 21 (6)

826 (2011) 442–453.

827 [2] X. Han, W. Tian, J. VanGilder, W. Zuo, C. Faulkner, An open source

828 fast fluid dynamics model for data center thermal management, *Energy*

829 and *Buildings* 230 (2021) 110599.

830 [3] X. Zhu, T. Shi, X. Jin, Z. Du, Multi-sensor information fusion based

831 control for VAV systems using thermal comfort constraints, *Building*

832 *Simulation* 14 (4) (2021) 1047–1062.

833 [4] X. Kong, Y. Chang, N. Li, H. Li, W. Li, Comparison study of thermal
834 comfort and energy saving under eight different ventilation modes for
835 space heating, *Building Simulation* 15 (7) (2022) 1323–1337.

836 [5] K. Gangisetti, D. E. Claridge, J. Srebric, M. T. Paulus, Influence of
837 reduced VAV flow settings on indoor thermal comfort in an ofice space,
838 *Building Simulation* 9 (1) (2016) 101–111.

839 [6] J. E. Castellini Jr, C. A. Faulkner, W. Zuo, D. M. Lorenzetti, M. D.
840 Sohn, Assessing the use of portable air cleaners for reducing exposure
841 to airborne diseases in a conference room with thermal stratification,
842 *Building and Environment* 207 (2022) 108441.

843 [7] F. Mohamadi, A. Fazeli, A review on applications of CFD modeling
844 in COVID-19 pandemic, *Archives of Computational Methods in
845 Engineering* (2022) 1–20.

846 [8] B. Jayaraman, E. U. Finlayson, M. D. Sohn, T. L. Thatcher, P. N. Price,
847 E. E. Wood, R. G. Sextro, A. J. Gadgil, Tracer gas transport under
848 mixed convection conditions in an experimental atrium: Comparison
849 between experiments and CFD predictions, *Atmospheric Environment*
850 40 (27) (2006) 5236–5250.

851 [9] S.-J. Cao, Challenges of using CFD simulation for the design and online
852 control of ventilation systems, Indoor and Built Environment 28 (1)
853 (2019) 3–6.

854 [10] L. Wang, Q. Chen, Applications of a coupled multizone-CFD model to
855 calculate airflow and contaminant dispersion in built environments for
856 emergency management, HVAC&R Research 14 (6) (2008) 925–939.

857 [11] W. Zuo, Q. Chen, Real-time or faster-than-real-time simulation of
858 airflow in buildings, Indoor Air 19 (1) (2009) 33.

859 [12] W. Zuo, Q. Chen, Fast and informative flow simulations in a building by
860 using fast fluid dynamics model on graphics processing unit, Building
861 and Environment 45 (3) (2010) 747–757.

862 [13] S. B. Pope, Computationally efficient implementation of combustion
863 chemistry using in situ adaptive tabulation, Combustion Theory and
864 Modelling 1 (1) (1997) 41–63.

865 [14] W. Tian, T. A. Sevilla, D. Li, W. Zuo, M. Wetter, Fast and self-learning
866 indoor airflow simulation based on in situ adaptive tabulation, Journal
867 of Building Performance Simulation 11 (1) (2018) 99–112.

868 [15] Q. Zhou, R. Ooka, Comparison of different deep neural network
869 architectures for isothermal indoor airflow prediction, Building
870 Simulation 13 (6) (2020) 1409–1423.

871 [16] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley,
872 S. Ozair, A. Courville, Y. Bengio, Generative adversarial nets, Advances
873 in Neural Information Processing Systems 27 (2014).

874 [17] R. Barth, J. Hemming, E. J. Van Henten, Optimising realism
875 of synthetic images using cycle generative adversarial networks for
876 improved part segmentation, Computers and Electronics in Agriculture
877 173 (2020) 105378.

878 [18] T. Iqbal, H. Ali, Generative adversarial network for medical images
879 (MI-GAN), Journal of Medical Systems 42 (11) (2018) 1–11.

880 [19] M. Mirza, S. Osindero, Conditional generative adversarial nets, arXiv
881 preprint arXiv:1411.1784 (2014).

882 [20] G. Antipov, M. Baccouche, J.-L. Dugelay, Face aging with conditional
883 generative adversarial networks, in: 2017 IEEE international conference
884 on image processing (ICIP), IEEE, 2017, pp. 2089–2093.

885 [21] Y. Ye, M. Strong, Y. Lou, C. A. Faulkner, W. Zuo, S. Upadhyaya,
886 Evaluating performance of different generative adversarial networks for
887 large-scale building power demand prediction, *Energy and Buildings* 269
888 (2022) 112247.

889 [22] Q. Zhang, A. Ferdowsi, W. Saad, M. Bennis, Distributed conditional
890 generative adversarial networks (GANs) for data-driven millimeter wave
891 communications in UAV networks, *IEEE Transactions on Wireless
892 Communications* 21 (3) (2021) 1438–1452.

893 [23] D. Chen, X. Gao, C. Xu, S. Chen, J. Fang, Z. Wang, Z. Wang,
894 FlowGAN: a conditional generative adversarial network for flow
895 prediction in various conditions, in: 2020 IEEE 32nd International
896 Conference on Tools with Artificial Intelligence (ICTAI), IEEE, 2020,
897 pp. 315–322.

898 [24] Y. Wang, W. Wang, G. Tao, H. Li, Y. Zheng, J. Cui, Optimization
899 of the semi-sphere vortex generator for film cooling using generative
900 adversarial network, *International Journal of Heat and Mass Transfer*
901 183 (2022) 122026.

902 [25] L. Gonog, Y. Zhou, A review: generative adversarial networks, in:

903 2019 14th IEEE conference on industrial electronics and applications
904 (ICIEA), IEEE, 2019, pp. 505–510.

905 [26] L. Sun, J. Chen, Y. Xu, M. Gong, K. Yu, K. Batmanghelich, Hierarchical
906 amortized gan for 3D high resolution medical image synthesis, IEEE
907 journal of biomedical and health informatics 26 (8) (2022) 3966–3975.

908 [27] M. D. Cirillo, D. Abramian, A. Eklund, Vox2Vox: 3D-GAN for brain
909 tumour segmentation, in: International MICCAI Brainlesion Workshop,
910 Springer, 2021, pp. 274–284.

911 [28] X. Zhao, F. Ma, D. Güera, Z. Ren, A. G. Schwing, A. Colburn,
912 Generative multiplane images: Making a 2d gan 3d-aware, in: European
913 Conference on Computer Vision, Springer, 2022, pp. 18–35.

914 [29] M. El-Kaddoury, A. Mahmoudi, M. M. Himmi, Deep generative models
915 for image generation: A practical comparison between variational
916 autoencoders and generative adversarial networks, in: International
917 Conference on Mobile, Secure, and Programmable Networking, Springer,
918 2019, pp. 1–8.

919 [30] S. Mokhtar, A. Sojka, C. C. Davila, Conditional generative adversarial
920 networks for pedestrian wind flow approximation, in: Proceedings of

921 the 11th Annual Symposium on Simulation for Architecture and Urban
922 Design, 2020, pp. 1–8.

923 [31] Y. Zheng, Y. Zhang, Z. Zheng, Continuous Conditional Generative
924 Adversarial Networks (cGAN) with Generator Regularization, arXiv
925 preprint arXiv:2103.14884 (2021).

926 [32] C. Blohm, H. C. Kuhlmann, The two-sided lid-driven cavity:
927 experiments on stationary and time-dependent flows, *Journal of Fluid
928 Mechanics* 450 (2002) 67–95.

929 [33] H. Kuhlmann, M. Wanschura, H. Rath, Flow in two-sided lid-driven
930 cavities: non-uniqueness, instabilities, and cellular structures, *Journal
931 of Fluid Mechanics* 336 (1997) 267–299.

932 [34] S. Albensoeder, H. C. Kuhlmann, Accurate three-dimensional lid-driven
933 cavity flow, *Journal of Computational Physics* 206 (2) (2005) 536–558.

934 [35] O. R. Burggraf, Analytical and numerical studies of the structure
935 of steady separated flows, *Journal of Fluid Mechanics* 24 (1) (1966)
936 113–151.

937 [36] U. Ghia, K. N. Ghia, C. Shin, High-Re solutions for incompressible flow

938 using the Navier-Stokes equations and a multigrid method, *Journal of*

939 *Computational Physics* 48 (3) (1982) 387–411.

940 [37] M. Khan, N. Delbosc, C. J. Noakes, J. Summers, Real-time flow

941 simulation of indoor environments using lattice Boltzmann method,

942 *Building Simulation* 8 (4) (2015) 405–414.

943 [38] T. Chiang, W. Sheu, R. R. Hwang, Effect of Reynolds number on the

944 eddy structure in a lid-driven cavity, *International Journal for Numerical*

945 *Methods in Fluids* 26 (5) (1998) 557–579.

946 [39] N. Ramanan, G. M. Homsy, Linear stability of lid-driven cavity flow,

947 *Physics of Fluids* 6 (8) (1994) 2690–2701.

948 [40] M. D. Zeiler, D. Krishnan, G. W. Taylor, R. Fergus, Deconvolutional

949 networks, in: 2010 IEEE Computer Society Conference on computer

950 vision and pattern recognition, IEEE, 2010, pp. 2528–2535.

951 [41] K. O’Shea, R. Nash, An introduction to convolutional neural networks,

952 *arXiv preprint arXiv:1511.08458* (2015).

953 [42] L. N. Smith, A disciplined approach to neural network

954 hyper-parameters: Part 1—learning rate, batch size, momentum,
955 and weight decay, arXiv preprint arXiv:1803.09820 (2018).

956 [43] D. P. Kingma, J. Ba, Adam: A method for stochastic optimization,
957 arXiv preprint arXiv:1412.6980 (2014).

958 [44] M. Wang, Q. Chen, Assessment of various turbulence models for
959 transitional flows in an enclosed environment (RP-1271), HVAC&R
960 Research 15 (6) (2009) 1099–1119.

961 [45] M. Wang, Q. Chen, On a hybrid rans/les approach for indoor airflow
962 modeling (rp-1271), HVAC&R Research 16 (6) (2010) 731–747.

963 [46] L. C. Jain, M. Seera, C. P. Lim, P. Balasubramaniam, A review of
964 online learning in supervised neural networks, Neural Computing and
965 Applications 25 (3) (2014) 491–509.

966 [47] B. Pérez-Sánchez, O. Fontenla-Romero, B. Guijarro-Berdiñas, A review
967 of adaptive online learning for artificial neural networks, Artificial
968 Intelligence Review 49 (2) (2018) 281–299.