#44 Pattern Discovery from Large-scale Computational Fluid Dynamic Data using Deep Learning

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Background

- Deep neural network architectures are used in:

Object Recognition	Speech Recognition
Scene Understanding	Biological & medical applications

- In our work, we apply **deep learning in design engineering** (specifically, microfluidic device or lab-on-a-chip design).
- Controlling shape and location of a fluid stream enables creation of structured materials, preparing biological samples, and engineering heat and mass transport.
- Recent work is capable of **manipulating cross sectional fluid shapes** by creating chaos by using **a sequence of pillars** of various diameters and positions in the fluid channel (Fig 1, 2).

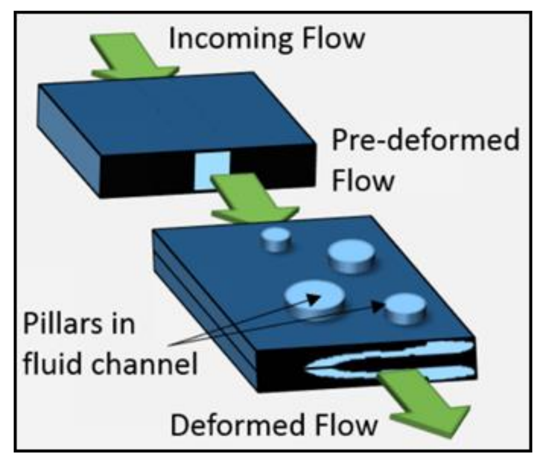


Fig 1: The forward problem: Sculpting fluid shapes with pillar sequences in fluid channel

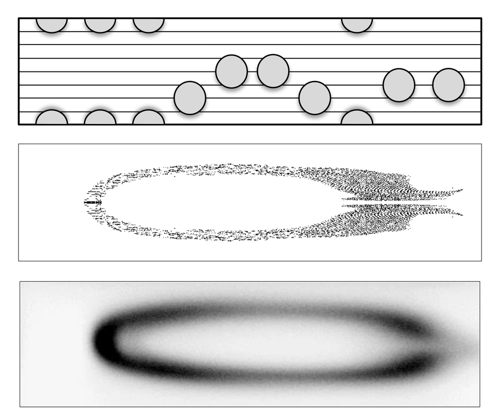


Fig 2: Pillar programs (top row), simulations (middle row) and experimental validation (bottom row).

- Although this approach allowed for sculpting complex fluid shapes, creating user-defined flow shapes for practical applications currently **requires laborious and time-consuming trial and error design iterations.**
- The ability to create a user-defined flow shape and **automatically determine a sequence of pillars** that yields this shape is a significant and impactful advance.
- Standard techniques that reformulate the inverse design problem is successful but **time consuming**, making their utility in real-time design suspect.
- We explore **deep learning (DL) models**, which can be **much faster than standard techniques**, to **serve as a map** between user defined flow shapes and corresponding sequence of pillars (Fig 3).
- To the best of our knowledge, this **is the first application of deep learning** to solving the inverse problem specifically in fluid mechanics.

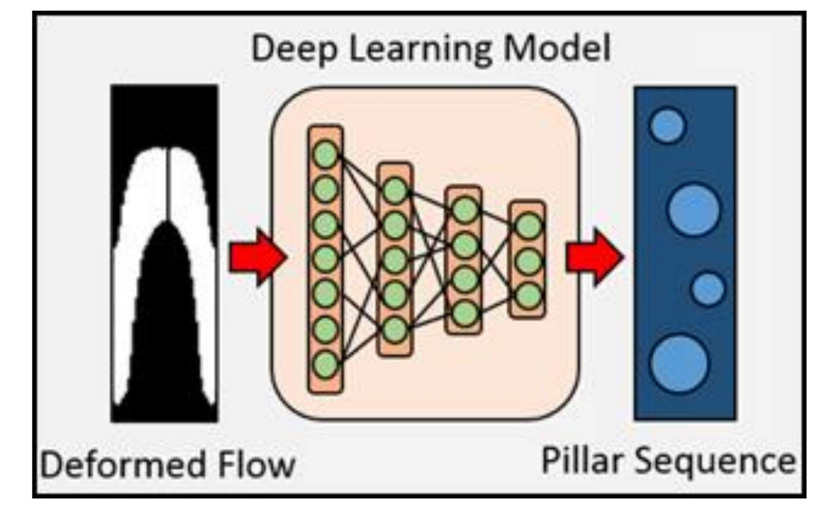


Fig 3: Solving the inverse problem with deep learning methods

Problem Statement

The problem is solved by the following approach:

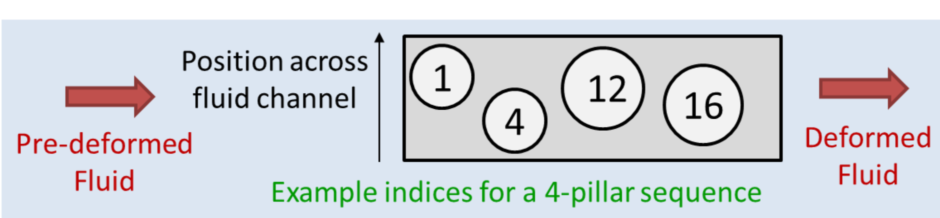


Fig 4: Discretization into indices

- **Discretizing pillar configuration as integers (Fig 4):** The combination of position and diameter of each pillar is assigned an index (or class). A *null* index is assigned when a pillar is absent at a particular location. This results in 33 classes per pillar in our experiments.
- **Solving the problem by classification:** The input is the desired flow shape (that can be drawn freehand). A convolutional neural network (CNN) extract pertinent features from the input images and simultaneously predicts the index of each pillars in the sequence which produces the desired shape (Fig 5).

Challenges:

- **Curse of dimensionality:** The number of possible sequences increases exponentially as the length of the sequence increases (Fig 6). Large volume of training data is required!

Solution:

- **On-the-fly data generation:** Provides sufficiently large volume of training data
- **Sobol-sequences for training data generation:** Instead of randomly sampling from the design space, using quasi-random Sobol sequences ensure more even coverage of the high-dimensional space and thus improves veracity, variety, and value of data.

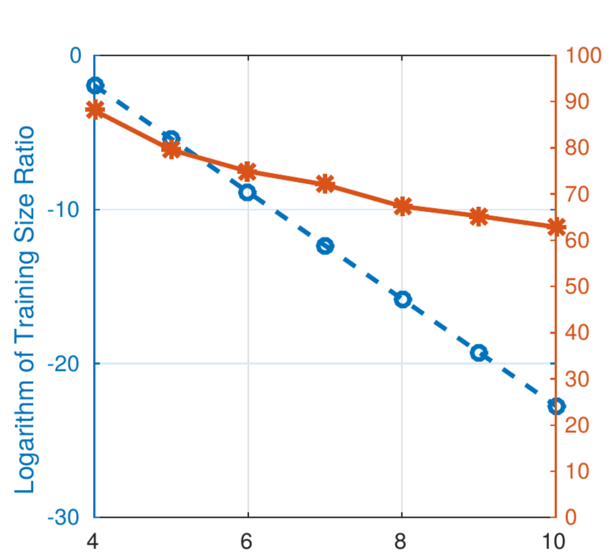


Fig 6: The 10-pillar sequence has 2^{32} ($\sim 10^{15}$) possible configurations but achieves an acceptable ~65% prediction accuracy following the use of Sobol sequences.

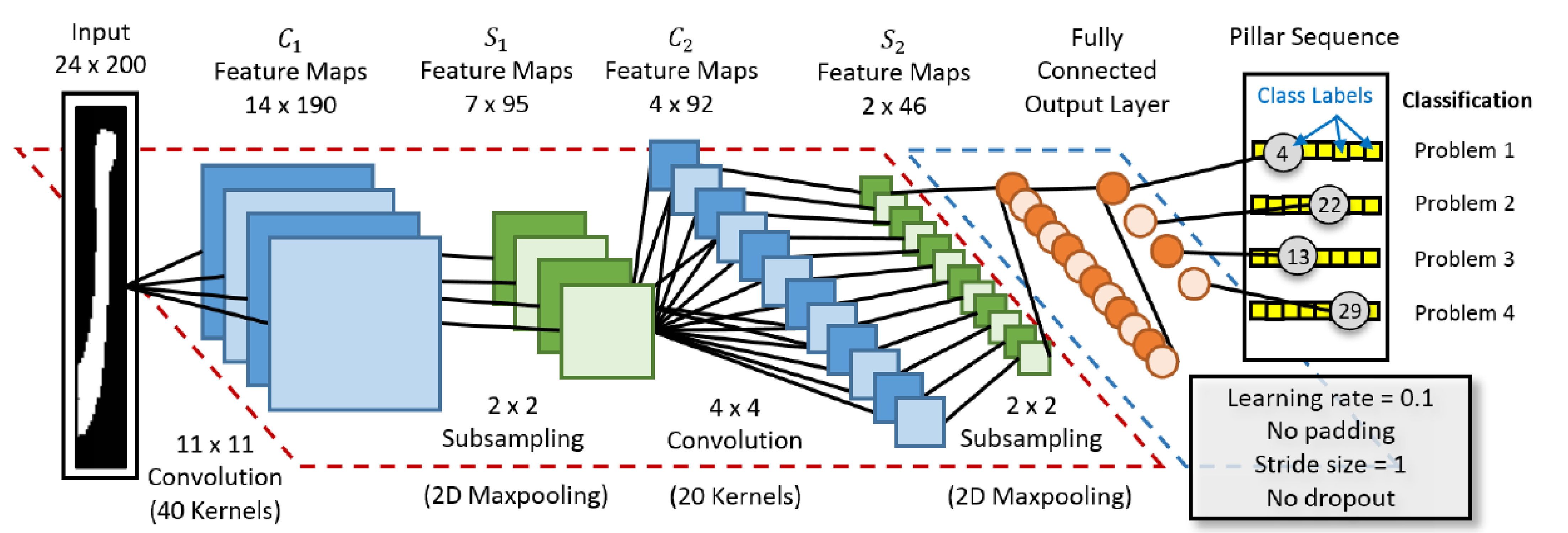


Fig 5: Implementation of the problem in the convolutional neural network with simultaneous multi-class classification (CNN-SMC)

Results & Broader Impacts

- Pixel Match Rate (PMR) is defined by the percentage of pixels matching in color between the desired flow shape and the reconstructed flow shape based on the predicted pillar sequence

Pixel Match Rate (PMR)	
Min	52.83%
Mean	88.09%
Median	89.92%
Max	100.00%
Percentage of Test Samples Exceeding PMR Threshold	
PMR >= 80 %	84.33%
PMR >= 85%	70.89%
PMR >= 90%	49.50%
PMR >= 95%	18.47%

Table 1: Prediction accuracy using current approach

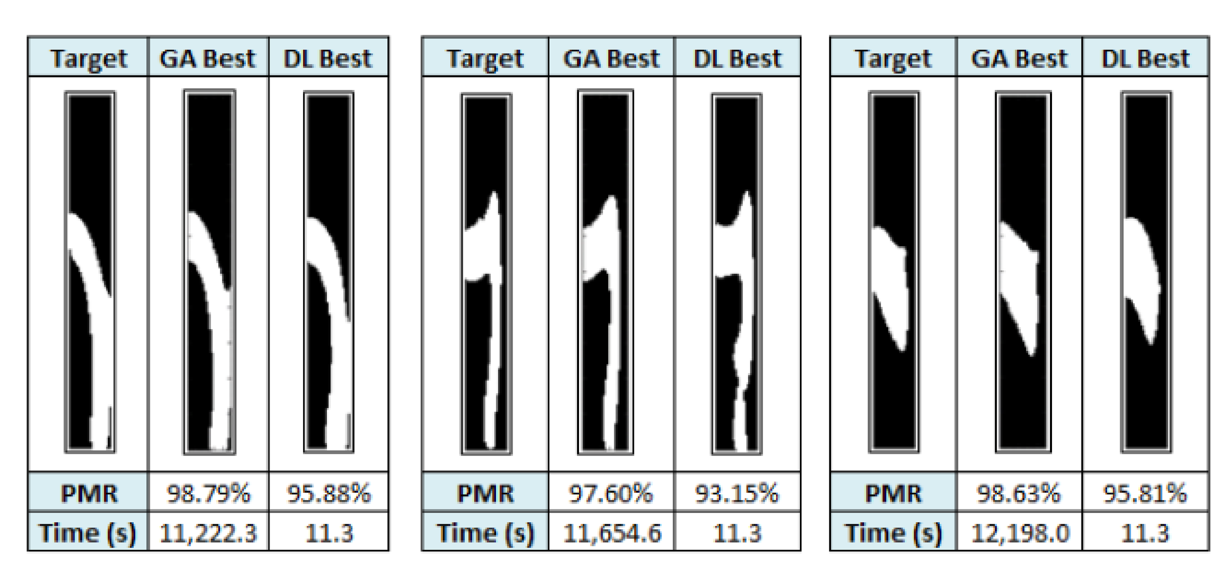
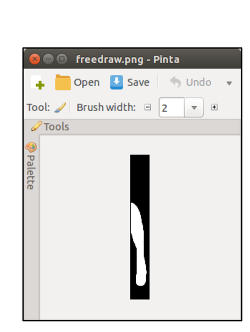
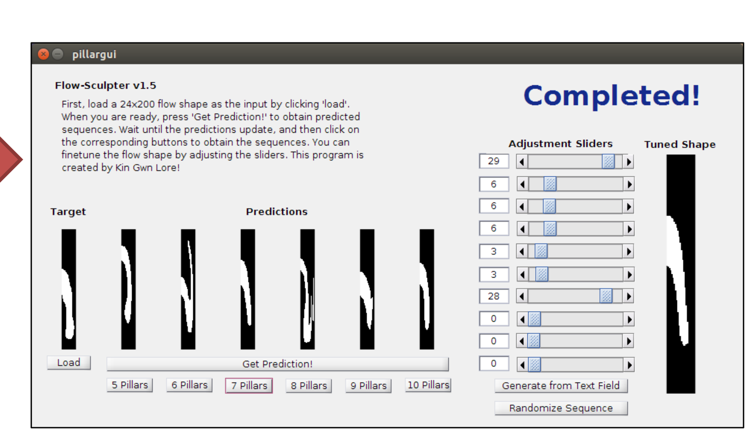


Table 2: Three comparison example of performance between DL-based tools and genetic algorithm (GA)-based methods

- Current state-of-the-art genetic algorithm **(GA)-based methods perform slightly better quantitatively**, but suffers from **long execution time**. DL-based methods can achieve acceptable accuracy (Table 1).
- DL-based methods can **expedite the design process by more than 600 times** compared to GA and present real-time design alternatives for lab-on-a-chip design (Table 2).
- A **computer-aided design (CAD) tool** can be developed that enables engineers to easily design fluid profiles for their applications:



User draws desired shape



CAD tool predicts pillar sequence that gives this shape

Manufacturing tubes for **optimal heat transfer**
Sculpting fluid streams for **guided chemical reactions**
Shaping fluids to wash cells in **biological applications**

The predicted sequence is used to manufacture fluid channels for various applications

- Capable of solving the inverse problem without full-scale Navier-Stokes simulations in the **order of mere seconds**, allowing **for real-time design**

Future Work

- Implementation of parallel processing on multiple GPUs to reduce training time with large volume of data
- Optimization of network hyper-parameters and architectures
- Investigation into the usage of other network types (e.g. Recurrent Neural Networks)
- Introduction of penalization term to penalize longer sequence, thus resulting in more financial savings

References

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