# Deep Learning in CFD

#### Ondřej Bublík

## NTIS - New Technologies for the Information Society Faculty of Applied Sciences, University of West Bohemia

December 2022

Deep Learning in CFD

## Motivation

- Full models:
  - solve the equations exactly
  - usually computationally expensive
- Surrogate (approximate) models:
  - similar behaviour to the original model
  - computationally cheaper
- Neural network:
  - highly nonlinear function with free parameters
  - the parameters are set to minimize the loss function
  - hight speed of evaluation
  - can be used as both cases: as a full or surrogate model

## Neural network libraries

#### • Keras + Tensorflow:

- excellent high-level API
- easy to learn with a simple way to build new architectures
- highly parallel pipelines with great scalability
- support for GPU, CPU and TPU
- trained models could by exported and used by different programming languages

### • PyTorch:

- easy to learn
- developed natively in Python
- support for GPU and CPU

伺 ト イヨト イヨト

## Convolution neural network

<ロ> <同> <同> < 同> < 同>

- convolution kernels (filters) slide along input features and provide responses known as feature maps
- shift (space) invariant



イロト イヨト イヨト イヨト

## Convolution layer - stride, kernel size, dilation

- stride governs how many cells the filter is moved in the input to calculate the next cell in the result
- larger kernel size leads to better results, but the number of unknowns increases





イロト イヨト イヨト イヨト

- valid the dimension of the outgoing feature map is reduced by the kernel size
- same output feature map has the same dimensions



イロト イヨト イヨト イヨト

## Convolution layer - examples



<ロ> <同> <同> < 同> < 同>

- when the input has more than one channels, the filter should have matching number of channels
- to calculate one output cell, convolution is performed on each matching channel, and the results are add together



イロト イヨト イヨト イヨト

tensorflow.keras.layers.Conv2D(filters, frame, activation, padding)

- a bias is added
- activation function such is applied





• • • • • • • •

臣

< ∃⇒

tf.keras.layers.MaxPooling2D(pool\_size, strides, padding)

tf.keras.layers.AveragePooling2D(pool\_size, strides, padding)

- reduce dimensions
- max pooling get max number
- average pooling get average number



イロト イヨト イヨト イヨト

## Flatten layer

tf.keras.layers.Flatten()

- used to convert the data into 1D arrays to create a single feature vector
- forward the data to a fully connected layer



臣

## Dense layer

tf.keras.layers.Dense(units, activation)

- fully connected layers connect every neuron in one layer to every neuron in another layer
- the flattened matrix goes through a fully connected layer to classify the images





ReLU(x) = max(0, x)

$$\mathsf{ELU}(x) = \begin{cases} x, & \text{if } x \ge 0\\ \alpha \left( e^x - 1 \right), & \text{otherwise} \end{cases}$$
  
Leaky ReLU(x) = max(0.1x, x

Activation functions:



Deep Learning in CFD

## Convolution neural network

- used for image/object recognition and classification
- convolutional layer reduces the high dimensionality of images without losing its information



イロト イヨト イヨト イヨト

## Convolution neural network - training

- The training sample has two part:
  - Input: matrix representing image
  - Output: probability vector  $[0, 0, \dots, 1, \dots, 0]$
- Three sets of samples need to be prepared:
  - training set used for training
  - validation set used for error monitoring
  - test set used for testing
- The loss function is usually defined as a **mean square error** between the predicted and desired output
- The gradient descent method is used for loss function minimization
- Various optimizers can be used to get better learning rate: RMSprop, Adam, SGD, ...

▲冊 ▶ ▲ 臣 ▶ ▲ 臣 ▶

## Convolution neural network - examples

- handwritten digit recognition
- from Gradient-Based Learning Applied to Document Recognition paper by Y. Lecun, L. Bottou, Y. Bengio and P. Haffner (1998)



- image recognition
- from ImageNet Classification with Deep Convolutional Neural Networks paper by Alex Krizhevsky, Geoffrey Hinton, and Ilya Sutskever (2012)



## Convolution neural network - shape classificatory

- image resolution: 128×128
- 1000 random circle/square samples



```
def enModel(Input):
    pooling_frame = (2, 2)
    frame = (3, 3)
    act = 'relu'
    n = 8
    deep = 5
    solverDeep = 3
    noUtput = 2
    # decoder
    layer = Input
    for 1 in range(deep): # 128 x 128 (1)-> 64 x 64 (2)-> 32 x 32 (3)-> 16 x 16 (4)-> 8 x 8 (5)-> 4 x 4 (6)-> 2 x 2
        layer = Conv2D((1+1) * n, frame, activation=act, padding='same')(layer)
        layer = MaxPeoling2D(pool_size=pooling_frame)(layer)
    decoded = Flatten()(layer)
```

```
# classificatory
s = decoded
for i in range(solverDeep):
    s = Dense(deep * n, activation=act)(s)
```

```
output = Dense(nOutput, activation='sigmoid')(s)
```

return output

・ロト ・回ト ・ヨト ・ヨト

- trained model was exported to the javascript
- simple node web server was created
- the image is generated on the frontend
- the prediction is realized using the node in the backend
- the result is send back to the frontend

## Convolution neural network - butterfly classification

- Input: coloured picture 64 x 64 pixels
- Output: probability vector
- Considered butterflies:
  - Babočka admirál Vanessa atalanta
  - Babočka bílé c Polygonia c album
  - Babočka bodláková Vanessa cardui
  - Babočka jilmová Nymphalis polychloros
  - Babočka kopřivová Aglais urticae
  - Babočka osiková Nymphalis antiopa
  - Babočka paví oko Inachis io
  - Babočka síťkovaná Araschnia levana
  - Babočka vrbová Nymphalis xanthomelas



#### Training set



イロト イヨト イヨト イヨト

## Encoder-decoder and U-Net

イロト イヨト イヨト イヨト

tf.keras.layers.UpSampling2D(size)

increases the dimensions



イロン イヨン イヨン イヨン

## Encoder-decoder, Autoencoder and U-Net

- The output has the same character as the input
- Encoder-decoder:
  - image recognition, detection, and segmentation
- U-net:
  - is Encoder-decoder with skip connection
- Autoencoder:
  - encoder-decoder with unsupervised learning
  - is trained to copy its input to its output
  - used for image denoising, and anomaly detection









## Prediction of steady flow field around airfoil

- Guo, X., Li, W., Iorio, F. Convolutional neural networks for steady flow approximation (2016) Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 13-17-August-2016, pp. 481-490. (419 citation)
- Convolution Neural Network was trained on the set of lattice Boltzmann simulations to produce the solution according to the boundary information



## Problem setup

- Inviscid fluid flow around airfoil, angle of attack  $\alpha = 0$ , Mach number  $M_{\infty} = 0.4$
- Structured C-mesh with 64 × 32 points, generated by elliptic mesh generator
- Airfoil shape is described using the Bezier curve with 8 control points



- First and last points are fixed on the airfoil tail
- Set of 1866 airfoils for various control points positions was created





Lift coefficient  $c_L = \oint_{\Gamma} p \, n_y \, \mathrm{d}I$ 

## Convolution Neural Network Architecture

- Input: C-mesh with 64 x 32 points
- **Output**: flow field  $(\varrho, p, u_x, u_y)$
- 106 324 trainable parameters
- Trained on the set of 1866 airfoils
- Keras and TensorFlow libraries, python interface



## Convolution Neural Network - keras model

```
def u_net(self, input):
    nSpec, n1, n2, dim = np.shape(input)
    nOutput = self.nOutput
    # huperparameters
    poolFrame = (2, 2)
    width = 1
    frame = (1 + 2 * width, 1 + 2 * width)
    actFun = 'relu'
    actFunOut = 'linear'
    nDown = 12
    nUp = 12
    deep = int(np.log(min(n1, n2)) / np.log(2))
    # encoder
    laver = input
    conv = [None] * deep # store layers for concatenation
    for i in range(1, deep);
        conv[i - 1] = Conv2D(i * nDown, frame, activation=actFun, padding='valid', trainable=self,trainableEncoder)(laver)
        laver = MaxPooling2D(pool size=poolFrame)(conv[i - 1])
    encoded = Conv2D(deep * nDown, frame, activation=actFun, padding='valid', trainable=self.trainableEncoder)(layer)
    # decoder
    layer = encoded
    for i in range(deep - 1, 0, -1):
        laver = UpSampling2D(poolFrame)(laver)
        conc = Conv2D(i * nUp, frame, activation=actFun, padding='valid')(laver)
        laver = concatenate([conc. conv[i - 1]])
    decoded = Conv2D(nOutput, frame, activation=actFunOut, padding='valid')(laver)
```

return decoded

## Results - Tests NACA Airfoils



4412

6615













э

## Results - Flow Field (top DNN, bottom CFD)



Deep Learning in CFD

æ

・ 回 ト ・ ヨ ト ・ ヨ ト

## Results - Pressure



4412















イロト イヨト イヨト イヨト

Absolute error  $|c_L^{CFD} - c_L^{CNN}| \ge 10^3$ 

$\alpha \setminus airfoil$	0012	0020	0030	2412	4412	6615	8607	9210
0	0.88	1.52	0.87	0.67	0.34	2.38	1.99	2.26
5	0.93	0.85	0.69	1.57	0.13	3.50	0.96	1.39
10	1.97	0.57	2.68	2.08	2.02	5.37	0.59	0.31
20	4.82	2.93	3.82	4.67	3.98	4.25	4.44	1.72

Relative error 
$$\frac{\left|c_{L}^{CFD}-c_{L}^{CNN}\right|}{\left|c_{L}^{CFD}\right|}$$
 x100

$\alpha \setminus airfoil$	0012	0020	0030	2412	4412	6615	8607	9210
0	-	-	-	7.00	1.78	9.71	5.91	5.08
5	2.57	2.63	2.60	3.45	0.24	6.12	2.07	4.76
10	2.89	0.93	5.30	2.71	2.39	6.29	0.75	0.56
20	4.51	3.00	4.54	4.11	3.32	3.52	3.88	1.92

▲ロト ▲御 ト ▲ 臣 ト ▲ 臣 ト 一臣 - のへで

## Conclusion

- Structured mesh with  $64 \times 32 = 2048$  cells
- The test set of 1866 NACA airfoils
- CFD solution:
  - DG method (FlowPro)
  - First order of spatial accuracy
  - Total CPU time of 1866 airfoils: 4.5hour
  - CPU time of one solution: 8.7s
  - (CPU time for the second order solution: 26s)

#### CNN solution:

• Total CPU time of 1866 airfoils: 10.7s

向下 イヨト イヨト

• CPU time of one solution: 0.0057s

 The convolution neural network provides 1500 times faster solution than classical CFD solver. (possible 4500 times faster than second order solution)

# Prediction of steady flow field in cascade, parametrization

## Main Neural Network Architecture - U-net



#### Main Neural Network Architecture - Convolution With Periodic Padding



Inlet and outlet



Top and bottom walls



Convolution filter application



(4回) (4回) (4回)
## Problem Setup

- Laminar fluid flow in blade cascade, angle of attack  $lpha=10^\circ$
- Mach numbers Ma = 0.9
- Reynolds numbers Re = 10000
- Structured grid with 64 × 32 points, generated by elliptic mesh generator
- Periodic boundary condition
- Blade shape is described by cubic spline with 6 control points



# Neural Network - Summary

- Input tensor  $[n_{spec}, n_1, n_2, 3]$ , (X, Y, walls) grid coordinates and wall markers  $(n_1 = 64 \times 32 = n_2 \text{ points})$
- Output tensor  $[n_{spec}, n_1, n_2, 4]$ : flow field  $(u_x, u_y, p, \varrho)$
- 402 928 trainable parameters
- Trained on the set of 136 random airfoils
- Keras and TensorFlow libraries, Python interface



#### Convolution Neural Network - keras model

```
def u_net(self, input):
    nSpec, n1, n2, dim = np.shape(input)
   nOutput = self.nOutput
   # huperparameters
   poolFrame = (2, 2)
   width = 1
   frame = (1 + 2 * width, 1 + 2 * width)
   actFun = 'relu'
   actFunOut = 'linear'
   nDown = 12
   nUp = 12
   deep = int(np.log(min(n1, n2)) / np.log(2))
   # encoder
   layer = input
   conv = [None] * deep # store layers for concatenation
   for i in range(1, deep):
       conv[i - 1] = Conv2D(i * nDown, frame, activation=actFun, padding='valid', trainable=self,trainableEncoder)(
            self.addPeriodicPadding(layer, width))
       layer = MaxPooling2D(pool_size=poolFrame)(conv[i - 1])
   encoded = Conv2D(deep * nDown, frame, activation=actFun, padding='valid', trainable=self.trainableEncoder)(
        self.addPeriodicPadding(laver, width))
   # decoder
   layer = encoded
   for i in range(deep - 1, 0, -1):
        layer = UpSampling2D(poolFrame)(layer)
       conc = Conv2D(i * nUp, frame, activation=actFun, padding='valid')(self.addPeriodicPadding(layer, width))
       layer = concatenate([conc, conv[i - 1]])
   decoded = Conv2D(nOutput, frame, activation=actFunOut, padding='valid')(self.addPeriodicPadding(layer, width))
```

```
return decoded
```

1

```
def addPeriodicPadding(self, T, width):
    # rows
    bottomRow = tf.slice(T, (0, 0, 0, 0), (tf.shape(T)[0], width, T.shape[2], T.shape[3]))
    topRow = tf.slice(T, (0, T.shape[1]-width, 0, 0), (tf.shape(T)[0], width, T.shape[2], T.shape[3]))
    T = tf.concat((bottomRow, T, topRow), axis=1)
    # colls
    leftCol = tf.slice(T, (0, 0, 0, 0), (tf.shape(T)[0], T.shape[1], width, T.shape[3]))
    rightCol = tf.slice(T, (0, 0, -0, 0), (tf.shape(T)[0], T.shape[1], width, T.shape[3]))
    rightCol = tf.slice(T, (0, 0, -0, 0), (tf.shape(T)[0], T.shape[1], width, T.shape[3]))
```

```
T = tf.concat((rightCol, T, leftCol), axis=2)
```

return T

イロト イポト イヨト イヨト

## Application - Blade Optimization

• Blade profile optimization for the inlet Mach number M = 0.95

• Target functional: max(
$$f(\mathbf{x})$$
),  $f(\mathbf{x}) = \frac{c_L(\mathbf{x})}{1+c_D(\mathbf{x})}$ ,  $c_L = \oint_{\Gamma} p n_y$ ,  $c_D = \oint_{\Gamma} p n_x$ 

- Algorithm of optimization:
  - First step roughly search the state space  $9^4 = 6561$  combinations of control points 13.3s of CPU time
  - Second step perform 100 steps of gradient descent method 32s of CPU time



#### Comparison of flow fields for optimal blade



FlowPro (CFD software)

Neural network prediction

- How to include parameters in the neural network?
- In general, the sooner is the better



э

• 3 >

- Used for parametrization of a main network
- Main network is trained for all combinations of flow parameters and resulting weights are stored
- Map flow parameters into main neural network weights
- Dense neural network one hidden layer



## Hyper Neural Network - Single Parameter Re

name	symbol	value
heat capacity ratio	$\kappa$	1.4
Training Reynolds numbers	Re	100, 500, 1000
Prandtl number	Pr	0.72
pressure ratio	$p_{\rm out}/p_{\rm ino}$	0.843
angle of attack	α	$15^{\circ}$

Re	Drag average err [%]	SD	Lift average err [%]	SD
100	1.9	1.2	1.1	0.5
250	3.6	3.7	4.1	1.3
500	3.9	1.4	2.4	1.4
750	3.3	2.3	2.7	2.0
1000	2.9	1.7	3.0	2.3

ヘロア 人間 アメヨア 人間 アー

E.

# Hyper Neural Network - Single Parameter Re



イロン 不同 とくほど 不同 とう

# Hyper Neural Network - Single Parameter Re







イロン 不同 とうほう 不同 とう

Deep Learning in CFD

# Prediction of unsteady flow field

- Hennigh, O., Lat-Net: Compressing Lattice Boltzmann Flow Simulations using Deep Neural Networks. (2017) arXiv e-prints arXiv:1705.09036 (61 citation)
- Time dependent solution compared with lattice Boltzmann simulation





# Neural network architecture

- The architecture is same as in the case of prediction steady flow field
- The solution of *n* time level is added as another input
- If the mesh is moving, the points coordinates in n+1 time level are also added as another input
- The outpus is the solution at *n* + 1 time level



臣

# Unsteady flow field prediction



< (1) × (1)

э.

#### Flow field prediction with moving mesh



イロン イヨン イヨン

### Vortex induced vibrations

Structure equation of motion:

$$\ddot{y} + 2\,\zeta\,\omega_n\,\dot{y} + \omega_n^2\,y = \frac{L}{m}$$

Lift force:

$$L = \oint_{\Gamma} \left( \sigma_{xx} \, n_x + \sigma_{yx} \, n_y \right) \, dS$$

- Parameters:
  - Damping ratio:  $\zeta = \frac{c}{2m\omega_n}$
  - Stiffness:  $k = m \omega_n^2$
  - Mass: m = 10
  - Damping: c = 0.25
  - Natural frequency:  $f_n = \frac{\omega_n}{2\pi} = f_{St}$
  - Strouhal frequency:  $f_{St} = \frac{\mu}{\varrho \propto L^2} 0.212 (\text{Re} - 21.2)$

- Convolution neural network predict unsteady flow-field with moving boundary
- Training frequencies and amplitudes:



Convolution neural network architecture:



臣

< ≣ ▶

# Vortex induced vibrations



CNN predicted unsteady flow field



イロト イヨト イヨト イヨト

Deep Learning in CFD

1.3

1.3

1.2

1.2 1.3

1.2

- The output values must be scaled to a range of around  $\pm 1$ 
  - for example: velocity range [0,400]  $ms^{-1}$  or pressure range [8 $e^5$ , 1 $e^6$ ] Pa
  - it is advantageous to consider the equations in dimensionless form
- If more outputs are present, their scales must be comparable
  - for example: dimensionless velocity range [0, 1] is not comparable with dimensionless pressure range [0.85, 1]
  - either the data must be rescaled or the weights in the loss function must be taken into account
- The input values scale must be comparable
  - for example: Mach number [0.1, 1] is not comparable with Reynolds number [100, 1e6]
  - instead of the real value the logarithm is taken  $log_{10}(Re) = [2, 6]$

(1日) (1日) (日) (日)

# Physic Informed Neural Network

< A ≥ < B

# Neural Network in CFD - Physic Informed Neural Network

- Raissi M., Perdikaris P., Karniadakis G., Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics, 2019, 378, pp. 686†"707 (2148 citation)
- Fully connected deep neural network is used for the solution approximation
- The loss function is computed according to PDE



Image: A matrix and a matrix

# Motivation

- Consider neural network as a solution function
- Use PDE in classical or weak form, together with boundary condition for evaluation of loss function ⇒ no need of any train data

イロト イヨト イヨト イヨト

### Motivation

- Consider neural network as a solution function
- Use PDE in classical or weak form, together with boundary condition for evaluation of loss function ⇒ no need of any train data

$$\begin{array}{c} \displaystyle \frac{\text{Boundary value problem:}}{\mathcal{L}\left(u, \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i \partial x_j}, \ldots\right) = \mathbf{0}, \quad x \in \Omega \\ & u = u_0, \quad x \in \Gamma_D \\ & \frac{\partial u}{\partial x_i} n_i = c, \quad x \in \Gamma_N \end{array}$$

イロン 不同 とくほど 不同 とう

æ,

## Motivation

- Consider neural network as a solution function
- Use PDE in classical or weak form, together with boundary condition for evaluation of loss function ⇒ no need of any train data







Activation functions: sigmoid(x) =  $\frac{1}{1 + e^{-x}}$ swish(x) =  $\frac{x}{1 + e^{-x}}$ mish(x) = x tanh(1 + e^x)



Deep Learning in CFD

#### Neural network architecture - dense neural network



臣

• 3 >

#### Neural network architecture - gradient layer



臣

< ∃⇒

# Neural network architecture - PINN



イロト イヨト イヨト イヨト

크

## PINN layers in code

#### Gradient layer

```
x, y = [ xy[..., i, tf.newaxis] for i in range(xy.shape[-1]) ]
with tf.GradientTape(persistent=True) as gg:
   gg.watch(x)
    gg.watch(v)
    with tf.GradientTape(persistent=True) as g:
       q.watch(x)
       g.watch(y)
       out = self.model(tf.concat([x, y], axis=-1))
       u = out[..., 0, tf.newaxis]
       v = out[..., 1, tf.newaxis]
       p = out[..., 2, tf.newaxis]
   u_x = g.batch_jacobian(u, x)[..., 0]
   u_v = q.batch_iacobian(u, v)[..., 0]
   v_x = q.batch_jacobian(v, x)[..., 0]
   v_y = g.batch_jacobian(v, y)[..., 0]
   p = q.batch |acobian(p, x)[..., 0]
   p_v = q.batch_iacobian(p, v)[..., 0]
   del q
u_xx = gg.batch_jacobian(u_x, x)[..., 0]
u_vv = gg.batch_iacobian(u_v, v)[..., 0]
v_x = qq.batch_jacobian(v_x, x)[..., 0]
v_yy = gg.batch_jacobian(v_y, y)[..., 0]
del aa
p_qrads = p, p_x, p_y
u_grads = u, u_x, u_y, u_x, u_y
v_grads = v, v_x, v_y, v_xx, v_yy
return u_grads, v_grads, p_grads
```

#### PINN layer

# compute gradients relative to equation
u\_grads, v\_grads, p\_grads = self.grads(xy\_eqn)
p, p.x, p\_Y = p\_grads
u, u\_x, u\_y, u\_xx, u\_yy = u\_grads
u, v\_x, v\_y, v\_xx, v\_yY = v\_grads

# compute equation loss

continuity = tf.square(u\_x + v\_y) u\_eqn = tf.square(u\*u\_x + v\*u\_y + p\_x/self.rho - self.nu\*(u\_xx + u\_yy)) v\_eqn = tf.square(u\*u\_x + v\*u\_y + p\_y/self.rho - self.nu\*(v\_xx + v\_yy))

イロト イヨト イヨト イヨト

2

#### Problem setup

#### Equations:

$$\begin{split} &\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \\ &u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} = \frac{1}{Re} \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \\ &u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial v} = \frac{1}{Re} \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \end{split}$$

#### Boundary conditions:

- inlet: *u* = 1, *v* = 0
- outlet: *p* = 0
- wall: u = 0, v = 0
- Control points:
  - 10000 equations points
  - 100 inlet points
  - 100 outlet points
  - 700 wall points





(日)

æ

< ∃⇒



PINN

CFD

#### difference

2

#### Results - Re = 100



CFD

PINN

difference

◆□> ◆□> ◆注> ◆注> 二注:



- 28 unknowns
- Error 2.173





< A > < 3

э.

- Dense net [8,4,4,8]
- 96 unknowns
- Error 2.064





▲ 御 ▶ ▲ 臣

э





< A > < 3

- Dense net
   [32,16,16,32]
- 1344 unknowns
- Error 0.051





▲ 御 ▶ ▲ 臣

문 🛌 🖻

- Dense net [64,32,32,64]
- 5248 unknowns
- Error 0.036





▲ 御 ▶ ▲ 臣

문 🛌 🖻
## Convergence

- Dense net [128,64,64,128]
- 20736 unknowns
- Error referential solution





< <sup>(17)</sup> ► <

< ∃⇒

æ

- The loss function is the key to creating a good model.
- In physical modelling, the construction of the loss function can be made with the help of:
  - partial differential equations
  - conservation laws (integral form)
  - constitutive laws
  - ...
- If the loss function does not depend on the training data, the neural network can be said to be a full model.
- The next goal will be to bring physics to the loss function of a convolutional network.

向下 イヨト イヨト