

# A CFD-based multi-fidelity surrogate model for prediction of flow parameters in a ventilated room

N. Morozova<sup>1</sup>, F.X. Trias<sup>1</sup>, V. Vanovski<sup>2</sup>, C. Oliet<sup>1</sup>  
and E. Burnaev<sup>2</sup>

1 - Heat and Mass Transfer Technological Centre (CTTC),  
Universitat Politècnica de Catalunya (UPC)

2 - I was asked to remove this affiliation

The 8th European Congress on Computational Methods in  
Applied Sciences and Engineering  
ECCOMAS Congress 2022  
5–9 June 2022, Oslo, Norway



# Outline

- 1 Introduction
- 2 Test case description
- 3 Numerical methods
- 4 Results
- 5 Conclusions

# Introduction

Simulations of indoor environment. State of the art

- Modern heating ventilation and air conditioning (HVAC) systems are required to maintain a trade-off between maximizing human thermal comfort and minimizing energy consumption in buildings.
- The air distribution in buildings is usually evaluated either by simplified reduced-order models or by CFD.
- Simplified models provide very rapid predictions but offer limited information due to assumptions required.
- CFD simulations are computationally too expensive.

# Introduction

Simulations of indoor environment. State of the art

- Modern heating ventilation and air conditioning (HVAC) systems are required to maintain a trade-off between maximizing human thermal comfort and minimizing energy consumption in buildings.
- The air distribution in buildings is usually evaluated either by simplified reduced-order models or by CFD.
- Simplified models provide very rapid predictions but offer limited information due to assumptions required.
- CFD simulations are computationally too expensive.

# Introduction

Simulations of indoor environment. State of the art

- Modern heating ventilation and air conditioning (HVAC) systems are required to maintain a trade-off between maximizing human thermal comfort and minimizing energy consumption in buildings.
- The air distribution in buildings is usually evaluated either by simplified reduced-order models or by CFD.
- Simplified models provide very rapid predictions but offer limited information due to assumptions required.
- CFD simulations are computationally too expensive.

# Introduction

## Simulations of indoor environment. State of the art

- Modern heating ventilation and air conditioning (HVAC) systems are required to maintain a trade-off between maximizing human thermal comfort and minimizing energy consumption in buildings.
- The air distribution in buildings is usually evaluated either by simplified reduced-order models or by CFD.
- Simplified models provide very rapid predictions but offer limited information due to assumptions required.
- CFD simulations are computationally too expensive.

# Introduction

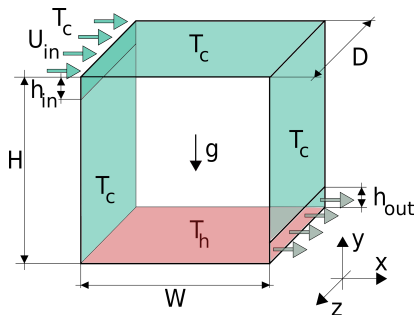
## Objectives of the study

- 1 Explore the capabilities of the surrogate modeling as a cheaper alternative to CFD for indoor environmental applications.
- 2 Reduce the computational cost of the dataset generation by implementing multi-fidelity approach.

# Physical problem

## Three-dimensional mixed convection in a ventilated cavity

- 3D ventilated room filled with air, where the floor is heated, side walls are cold, front and rear walls are periodic. The inlet flow is cold.
- Experimental parameters:
  - ① Cavity width aspect ratio  $A_W$ ;
  - ② Froude number  $Fr = U_{in}/U_{buo}$ ;
  - ③ Rayleigh number  $Ra_H = g\beta\Delta TH^3/(\nu\alpha)$ .





# Problem description

## Configuration of the experiments

### Experimental parameters

$A_w$	0.25, 0.50, 1.00, 2.00, 4.00
$Ra_H$	$1.5 \times 10^8$ , $6.0 \times 10^8$ , $2.4 \times 10^9$ , $9.6 \times 10^9$
$Fr$	0.15, 0.20, 0.25, ..., 0.55, 0.60, 0.70, ..., 1.50, 1.60

### CFD simulations

Total number of low-fidelity (LF) simulations - 360

Total number of high-fidelity (HF) simulations - 240

Total number of simulations - 600

# Problem description

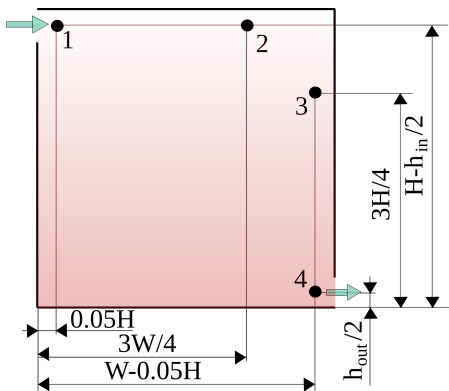
## Input-output parameters

### Input parameters

- 1  $A_w$
- 2  $T_1, \dots, T_4$
- 3  $V_1, \dots, V_4$

### Output parameters

- 1 Nusselt number on the hot wall -  $\langle Nu \rangle$
- 2 Average enstrophy -  $\langle \Omega \rangle$



<sup>1</sup>N. Morozova, F. X. Trias, R. Capdevila, E. Schillaci and A. Oliva.

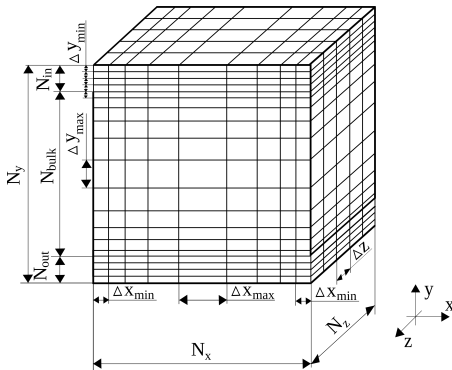
*A CFD-based surrogate model for predicting flow parameters in a ventilated room using sensor readings.* Energy Build, **266**:112146, 2022.

# Numerical methods

## CFD simulations

### Automatic mesh generation

- 1  $\Delta x_{max} = \Delta y_{max} \approx C_r \eta Gr_0$
- 2  $\Delta y_{min} \approx C_r \frac{h_{in}}{2} Re_{\tau}^{-1}$
- 3  $\Delta x_{min} = 4 \Delta y_{min}$
- 4  $\gamma_x, N_x, \gamma_y, N_{bulk}$  - are found iteratively using the hyperbolic tangent function
- 5  $N_z = 1.1D / \Delta y_{max}$



### Grid resolutions

- $C_r = 3$  - high-fidelity simulations
- $C_r = 6$  - low-fidelity simulations

# Numerical methods

## Surrogate models - 1

- The work is based on the Gaussian process regression (GPR).
- All of the models use an open-source library scikit-learn.

## Single-fidelity models

- **HF-GPR** - a model trained only high-fidelity (HF) data;
- **LF-GPR** - a model trained only on low-fidelity (LF) data.
- **HFLF-GPR** - a model trained on a mix of LF and HF data without distinguishing the data fidelity.

# Numerical methods

## Surrogate models - 1

- The work is based on the Gaussian process regression (GPR).
- All of the models use an open-source library scikit-learn.

## Single-fidelity models

- **HF-GPR** - a model trained only high-fidelity (HF) data;
- **LF-GPR** - a model trained only on low-fidelity (LF) data.
- **HFLF-GPR** - a model trained on a mix of LF and HF data without distinguishing the data fidelity.

# Numerical methods

## Surrogate models - 1

- The work is based on the Gaussian process regression (GPR).
- All of the models use an open-source library scikit-learn.

### Single-fidelity models

- **HF-GPR** - a model trained only high-fidelity (HF) data;
- **LF-GPR** - a model trained only on low-fidelity (LF) data.
- **HFLF-GPR** - a model trained on a mix of LF and HF data without distinguishing the data fidelity.

# Numerical methods

## Surrogate models - 2

### GPR with linear correction (LCGPR)

- 1 Train a single-fidelity model on LF data and test it on HF data -  $M_l(\mathbf{X}_l, \mathbf{y}_l) = \tilde{\mathbf{y}}_h$ .
- 2 Estimate an error ( $\Delta\mathbf{y}_h$ ) between the test results and the actual high-fidelity data and train a linear regression model  $\Delta M(\mathbf{X}_h, \Delta\mathbf{y}_h)$  to predict this error.
- 3 Correct the predictions of low-fidelity surrogate model for the the step one -  $M_l(\mathbf{X}_h)$  using the error correction model from the step two.

# Numerical methods

## Surrogate models - 2

### GPR with linear correction (LCGPR)

- 1 Train a single-fidelity model on LF data and test it on HF data -  $M_l(\mathbf{X}_l, \mathbf{y}_l) = \tilde{\mathbf{y}}_h$ .
- 2 Estimate an error ( $\Delta \mathbf{y}_h$ ) between the test results and the actual high-fidelity data and train a linear regression model  $\Delta M(\mathbf{X}_h, \Delta \mathbf{y}_h)$  to predict this error.
- 3 Correct the predictions of low-fidelity surrogate model for the the step one -  $M_l(\mathbf{X}_h)$  using the error correction model from the step two.



# Numerical methods

## Surrogate models - 2

### GPR with linear correction (LCGPR)

- 1 Train a single-fidelity model on LF data and test it on HF data -  $M_l(\mathbf{X}_l, \mathbf{y}_l) = \tilde{\mathbf{y}}_h$ .
- 2 Estimate an error ( $\Delta\mathbf{y}_h$ ) between the test results and the actual high-fidelity data and train a linear regression model  $\Delta M(\mathbf{X}_h, \Delta\mathbf{y}_h)$  to predict this error.
- 3 Correct the predictions of low-fidelity surrogate model for the the step one -  $M_l(\mathbf{X}_h)$  using the error correction model from the step two.

# Numerical methods

## Surrogate models - 3

### Multi-fidelity GPR (MFGPR) or co-kriging

It estimates for a poorly sampled variable  $\mathbf{y}_l(\mathbf{x})$  with the help of a well-sampled variable  $\mathbf{y}_h(\mathbf{x})$ :

$$\mathbf{y}_l(\mathbf{x}) = f_l(\mathbf{x}) + \epsilon_l$$

$$\mathbf{y}_h(\mathbf{x}) = \rho y_l(\mathbf{x}) + y_d(\mathbf{x})$$

# Numerical methods

## Metrics

### Mean relative prediction error (MRE)

$$MRE(\phi) = \frac{1}{N} \sum_{i=1}^N \frac{|\phi_{CFD} - \phi_{SM}|}{|\phi_{CFD}|}$$

We assume that less than **10% MRE** is acceptable for this model.

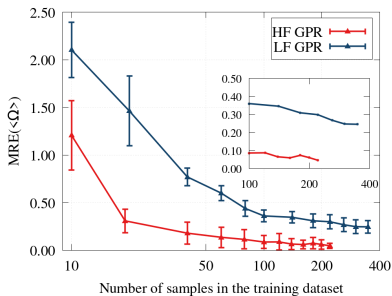
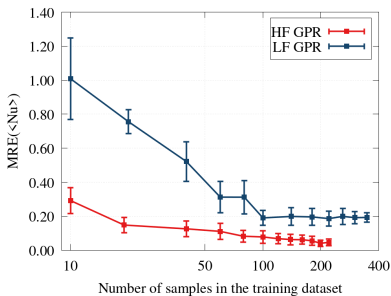
# Results

## Single-fidelity models

### Average computational cost

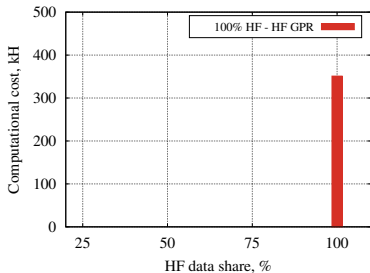
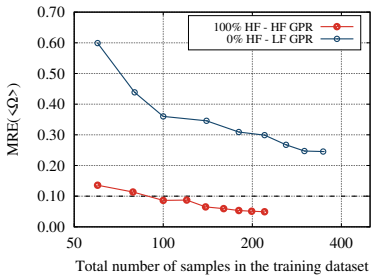
2700 core-hours - a high-fidelity simulation

285 core-hours - a low-fidelity simulation



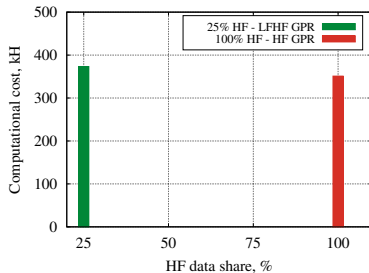
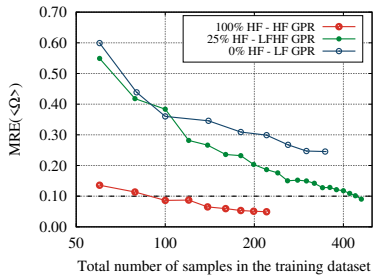
# Results

## HFLF GPR model



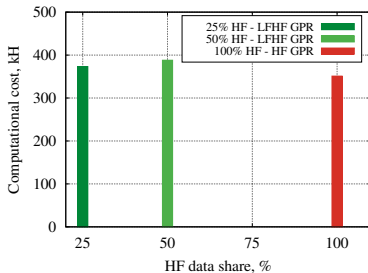
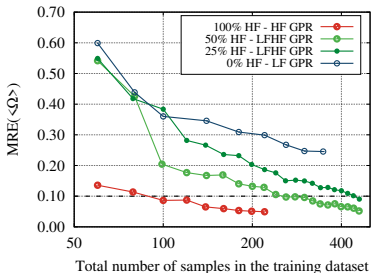
# Results

## HFLF GPR model



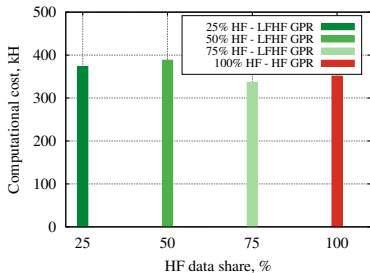
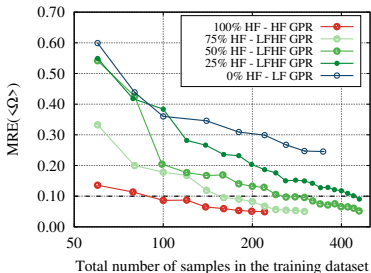
# Results

## HFLF GPR model



# Results

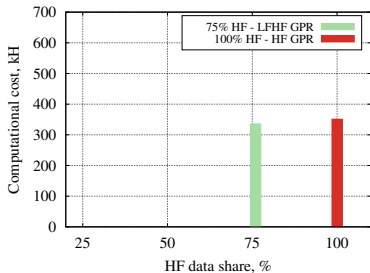
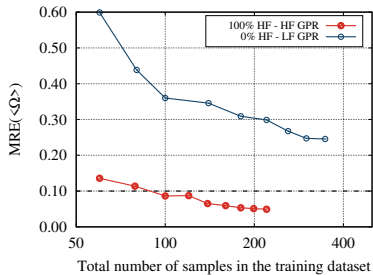
## HFLF GPR model





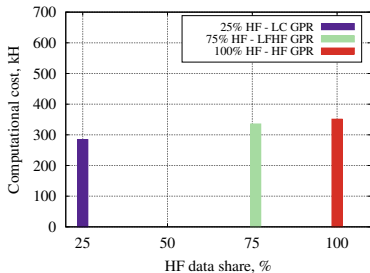
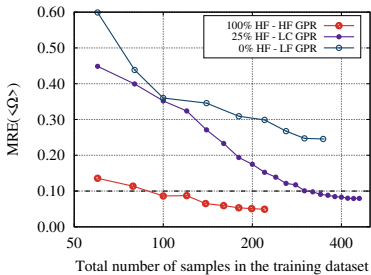
# Results

## LC GPR model



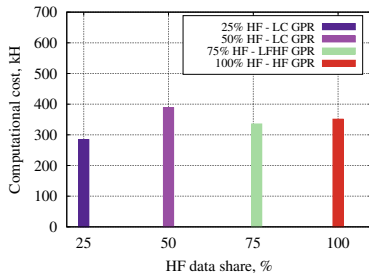
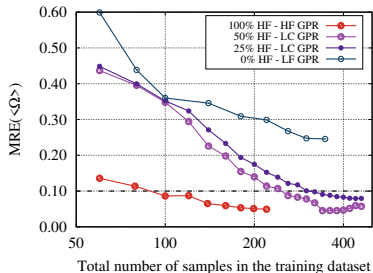
# Results

## LC GPR model



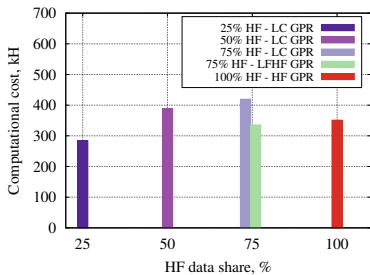
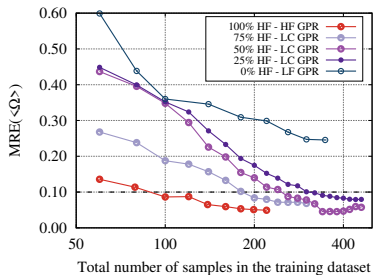
# Results

## LC GPR model



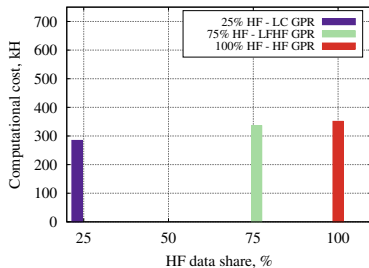
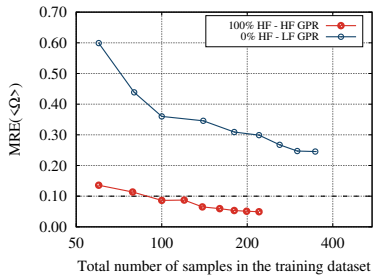
# Results

## LC GPR model



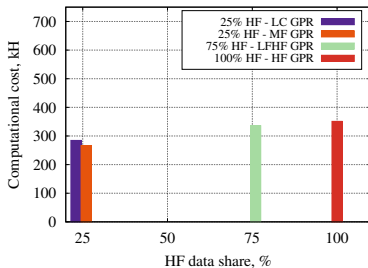
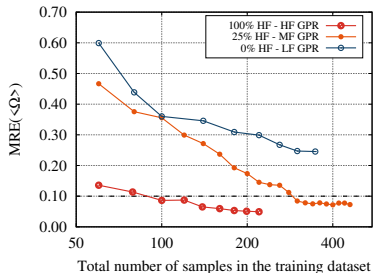
# Results

## MF GPR model



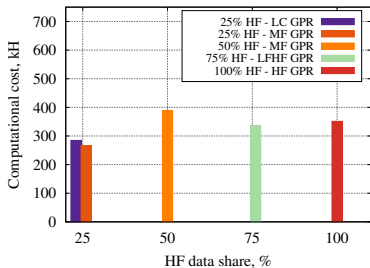
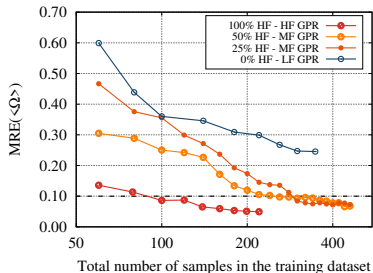
# Results

## MF GPR model



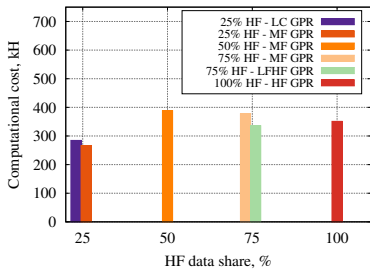
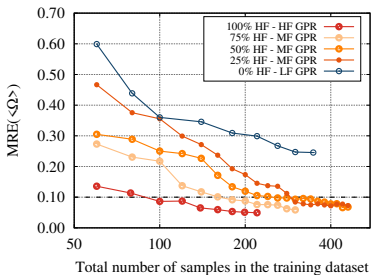
# Results

## MF GPR model



# Results

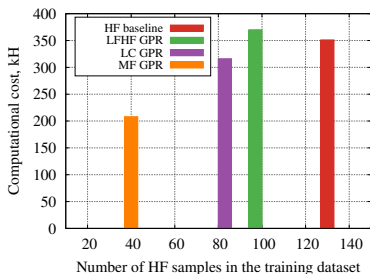
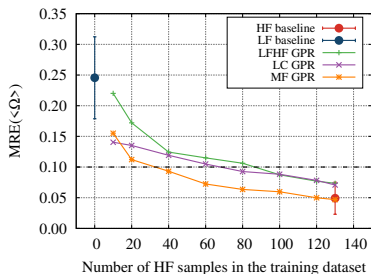
## MF GPR model





# Results

MRE of the average entrophy  $\langle \Omega \rangle$  for different number of HF training samples using different surrogate models



# Results

## Summary of the obtained results

Model	Samples			Kh	MRE	
	HF	LF	total		$\langle Nu \rangle$	$\langle \Omega \rangle$
HF GPR	130	-	130	351	$0.046 \pm 0.02$	$0.046 \pm 0.03$
LF GPR	-	350	350	100	$0.193 \pm 0.03$	$0.246 \pm 0.07$
HFLF GPR	120	40	160	335	$0.042 \pm 0.06$	$0.093 \pm 0.05$
LC GPR	75	225	240	285	$0.112 \pm 0.06$	$0.100 \pm 0.05$
MF GPR	40	350	380	208	$0.092 \pm 0.04$	$0.093 \pm 0.05$

# Conclusions

## Conclusions - 1

- The developed surrogate model provides almost instant accurate predictions using an ordinary office computer.
- The input data of the developed model is structured to take the values of temperature and velocity in the locations, which could be replaced by sensor readings.
- The main computational burden of the surrogate model is the cost of its development because, at this step, a comprehensive set of HF data is required.
- We spent 650Kh on 240 HF CFD simulations and 100Kh on 350 LF simulations.



# Conclusions

## Conclusions - 1

- The developed surrogate model provides almost instant accurate predictions using an ordinary office computer.
- The input data of the developed model is structured to take the values of temperature and velocity in the locations, which could be replaced by sensor readings.
- The main computational burden of the surrogate model is the cost of its development because, at this step, a comprehensive set of HF data is required.
- We spent 650Kh on 240 HF CFD simulations and 100Kh on 350 LF simulations.

# Conclusions

## Conclusions - 1

- The developed surrogate model provides almost instant accurate predictions using an ordinary office computer.
- The input data of the developed model is structured to take the values of temperature and velocity in the locations, which could be replaced by sensor readings.
- The main computational burden of the surrogate model is the cost of its development because, at this step, a comprehensive set of HF data is required.
- We spent 650Kh on 240 HF CFD simulations and 100Kh on 350 LF simulations.

# Conclusions

## Conclusions - 1

- The developed surrogate model provides almost instant accurate predictions using an ordinary office computer.
- The input data of the developed model is structured to take the values of temperature and velocity in the locations, which could be replaced by sensor readings.
- The main computational burden of the surrogate model is the cost of its development because, at this step, a comprehensive set of HF data is required.
- We spent 650Kh on 240 HF CFD simulations and 100Kh on 350 LF simulations.



# Conclusions

## Conclusions - 2

- The use of multi-fidelity models reduced the computational cost considerably.
- Even a simple HFLF GPR model is less computationally expensive than the baseline HF GPR model.
- More sophisticated multi-fidelity models like LC GPR and MF GRP required at least 1.5 times less computational resources than the HF GPR model.
- The MF GRP has shown the best trade-off between computational cost and accuracy among studied multi-fidelity models.

# Conclusions

## Conclusions - 2

- The use of multi-fidelity models reduced the computational cost considerably.
- Even a simple HFLF GPR model is less computationally expensive than the baseline HF GPR model.
- More sophisticated multi-fidelity models like LC GPR and MF GRP required at least 1.5 times less computational resources than the HF GPR model.
- The MF GRP has shown the best trade-off between computational cost and accuracy among studied multi-fidelity models.



# Conclusions

## Conclusions - 2

- The use of multi-fidelity models reduced the computational cost considerably.
- Even a simple HFLF GPR model is less computationally expensive than the baseline HF GPR model.
- More sophisticated multi-fidelity models like LC GPR and MF GRP required at least 1.5 times less computational resources than the HF GPR model.
- The MF GRP has shown the best trade-off between computational cost and accuracy among studied multi-fidelity models.

# Conclusions

## Conclusions - 2

- The use of multi-fidelity models reduced the computational cost considerably.
- Even a simple HFLF GPR model is less computationally expensive than the baseline HF GPR model.
- More sophisticated multi-fidelity models like LC GPR and MF GRP required at least 1.5 times less computational resources than the HF GPR model.
- The MF GRP has shown the best trade-off between computational cost and accuracy among studied multi-fidelity models.

# Conclusions

## Future work

- Study the generalization properties of the developed methodology.
- Adapt the existing methodology to a direct prediction of comfort parameters, such as predicted mean vote.
- A more broad study on a proper choice of data fidelity is required.
- The model could be further analyzed in terms of extrapolation capabilities.

# THANK YOU FOR YOUR ATTENTION!

## Ready for your questions!

