Data-driven prediction of flow parameters in a ventilated cavity using high-fidelity CFD simulations

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Nina Morozova

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Outline

1) Introduction
2) Test case and model description
3) Results
4) Discussion
5) Conclusions
6) Recent advances
7) Future work
Introduction

• The outburst of COVID-19 has highlighted the importance of ensuring adequate indoor air quality to reduce the risk of infection contamination in confined spaces.

• Proper design and precise control of air parameters are essential for ensuring indoor air quality.

• Fast and accurate computations of indoor airflow are crucial for testing different design options or performing model predictive control (MPC).
Traditional indoor airflow models

• **Multizone (airflow network) models** - low computational cost but not applicable for complex flows.

• **Zonal models** - moderate computational cost and moderate accuracy, but high case dependence.

• **Computational Fluid Dynamics (CFD)** - high computational cost and high accuracy.
Data-driven models (DDMs)

• Find relations between system state variables without explicit knowledge of the physical behavior of the system using data analysis.

• A comprehensive set of the high-quality input-output dataset is needed to train these models for all possible working conditions.

• Difficulties in obtaining high-fidelity training data are compensated by the resulting model's high accuracy and low computational cost.

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Objectives of the work

1) Develop machine learning based DDM, which uses the data from high-fidelity CFD simulations.

2) Investigate the capabilities and limitations of this model as a cheaper alternative to CFD, taking into account specific requirements for indoor environmental applications.
Governing equations

\[
\nabla \cdot \mathbf{u} = 0
\]
\[
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \nabla^2 \mathbf{u} - \frac{1}{\rho} \nabla p + \beta \mathbf{g} (T - T_0)
\]
\[
\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \alpha \nabla^2 T,
\]

where \( \mathbf{u} \) is the velocity vector, \( t \) the time, \( p \) the pressure, \( T \) the temperature, \( T_0 \) the reference temperature, \( \nu \) the kinematic viscosity, \( \rho \) the density, \( \mathbf{g} \) the gravitational acceleration, \( \beta \) the thermal expansion coefficient and \( \alpha \) the thermal diffusivity.
Physical problem

\[ A_D = \frac{D}{W} = 0.3 \]
\[ A_{in} = \frac{h_{in}}{H} = 0.017 \]
\[ A_{out} = \frac{h_{out}}{H} = 0.023 \]
\[ Pr = 0.71 \]
\[ Ra_H = 2.4 \times 10^9 \]

\[ A_H = \frac{H}{W} = [0.25, 0.5, 1, 2, 4] \]

\[ Fr = [1.10, 1.50, 2.00, ..., 5.00, 5.24, 5.50, ..., 10.00] \]
Model input data

\[ A_D = \frac{D}{W} = 0.3 \]
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Model output data

Nusselt number on the hot wall -

\[ <Nu> = -\frac{1}{A} \int_A \frac{\partial T}{\partial y} \, dA \quad \text{at} \quad y = 0 \]

Average cavity temperature -

\[ <T_v> = \frac{1}{V} \int_V T \, dV \]

Flow separation point -

\[ x_{sep} = x, \quad \text{at} \quad <\tau_W> = \int \frac{\partial u}{\partial y} \, dz = 0, \quad y = H, \]

Average kinetic energy -

\[ <E> = \frac{1}{V} \int_V \frac{u^2}{2} \, dV \]

Average enstrophy -

\[ <\Omega> = \frac{1}{V} \int_V \omega^2 \, dV, \]
Details of the CFD simulations

- **LES-S3PQ** turbulence model with second-order symmetry-preserving staggered discretization.
- All simulations run for 500 non-dimensional time units.

<table>
<thead>
<tr>
<th>( N_x )</th>
<th>( N_y )</th>
<th>( N_z )</th>
<th>( N_{\text{tot}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>100 ( \times A_H )</td>
<td>160</td>
<td>32</td>
<td>( 5.12 \times 10^5 \times A_H )</td>
</tr>
</tbody>
</table>

- 100 CFD simulations.
- 15% - for testing and 85% - for training.
Accuracy metrics

Relative error

$$RE(\phi) = \frac{|\phi_d - \phi_p|}{|\phi_d|},$$

Mean relative error

$$MRE(\phi) = \frac{1}{N} \sum_{i=1}^{N} RE(\phi)$$

We assume that the less than 15% RE is acceptable for this model.
Artificial neural network

- Densely connected ANN with layer configuration of 20-16-5.
- Rectified linear activation function (ReLU).
- 10-fold cross validation.
Model performance on varying number of samples in training dataset

![Graph showing model performance on varying number of samples in training dataset]
Model performance on different probe combinations

<table>
<thead>
<tr>
<th>Probes removed</th>
<th>$\langle Nu \rangle$</th>
<th>$\langle TV \rangle$</th>
<th>$x_{sep}$</th>
<th>$\langle E \rangle$</th>
<th>$\langle \Omega \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>none</td>
<td>0.144</td>
<td>0.018</td>
<td>0.014</td>
<td>0.086</td>
<td>0.095</td>
</tr>
<tr>
<td>3</td>
<td>0.146</td>
<td>0.023</td>
<td>0.067</td>
<td>0.082</td>
<td>0.102</td>
</tr>
<tr>
<td>3,4</td>
<td>0.154</td>
<td>0.051</td>
<td>0.068</td>
<td>0.093</td>
<td>0.118</td>
</tr>
<tr>
<td>3,4,6</td>
<td>0.197</td>
<td>0.076</td>
<td>0.084</td>
<td>0.145</td>
<td>0.144</td>
</tr>
<tr>
<td>3,4,6,7</td>
<td>0.343</td>
<td>0.165</td>
<td>0.115</td>
<td>0.195</td>
<td>0.228</td>
</tr>
</tbody>
</table>
RE of $<\text{Nu}>$ and $<T_Y>$ for different combinations of Fr and $A_H$
RE of $<x_{sep}>$ for different combinations of Fr and $A_H$
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Discussion. Dataset generation

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• The dataset should be increased, in order to develop a more reliable model.
Discussion. Model advantages and disadvantages

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- These models work better with simple geometries.

- DDMs could be used for applications where a combination of fast and accurate predictions is required.
Conclusions

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3) The accuracy for some of the most complex flow configurations was insufficient.
Conclusions

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2) The developed DDM provides rapid and accurate predictions using an ordinary office computer.

3) The accuracy for some of the most complex flow configurations was insufficient.

4) More high-fidelity data is required to construct a robust and reliable model.
## Recent advances

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<table>
<thead>
<tr>
<th>$Ah$</th>
<th>Ra</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$1.5 \times 10^8$</td>
</tr>
<tr>
<td>0.25</td>
<td>FG</td>
</tr>
<tr>
<td>0.50</td>
<td>FG</td>
</tr>
<tr>
<td>1.00</td>
<td>FG</td>
</tr>
<tr>
<td>2.00</td>
<td>FG</td>
</tr>
<tr>
<td>4.00</td>
<td>CG</td>
</tr>
</tbody>
</table>

$Fr = [1.00, ..., 10.00]$  

- Total number of coarse-grid (CG) simulations 120  
- Total number of fine-grid (FG) simulations 240
Recent advances

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<table>
<thead>
<tr>
<th>Model</th>
<th>MRE</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$&lt;N_u&gt;$</td>
</tr>
<tr>
<td>ANN</td>
<td>0.012</td>
</tr>
<tr>
<td>SVR</td>
<td>0.010</td>
</tr>
<tr>
<td>GBR</td>
<td>0.018</td>
</tr>
<tr>
<td>GPR</td>
<td>0.034</td>
</tr>
</tbody>
</table>
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Future work

• Adapt the model to the necessities of MPC.

• Investigate the possibilities of constructing multi-fidelity models by combing fine and coarse grid CFD.

• Study the extrapolating capabilities of DDMs.
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