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A Computational Toolchain for the Automatic Generation of Multiple Reduced-Order Models from CFD Simulations

Thibault Marzullo*
Department of Mechanical Engineering
National University of Ireland, Galway
E-mail: t.marzullo1@nuigalway.ie

Marcus M. Keane
Department of Civil Engineering
National University of Ireland, Galway
E-mail: marcus.keane@nuigalway.ie

Marco Geron
School of Mechanical and Aerospace Engineering
Queen's University Belfast
E-mail: m.geron@qub.ac.uk

Rory F.D. Monaghan
Department of Mechanical Engineering
National University of Ireland, Galway
E-mail: rory.monaghan@nuigalway.ie

ABSTRACT

The present study aims to develop a systematic tool chain for automatically extracting accurate Reduced-Order Models (ROMs) from Computational Fluid Dynamics (CFD) simulations for use in the design and operation of near-zero energy buildings, with a higher accuracy than traditional zonal models but at a fraction of the computational cost of CFD. This study assesses the accuracy and time to solution of ROMs when solved for different Boundary Conditions (BCs) in order to define the usability envelope of the automatically extracted ROMs. The parameters used in this study are inlet temperatures and mass flow rates. Results show that the absolute error can be kept under 0.5K for changes in temperature of up to ±15K and under 0.25K for changes in mass flow rates of up to ±45% of the original value. The results show that this method has potential for applications in the built environment where its accuracy and low computational cost can bridge a gap between low order RC models and high order CFD, further improving energy efficiency in smart buildings.

KEYWORDS

CFD, reduced, order, zonal, automatic, indoor, MPC

INTRODUCTION

Sustainability, as defined by the ASHRAE Handbook of Fundamentals [1], is "providing for the needs of the present without detracting from the ability to fulfil the needs of the future". A key approach to improve the sustainability of energy use is the reduction of waste through careful planning, optimization and management of demand. In the built environment, the use of models of building thermal conditions during both the design and operation phases is recognised as a powerful method to increase energy efficiency and reduce energy demand [2].

These computer models can be grouped into three categories: (1) physics-based models, (2) experimental models, and (3) mixed models [3]. Physics-based (theoretical) models describe in detail the studied system and its subsystems, and define an output based on mathematical equations constrained by physical laws. They are typically used during the preliminary design and energy audit phases. Experimental models on the other hand are tailored to a particular system. Through experimentation, the system's response to various inputs is evaluated and the model is developed accordingly. Finally, mixed models are physics-based models for which parameters are estimated using statistical and/or experimental analysis. Among physics-based models, Computational Fluid Dynamics (CFD) is a powerful and increasingly widespread tool for simulating fluid domains, which yields models of high fidelity [4], [5]. However, its large computational expense renders it too time-consuming for operational, and even some design, tasks [6], [7]. Designers and operators therefore often choose lower fidelity but faster methods when available [8].
In order to overcome some of these issues we propose a tool chain called CFD-ROM (Computational Fluid Dynamics – Reduced Order Model), which will automatically extract ROMs from CFD simulations and solve them rapidly for a wide range of conditions, including those for which no CFD solutions are available. The method aims to develop ROMs that will retain a high level of accuracy, similar to the CFD simulations, but at a significantly lower computational cost [9]. This will bridge the gap between lower order models and CFD, allowing operators and designers access to simplified yet accurate multi-zonal models that can be extracted automatically and without expertise, and solved in real time.

METHODOLOGY

The proposed method for ROM generation automatically extracts a multi zonal model from a CFD simulation, which can then be solved for boundary condition parameters different from the original CFD. The main advantages of this method are the level of automation, which allows generation of ROMs with minimal user input and expertise; the level of fidelity compared to CFD, which enables the ROM to retain most of the CFD simulation's accuracy; and finally the computational cost, which allows the generation of ROMs in under 60 seconds and their solution in under 0.95 seconds.

The CFD-ROM method consists in 6 main steps as shown in Figure 1: (1) the results of a CFD simulation are imported, (2) CFD computational cells are clustered together to create zones, which are uniform volumes of air, (3) interactions between zones and between zones and domain boundaries are processed, (4) a ROM is generated and (5) solved, and finally (6) the solved ROM is remapped back to the CFD domain.

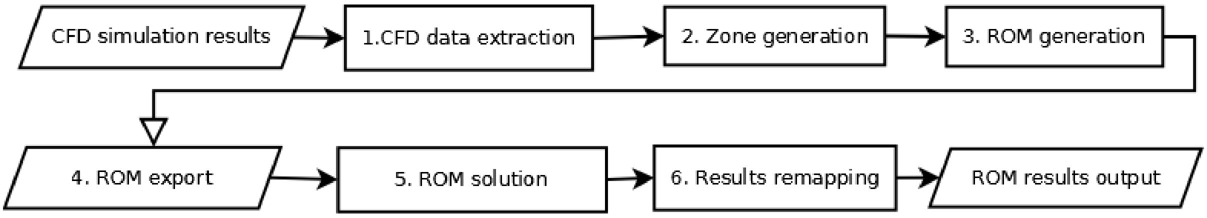


Figure 1: CFD-ROM method flowchart outlining the main steps of the method.

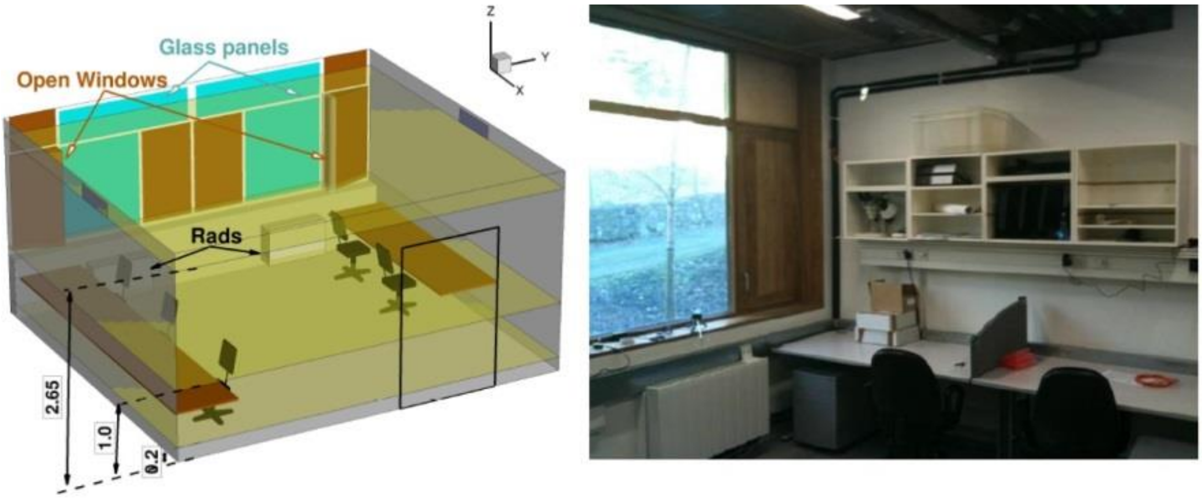


Figure 2: Numerical and physical domain of the ERI building office modelled in CFD

This section presents the methods used in the development of the algorithms in Python [10] for extraction and solution of the ROMs. Firstly, it presents the CFD simulations on which the ROMs have been tested and assessed, then the principles of zone generation, ROM generation and solution are explained.

CFD Simulations and Validation

The data used in this comparative study are taken from the previously validated CFD model of a north-facing office in the Environmental Research Institute (ERI) building at University College Cork (UCC) shown in Figure 2 [11]. CFD models were developed using Phoenics [12] modelling software to generate a database of test cases. For all simulations, turbulence is modelled using the steady state Reynolds Average Navier-Stokes (RANS) approach coupled with the Re-Normalisation Group (RNG) k-ε turbulence model. Air is modelled as an incompressible ideal gas. Phoenics utilises an immersed body technique and consequently the domain is discretized using a Cartesian structured grid with 1,572,165 cells (115x147x93). Constant temperature boundary conditions have been utilised for the ceiling, the floor, and east and west walls. All other objects are considered adiabatic. All CFD simulations used have been validated with experimental data and previously published [11].

The CFD domain energy sources are listed in Table 1. In the case used for this study, the windows and door are closed and the two convectors are on. The domain includes two air vents located on the east and west walls close to the ceiling. The two convectors are located on the north wall, close to the windows.

Table 1: CFD simulation base boundary conditions

Boundary	Comment	Type	Base value
Convectors			
East convector		Air inlet	$T_{Econvector}$ = 45 °C $\dot{m}_{Econvector}$ = 0.048 kg.s^{-1}
West convector		Air inlet	$T_{Wconvector}$ = 45 °C $\dot{m}_{Wconvector}$ = 0.048 kg.s^{-1}
Walls			
Ceiling		Constant temperature	$T_{ceiling}$ =23.2 °C
Floor		Constant temperature	T_{floor} =18 °C
East wall		Constant temperature	T_{Ewall} =20 °C
West wall		Constant temperature	T_{Wwall} =20 °C
Windows			
East window	Closed	Air inlet	$T_{Ewindow}$ = 9.35 °C $\dot{m}_{Ewindow}$ = 0 kg.s^{-1}
West window	Closed	Air inlet	$T_{Wwindow}$ = 8.3 °C $\dot{m}_{Wwindow}$ = 0 kg.s^{-1}
Other openings			
East vent		Opening	T_{Event} = 20.2 °C P_{Event} = 1.013 x10^5 Pa
West vent		Opening	T_{Wvent} = 20.7 °C P_{Wvent} = 1.013 x10^5 Pa
Door	Closed		$\dot{m}_{door}$ = 0 kg.s^{-1}

Zone Generation

As stated previously, ROMs are achieved by further discretizing the CFD domain by clustering computational cells together depending on their position and their zone criterion. Zone criteria are any variable for which clustering is demanded: temperature, density, air velocity, etc. The method currently uses one criterion at a time, and the ROMs presented in this study have been generated with cell temperature as the zone criterion.

Firstly, zone-types are defined. A zone-type is a group of cells which zone criterion belongs to an interval of, in this study, temperatures. Such intervals are defined as follows: first the mean value of the temperature is processed over the entire CFD domain. Two zone-types are then defined: a zone-type containing all the cells which temperature is higher than the mean value, and another containing all the cells which temperature is lower or equal to the mean value. Subsequently the zone-types are iteratively subdivided in smaller zone-types, according to the mean value of temperature within each zone-type.
As a result, 2^n zone-types are defined, with n the number of times this process is repeated. The user has control over the number of zone-types as this affects the discretization process. More zone-types allow a higher fidelity to the original CFD, but higher computational costs incur as discussed later in the Results section.

Once zone-types have been defined for the ROM, the algorithm starts assigning cells to zones as shown in Figure 3. A zone is a cluster of computational cells which (1) are adjacent and (2) belong to the same zone-type. The algorithm starts by creating an empty zone, and populates it with the first computational cell it finds.

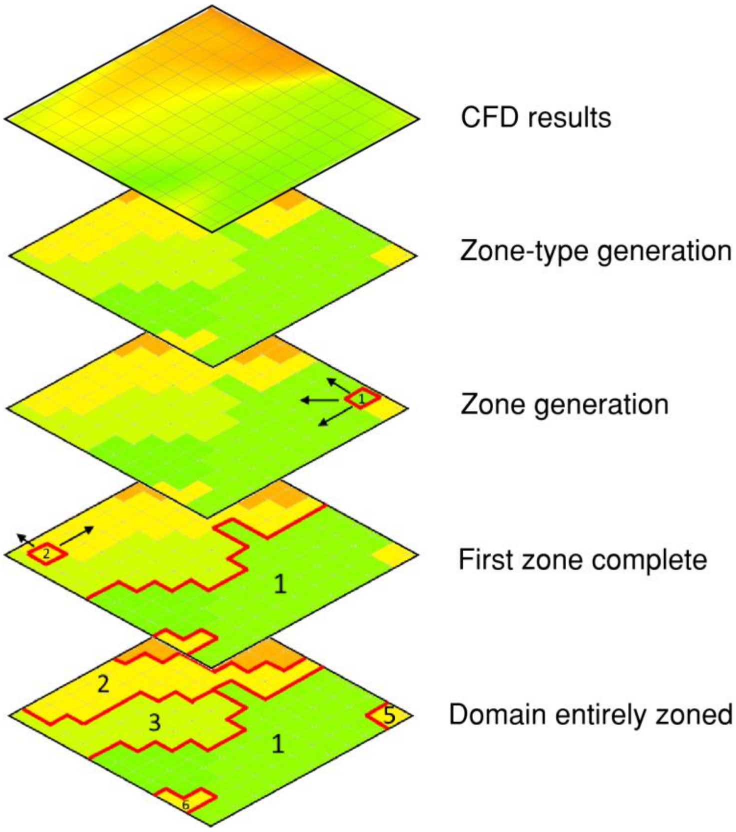


Figure 3: Representation of the zone generation algorithm in 2 dimensions. The algorithm first defines zone-types and then assigns all adjacent cells of the same zone-type to a new zone.

The cells adjacent to this initial cell are scanned, and if they belong to the same zone-type they are added to the zone. The same process is repeated for all the cells in the same zone, until no more suitable cells are found.

At that point the algorithm creates a new zone and repeats the process until all the cells of the domain are assigned to a zone.

Computationally, at this point the original CFD domain has been discretized from the original large number of cells to the final reduced number of zones. In order to generate a ROM it is then necessary to process interactions between zones, and between zones and domain boundaries.

ROM Generation

The first step in ROM generation is to consider zones as uniform volumes in the CFD domain. The average values of temperature, density, pressure, etc. are computed over the cells belonging to each zone in order to obtain the uniform zone properties.

Next, the zone-zone interactions must be computed. The algorithm calculates the mass flow rates at the zone-zone interfaces by selecting all cells which have a neighbour assigned to a different zone, and computing the unitary mass flow rate at the interface between these two neighbouring cells. The total mass flow rate between zones is calculated as the sum of all the unitary mass flow rates at the zone-zone interface.

After computing the zone-zone interactions, the algorithm detects the sources of energy such as air inlets, non-adiabatic walls, etc. Similarly to zone-zone interactions, the mass flow rates of inlets/outlets into each zone are computed at their interface and the total mass flow rate between an inlet/outlet and a zone is the sum of all unitary mass flow rates.

Finally, the thermal boundaries such as non-adiabatic walls are assumed uniform, they are assigned an average temperature and a constant UA depending on their contact area with each zone.

ROM Solution

Currently, the ROMs are solved with Sinda/FLUINT [13], a commercial software for finite-difference, lumped parameter fluid flow analysis of complex systems.

The data generated from zone properties and interactions with the domain are compiled to respect Sinda/FLUINT's input format: (1) zones are translated into "tanks", which are lumps of constant volume and uniform properties (temperature, density, pressure); (2) inlets and outlets are translated into "plena", which are similar lumps but with infinite volume; and (3) walls and other purely thermal sources are translated to thermal nodes, with uniform temperature.

A network is then created, linking these elements through corresponding interactions: mass exchange between fluid lumps, and heat exchange between fluid lumps and thermal nodes. Mass exchanges are computed directly from the mass flow rates at zone-zone interfaces found previously, and heat exchanges are computed from a constant UA defined between each zone and thermal boundary.

Once the model is solved, Sinda/FLUINT returns the steady-state solution with properties for each lump which can then be mapped back to the original CFD domain for comparison.

Error measurement

The present study uses the weighted mean absolute error in Kelvin (WMAE), shown in Equation 1. The weighting corresponds to the volume of each cell relative to the total volume of the domain, in order to account for varying cell volumes especially close to the boundaries where the CFD mesh is finer.

$$WMAE = \sum_{i=0}^{n} \frac{V_i \times |T_{CFDi} - T_i|}{V_{domain}} \tag{1}$$

Where n is the number of cells in the domain, V_i *is the volume of cell i,* V_{domain} *is the total volume of the domain,* T_{CFDi} *is the original CFD temperature of cell i, and* T_i *is the temperature assigned to the cell after solving the ROM.*

RESULTS

A previous study [9] by the authors assessed the accuracy of various zone generation algorithms. This study presents the results obtained when modifying the parameters of a ROM to predict temperature distributions for BCs that differ from the ones of the original CFD simulations.

In order to achieve this, a set of CFD simulations was generated. For the same computational domain, simulations were ran featuring different inlet temperatures and mass flow rates. Table 2 presents the sets of parameters for boundary conditions used in this study. The cases range from T-10 to T+15 for temperature, including T+5b where the temperature of the west convector only is modified leaving the east one to 45°C (the base temperature); and from M-45% to M+100% for mass flow rates at the convectors.

Table 2: list of boundary conditions parameters used in MultiROM and MultiCFD

Variable	Cases	Values
Temperature ($T_{convector}$)	T-10	35°C
	T-5	40°C
	Base	45°C
	T+5b	50°C (West) & 45°C (East)
	T+5	50°C
	T+10	55°C
	T+15	60°C
Mass flow rates ($\dot{m}_{convectors}$)	M-45%	0.0528 $kg.s^{-1}$
	M-30%	0.0672 $kg.s^{-1}$
	Base	0.096 $kg.s^{-1}$
	M+30%	0.1248 $kg.s^{-1}$
	M+45%	0.1392 $kg.s^{-1}$
	M+60%	0.1536 $kg.s^{-1}$
	M+100%	0.192 $kg.s^{-1}$

ROMs have been generated for zone numbers ranging from 2 to 51 in order to define at which point the error starts converging around a minimal value. The error quickly decreases for 2-11 zones then stabilizes around 22 zones and is nearly constant thereafter as shown in Figure 4 along with the corresponding solution times. Therefore, the ROMs presented in this study are in the 20-25 zones range, the range being due to the fact that while the user can demand a certain number of zones, there are occasionally a limited number of odd zones created to accommodate large temperature gradients in the domain.

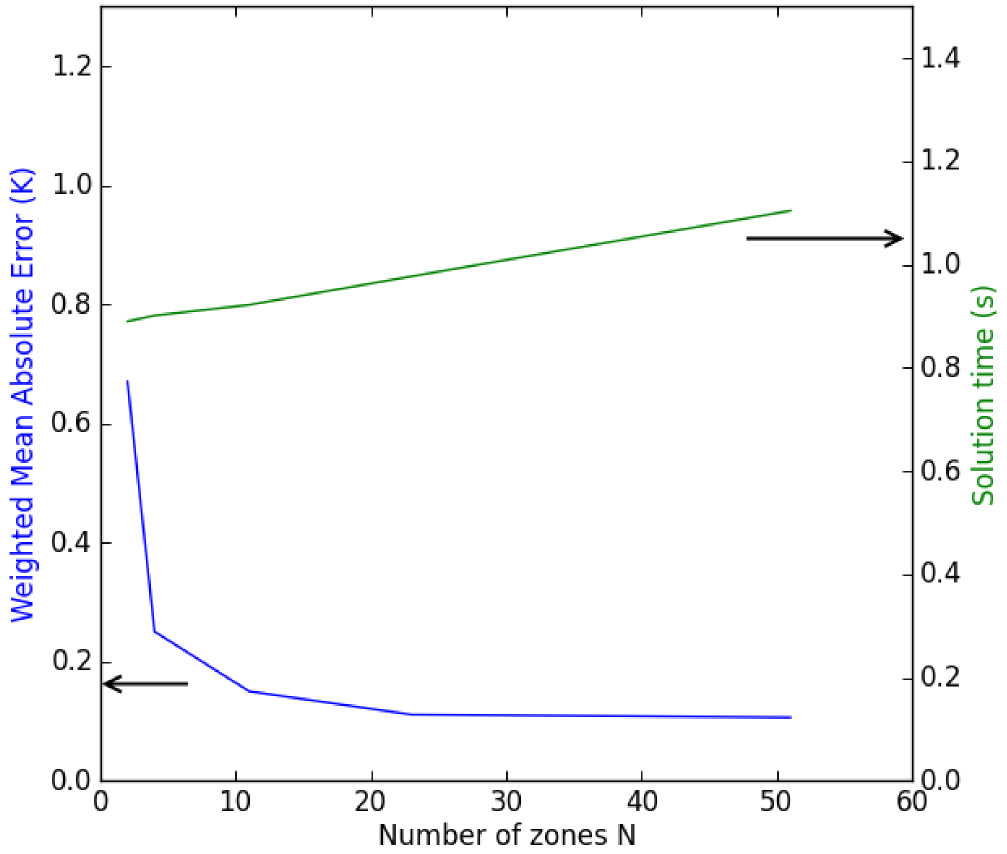


Figure 4: ROM size independence study.

ROM accuracy when varying BC parameters

In order to measure the effect that changing the ROM parameters has on accuracy and assess the usability envelope of ROMs, for each case two ROMs were generated. The first, called "MultiCFD", is generated directly from the corresponding CFD case and no parameters are changed before solving it. It serves as a basis for estimating the relative accuracy of the second, called "MultiROM", which is a ROM generated from the base CFD case and subsequently modified to match the new BC parameters. Developing a method for generating flexible and accurate MultiROMs is the main objective of this research, in order to provide designers and operators with a tool that would allow them to simulate the built environment when multiple CFD simulations are either unavailable or unpractical.

The modelled office and its corresponding CFD simulation features two convectors for which a temperature and air velocity are defined. This study assesses the accuracy of ROMs when (1) the convectors temperature $T_{convector}$, and (2) their mass flow rate $\dot{m}_{convector}$ are changed. The ROMs are extracted from the "base" CFD case, then their parameters are changed to match the other CFD cases, the ROMs are solved and finally their outputs are compared to the corresponding CFD case results.

The first test was to replicate previous results by the authors obtained when varying only temperatures by ±10K around the base temperature, then to reach +15K of variation around the base temperature. Figure 5 shows the absolute error for each case, in both MultiCFD and MultiROM scenarios. The ROMs show a good level of accuracy when solved for this range of parameters, considering the ± 0.6K uncertainty range of temperature sensors commonly met in the built environment [14].

The second, and novel, set of results was generated by varying the convectors mass flow rates. In order to achieve this, an additional function was added to the code to ensure that the ROM mass flow rates were all balanced, as changing the inlets mass flow rates would alter the balance. This step is done in a purely mathematical manner, where zone by zone the inflows and outflows are iteratively balanced to match the new BCs. The results are presented in Figure 6 and show that up to ±45% of change in mass flow rates at the convectors, the ROM still has an absolute error under 0.5K versus 0.11K of error for the base, unmodified case – with the exception of the +45% case with 0.84K of absolute error. This again falls into the uncertainty range of common temperature sensors.

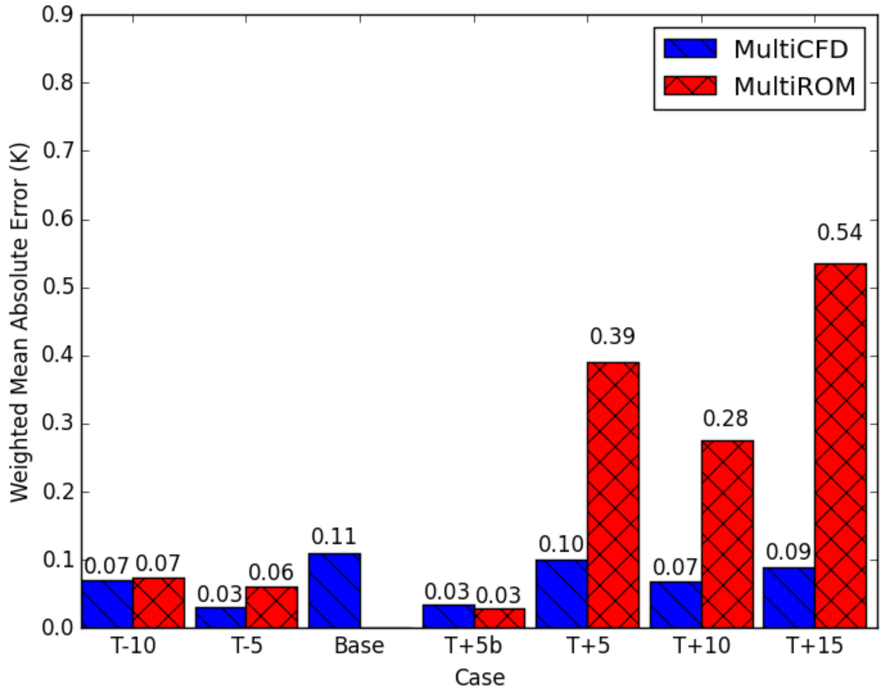


Figure 5: MultiCFD and MultiROM error when changing BC temperatures.

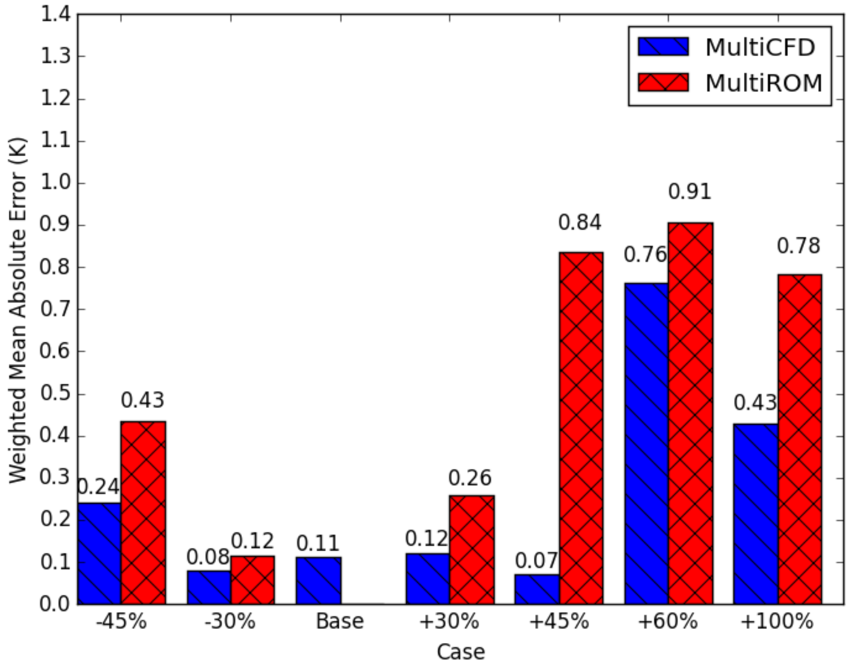
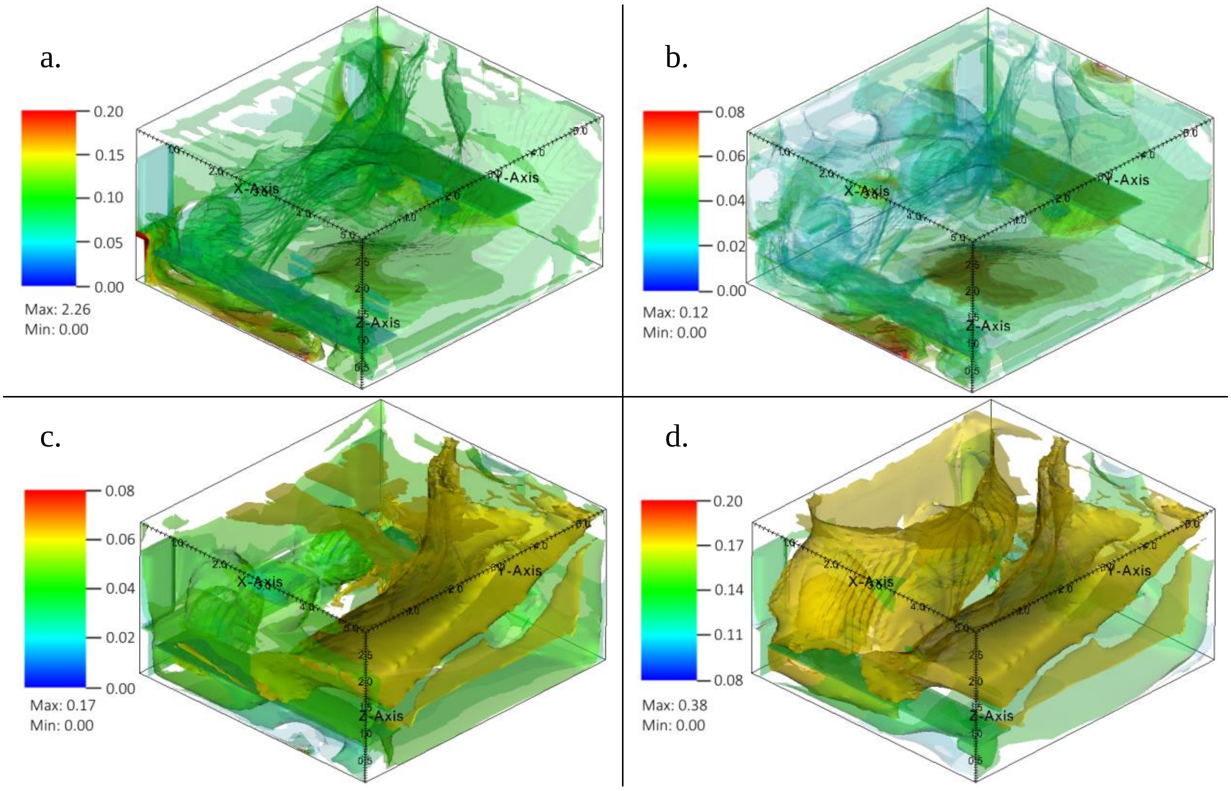


Figure 6: MultiCFD and MultiROM error when changing BC mass flow rates



Error plots

A study of the local error was done in order to assess more finely the fidelity of the ROMs against the original CFD simulations. Figure 7 shows semi-opaque iso-surface plots of the ṁ-45% to ṁ+45% cases. No peaks in local error stand out, except for a very limited amount of odd cells certainly due to minor computational errors such as the assignment of a cell to the wrong zone. Results are identical for the T-10 to T+15 cases, suggesting that the algorithm is able to accurately capture the domain's thermal distribution, including the volumes with high temperature gradients such as above and around the convectors.

Figure 7: Iso-surface WMAE (in K) plots of cases (a) ṁ-45%, (b) ṁ-30%, (c) ṁ+30% and (d) ṁ+45%.

DISCUSSION

This study showed that it is possible to extract multi-zonal ROMs from CFD simulations with high fidelity and in real time. These findings can be mitigated by the relative simplicity of the case displayed in this study, where only two convectors and two vents are present in the domain. Further research must be done on other indoor environments, such as open-space offices, theatre rooms, sports complexes, etc. in order to assess the usability of the method in more complex environments featuring larger spaces and openings, air vents, HVAC outlets, which could affect the accuracy of the ROMs.

In both studies, when varying temperature and mass flow rates the ROMs are generally more accurate when lowering the parameters values than they are when the values are increased. When solving for different BCs, the parameters computed on the base case are not valid anymore and lead to increasing error as the new ROM differs more and more from the base case. This is likely caused by the assumptions made when compiling the model for Sinda/FLUINT, namely the constant values assigned to zone-zone mass flow rates and wall heat transfers. An improvement upon the current iteration of the method will be the implementation of variable mass flow rates and heat transfers. The asymmetrical change in error, lower when temperatures are colder and mass flow rates weaker, may be due by the fact that the domain becomes more and more uniform as the energy flow in the domain is lower.

Nevertheless, the results are encouraging when considering the usual ±0.6K uncertainty of temperature sensing techniques in the built environment [14]. The possibility to change boundary temperatures by ±15K and mass flow rates by ±45% while maintaining an acceptable level of accuracy allows the consideration of, for example, thermal comfort and HVAC control as potential applications for which further research must be done.

Additionally the authors consider the inclusion of multiple-criteria zone generation, versus the current single-criterion zone generation, as an important upgrade to the algorithm which may improve its accuracy especially when mass flow rates must be changed.

CONCLUSION

The accuracy of CFD is recognized to have a potentially substantial impact on building energy consumption through methods such as virtual sensing [15]. Unfortunately, the computational costs involved in solving a CFD model render it unpractical for real-time applications such as BEMS. This study proposed a method capable of extracting ROMs from CFD simulations and solving them in near real-time, for boundary conditions that were different from the original CFD BCs. These multi-zonal ROMs have an accuracy comparable to the uncertainty in sensing equipment used in the built environment, thus rendering them useful in applications such as virtual sensing. This study showed a good level of accuracy when solving ROMs in real time for BCs different from the original CFD simulation. This enables the use of CFD-ROM for thermal comfort assessment, BEMS, and applications where the unavailability of real-time multi-zonal models is detrimental.

The next steps in the development of the CFD-ROM toolchain are: (1) the generation of ROMs for different indoor environments, such as large spaces; (2) the investigation of techniques that would improve ROMs accuracy when solving for different inlet mass flow rates; (3) the development of a tailored solver in the open-source language Modelica [16].

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NOMENCLATURE

BC	*Boundary Condition*
BEMS	*Building Energy Management System*
CFD	*Computational Fluid Dynamics*
CFD-ROM	*Computational Fluid Dynamics – Reduced Order Model*
$\dot{m}$	*Mass flow rate (in kg.s-1)*
MultiCFD	*ROM extracted and solved for the same BCs*
MultiROM	*ROM extracted and solved for different BCs*
P	*Pressure (in Pa)*
RANS	*Reynolds Average Navier-Stokes*
RNG	*Re-Normalisation Group*
ROM	*Reduced Order Model*
T	*Temperature (in °C)*
WMAE	*Weighted Mean Absolute Error (in K)*

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