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Calibrating models for MPC of energy systems in buildings using an adjoint-based sensitivity method

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Abstract

For several years, Model Predictive Control (MPC) is depicted in the literature as a promising way to increase buildings' energy efficiency during operation. This model-based control technique uses the optimal control theory to provide a constraint compliant, anticipative control, maximizing performance criteria. However, building and calibrating a reliable model for a real application is difficult, costly and time-consuming. Indeed, it requires hard expert work to retrieve all the building's data and tune the corresponding model. This prevents MPC to be widespread in Building Management Systems.

In this paper, we propose a MPC formulation where all the optimization problems included in a MPC strategy (calibration, estimation, optimal control) are performed efficiently using gradient-based techniques and adjoint-based gradient computations. This formulation relies on an automated "white-box" modeling technique (with partial-differential equations) using Building Information Model (BIM - using gbXML standard here) files parsing. We also show that making extensive use of adjoint models in MPC opens opportunities for fast sensitivity analysis, which can, for instance, help to choose which parameters to calibrate.

Keywords: building simulation; Model Predictive Control; gradient-based optimization; estimation; instrumentation; model calibration; inverse problems; adjoint model

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Nomenclature

Building model notations

θ Vector of temperature nodes

ϑ Subset vector of temperature nodes

20 \mathbf{A}, \mathbf{B} Building's state space matrices

\mathbf{p} Vector of constant parameters

\mathbf{u} Vector of thermal inputs (time dependant)

Mathematical Notations

$\int_{t \in \mathbf{T}} x \cdot dt$ Integration of x over time interval \mathbf{T}

25 \sum Sum symbol (of all vector elements if provided without indices)

\mathbf{A} Matrices in bold italic upper case

\mathbf{A}^T Transposition of matrix A

\mathbf{v} Vectors in bold italic lower case

\mathbf{v}^* Adjoint of vector v

30 \mathbf{v}^T Transposition of vector v

\mathbf{v}_i i^{th} element of vector \mathbf{v}

$argmin$ Argument of the minimum of a given function

$J_{purpose}$ Cost function (scalar) with optimization purpose in subscript

Vector spaces

35 $\mathcal{P} = \mathbb{R}^j$ Space of model scalar parameters (thermal coefficients...)

$\mathcal{S} = [L^2(T)]^k$ Space of model states (k temperatures as square integrable functions over time interval T)

$\mathcal{U} = [L^2(T)]^i$ Space of model inputs (i square integrable time functions)

$\mathcal{V} = [L^2(T)]^l$ Space of time dependant parameters (l square integrable time functions)

1. Introduction

40 1.1. MPC in buildings

Model Predictive Control is an advanced control technique initiated by Richalet [1], and generalized by Clarke [2], to implement the optimal control theory to real-time control of dynamic systems. It was first applied to industrial applications (petroleum industry), and then in many other fields (robotics, avionics...).

Classical optimal control is an open-loop control. It consists in optimizing a command law over a prediction horizon, according to a dynamic model of the controlled system, and supposed initial conditions and solicitations predictions. Unfortunately, these elements are often subject to errors and uncertainties. A MPC strategy consists in adding some feedback to optimal control to reduce the impact of such uncertainties and perturbations.

A full MPC strategy can be divided in four steps (figure 1):

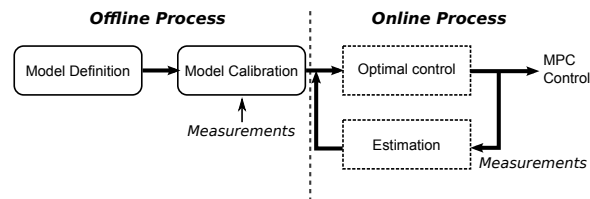


Figure 1: MPC strategy

50 Offline steps

- **Model definition:** There are many ways to build up the model representing the behavior of the controlled system. This model can be physical, using differential equations deduced from an analysis of the building structure, or purely numerical (“black-box model”) such as ARX statistical models or neural networks. Physical models can come with different levels of definition, according to the simplifying hypothesis. Detailed zonal-nodal models [3, 4] are used intensively in well-known building simulation software (EnergyPlus, TRNSYS...) under the denomination of “white-box models”. Low order physical models, also called “grey box models”, use a more simplifying hypothesis (for example, the electrical RC network analogy [5]), and are often easier to handle for control purposes.

- **Model calibration:** The calibration phase consists in finding a set of model parameters values such as the model response matches with *in situ* measurements. For black-box models, parameters are always unknown and a calibration phase is mandatory. The calibration of such models takes generally advantage from their structure (backpropagation for neural networks, subspace methods for linear systems...). Physical models are often subject to modeling errors and parameter uncertainty, and a calibration step helps to reduce output errors.

Since we have a model with a response close to reality, we can use it sequentially in optimal control steps, and state estimation phases giving feedback in the control process.

- Optimal control:** The optimal control phase consists in computing a control law maximizing a performance criterion over a prediction horizon. In the case of constrained optimization, the user can define constraints on system inputs and outputs, that will be taken into account during the optimization process. Unlike standard regulation control techniques, this kind of formulation can directly take into account control constraints, consumed energy and comfort criterion. Several mathematical frameworks were developed to solve optimal control problems, like Pontryagin’s principle [6], the theory of dynamic programming [7] or the optimal control theory of systems governed by partial differential equations [8].
- Estimation:** To deal with the open-loop nature of optimal control, computed control laws are repeatedly updated with an initial state and corrected parameters provided by a state estimation step. Indeed, if the number of model states is high (e.g. the number of temperature points simulated by a thermal model), providing a sensor for each state can be difficult and costly. State estimation techniques can use the control model to estimate states and parameters complying the best with local measurements.

The imbrication of these two sequential steps is summarized in figure 2. At each time t_k , one can perform a state estimation from past measurements and applied inputs. Then one computes an optimal command law over the prediction horizon $[t_k, t_k + t_f]$ with the estimated state as initial condition. This command is applied until the next update step at the time $t_{k+1} < t_k + t_f$. As the prediction horizon is always pushed forward, it is also called the “receding horizon”.

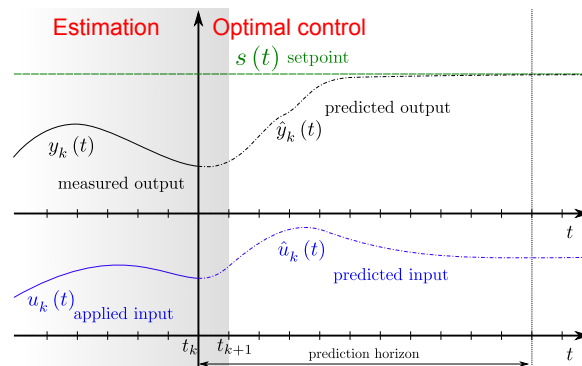


Figure 2: MPC: online steps and receding (prediction) horizon

Many studies advocate the potential of MPC to generate energy savings in buildings during operation.

The study [9], for instance, implements a MPC strategy generating 20% more energy savings than a weather-compensated feedforward control strategy. Ph.D. investigations of [10] indicate energy gains between a range of 5% to 20% for Distributed MPC strategies towards standard regulation techniques while preserving thermal comfort. Such ranges are commonly found in literature ([11, 12]). However, deploying MPC in buildings is not straightforward, and one can often struggle with two major obstacles :

- Building and tuning a precise dynamic model is a complex task. Standard building simulation software (EnergyPlus, Comfie Pléiades, TRNSYS...) can help to build deterministic physical models, but assume one perfectly knows the building's structure and physical parameters, often subject to important uncertainties [13, 14, 15, 16]. Such uncertainties usually lead to a bad evaluation of energy performance [17, 18]
- It is also difficult to predict the building's thermal solicitations. Weather forecasts present an increasing bias with time and are subject to microclimate variations. Predictions of use can also lack reliability, and can lead to erroneous anticipation of setpoints and internal gains.

1.2. Model calibration for MPC

To face uncertainties in MPC, model calibration is often mandatory. Many model calibration techniques exist in the literature, and they are highly dependent on model choices (one can refer to the review [19] for application in buildings energy simulation). For example, neural network models are calibrated by dedicated back-propagation techniques. "Subspace" methods are applied on specific stochastic linear models and ARIMA models are specific polynomial models often used for time series prediction. A more generic and theoretical background, applicable to physical models, can be found in the inverse problems' literature.

All these techniques imply at some point to choose specific measurements that one wants to minimize the error with. For some of them (particularly in the case of physical models), one also has to choose parameters to calibrate. Since a model is used for MPC, it must provide the best prediction performance of the outputs used in the control cost function. Calibration and estimation steps aim to reduce prediction errors along with the control procedure. This implies the use of a good calibration technique properly used and associated with appropriate *in situ* measurements.

In practice, applying a calibration strategy with good results is challenging and leads to several issues:

- For black-box models, one generally needs a huge amount of data for calibration, since there is no physical meaning in parameters that could lead to preconditioning. Besides, they are often prone to overfitting.

• For white-box models, the parameter number can be high, which can increase computation time, performance, and even compromise the convergence of the calibration problem. Besides, most well known white-box modelers encapsulate models in a simulation engine that doesn't provide any gradient, preventing the use of efficient gradient-based techniques. Tools like GenOpt [20] provide solutions when derivatives are not available, but having access to derivatives alongside simulations can lead to significant improvements in convergence speed. The reader can refer to [21] for a review on simulation-based calibration techniques applied to buildings.

• In many cases, the choice of sensors is induced by common sense and technical limitations. However, this choice can have quite important effect on control performance, as one will see further in this study.

1.3. Objectives and structure of the paper

We have two main objectives in this work:

- First, we show that there are powerful mathematical frameworks to efficiently include gradient computation in building simulation models. Such a gradient can be of great interest in MPC.
- Then, in the case of simulation-based calibration, we highlight the impact that parameters and sensors choice can have, and how we can use gradient-based techniques to help this choice.

To do so, we present here a theoretical framework for MPC and calibration in buildings using zonal-nodal modelization and the adjoint method for fast gradient computations. Then, using this approach, we show on a test case how choosing identified parameters and sensors for each step of the MPC process can impact final performance. From these observations, we propose a method taking advantage of the adjoint method to compute sensitivity indices and select the most influential parameters for MPC.

2. Theory: MPC using zonal-nodal models and the adjoint method

In this theoretical section, we remind the theory of zonal-nodal modeling for buildings. Then, we introduce a general MPC formulation based on successive optimization problems and show how an adjoint-based gradient method can solve them efficiently.

2.1. Building modelization

A building and its environment can be modeled using a standard zonal-nodal model, quite common in the state-of-the-art of building simulation software [3, 4]. This modelization technique consists in representing

each building part by a set of interconnected temperature “nodes”, and is a particular discretization of heat transfer equations with simplifying hypotheses:

- Environment: all meteorological parameters (temperature, cloud coverage, solar irradiance) are involved in model boundaries equations.
- 150 • Zones: Volumes where all physical properties (pressure, humidity, temperature...) are considered homogeneous. Consequently, zones have a unique temperature node. Generally, a zone includes the air and the furniture of a room. A zone can include several rooms and walls if thermal exchanges between them are sufficient. A large room with heterogeneous temperatures can also be subdivided into several zones.
- 155 • Walls and surfaces: Building envelope parts where heat conduction is supposed unidirectional. Walls equations are obtained by applying finite elements discretization of the heat transfer equation along with wall depth.
- HVAC Systems: Heating, Ventilation, and Air-Conditioning systems are modeled by a state-space equation where the state vector contains some temperatures of the system.

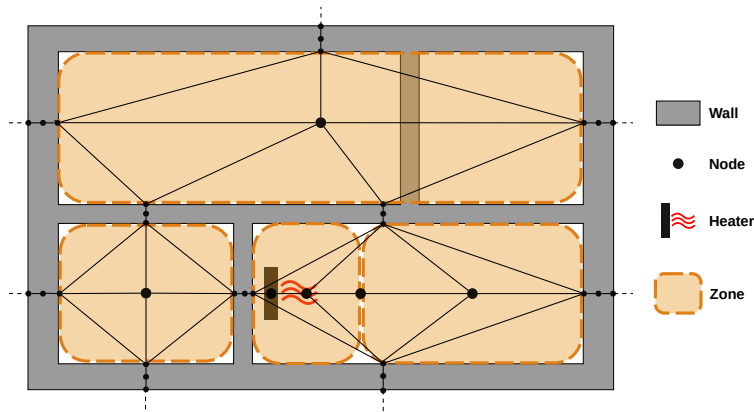


Figure 3: Zonal-Nodal modelization

160 Due to heat transfers (radiation, conduction and convection), the equation of each part is more or less connected with the others. Consequently, all equations can be compiled in a global state equation, where the state vector contains all the node temperatures of the system :

$$\frac{d\boldsymbol{\theta}}{dt} = \mathbf{A}\boldsymbol{\theta} + \mathbf{B}\mathbf{u} \quad (1)$$

where $\boldsymbol{\theta}$ is the vector of temperature nodes, \mathbf{u} the thermal inputs vector of the system (boundary temperatures and heat flows), \mathbf{A} and \mathbf{B} the matrices of coefficients due to thermal mass and thermal

165 transfers.

If one considers the general spaces defined in the nomenclature, then $\boldsymbol{\theta} \in \mathcal{S}$, $\mathbf{u} \in \mathcal{U}$. Besides, \mathbf{A} and \mathbf{B} are build up from elements of vectors in \mathcal{P} and \mathcal{V} and therefore can be time-dependant.

2.2. MPC as a set of optimization sub-problems

As seen in 1.1 on page 3, a MPC strategy can be decomposed in several sub-problems: model definition, 170 model calibration, estimation, and optimal control. The first one is an expert task and invokes the use of specific modeling knowledge. However, calibration, estimation, and optimal control can all be seen as optimization problems, and consequently be solved similarly. The following examples show how we can formulate these three steps and the next section generalizes this approach.

2.2.1. Calibration

175 For each built model, there is error induced by modelling hypothesis and parameters bias. Calibration techniques are often used to estimate exact parameter values for uncertain, missing parameters, or for thermal property assessment. In our case, the model is preconditioned by the knowledge one have on the building, but our goal here is to fit simulation results with corresponding measurements. Besides, one wants parameters to keep a physical meaning, but there may be some flexibility on their values. With these 180 assumptions, one can choose a set of parameters to calibrate in order to fit the simulation results with a set of measurements, and can consequently represent the calibration problem by the following optimization problem:

$$\begin{cases} \mathbf{p}^\circ = & \underset{\mathbf{p} \in \mathcal{P}}{\operatorname{argmin}} J_{cal}(\mathbf{p}) \\ J_{cal} = & \frac{1}{2} \sum \int_{t \in \mathbf{T}_{cal}} (\boldsymbol{\vartheta}(t) - \boldsymbol{\vartheta}_{mes}(t))^2 dt + \mathcal{R} \\ \mathcal{R} = & \frac{\epsilon}{2} \sum (\mathbf{p} - \hat{\mathbf{p}})^2 \end{cases} \quad (2)$$

Here, one wants to find the vector of parameter values $\mathbf{p} \in \mathcal{P}$ minimizing J_{cal} , the quadratic cost (scalar) associated with the discrepancy between temperature measurements vector $\boldsymbol{\vartheta}_{mes}$ and the corresponding 185 simulated temperatures $\boldsymbol{\vartheta}$ during the calibration time interval \mathbf{T}_{cal} . J_{cal} contains a Tikhonov regularization term \mathcal{R} to help problem solving. This term implies that unknown parameters are not too far from their initial guess $\hat{\mathbf{p}}$.

This approach was successfully experimented in inverse heat transfer problems [22, 23] and also used by our team on building thermal audit for retrofit [24, 25].

190 One major difficulty in this approach consists in finding sets of measurements and parameters providing the best performance for the considered application. This issue will be discussed further in this paper.

2.2.2. Estimation

Most of the time, the calibration phase is not enough to compensate for all modeling errors. If we suppose we have the correct model inputs and initial states, one will observe an increasing deviation of the simulation results against reality. To compensate for this deviation, we have to re-estimate some well-chosen parameters regularly. Then, the estimation phase is also a calibration problem but with a reduced number of parameters and measurements.

$$\left\{ \begin{array}{l} \boldsymbol{\theta}^\circ(t) = \boldsymbol{\theta}(t, \mathbf{q}^\circ) \\ \mathbf{q}^\circ = \arg \min_{\mathbf{q} \in \mathcal{U}_{gains}} (J_{estim} + \mathcal{F}) \\ J_{estim} = \frac{1}{2} \Sigma \int_{t \in \mathbf{T}_e} (\boldsymbol{\vartheta}(\mathbf{q}, t) - \boldsymbol{\vartheta}_{mzone}(t))^2 dt \\ \mathcal{F} = \frac{\varepsilon}{2} \Sigma \int_{t \in \mathbf{T}_e} \mathbf{q}^2 dt \end{array} \right. \quad (3)$$

In this case, we choose to compensate for the deviation with “corrective” internal heat gains $\mathbf{q}^\circ \in \mathcal{U}_{gains} \subset \mathcal{U}$, minimizing J_{estim} the quadratic error against zone temperature measurements vector $\boldsymbol{\vartheta}_{mzone}$ over the estimation time interval \mathbf{T}_e . Since internal gains are time-dependant parameters, the regularisation term \mathcal{F} features integration over time. Then, temperatures estimation $\boldsymbol{\theta}^\circ$ is the simulation result of our building model with internal gains substituted by computed corrective gains \mathbf{q}° .

The choice of estimating \mathbf{q} is motivated by the high uncertainty on this input (it is almost impossible to measure in a “standard” environment (ie. not an extensively monitored lab experiment)). Besides, we observed on various simulations that $\boldsymbol{\vartheta}_{mzone}$ is very sensitive to \mathbf{q} , so these temperatures seemed to be the minimal measurements necessary for such estimation. Correction of internal gains can also have a corrective effect on system states.

2.2.3. Optimal control

In the optimal control problem, we want to find parameters minimizing a cost associated with comfort and consumption measurements. In our test case, we wanted to optimize thermal comfort towards used power. Then we formulated the control problem as the following optimization problem:

$$\left\{ \begin{array}{l} \mathbf{u}_{heaters}^\circ = \arg \min_{\mathbf{u}_{heaters} \in \mathcal{U}_h} J_c(\mathbf{u}_{heaters}) \\ J_c = aJ_{comf} + bJ_{power} \\ J_{power} = \frac{1}{2} \Sigma \int_{t \in \mathbf{T}_c} \mathbf{u}_{heaters}^2 dt \\ J_{comf} = \frac{1}{2} \Sigma \int_{t \in \mathbf{T}_c} \mathbf{o}_c(\mathbf{t}) (\boldsymbol{\vartheta}(\mathbf{u}_{heaters}, t) - \boldsymbol{\vartheta}_{set}(t))^2 dt \\ \mathbf{0} \leq \mathbf{u}_{heaters} \leq \mathbf{u}_{heaters_{max}} \end{array} \right. \quad (4)$$

In this case we want to compute the optimal power of heaters $\mathbf{u} \in \mathcal{U}_h \subset \mathcal{U}$ minimizing the cost function

J_c over the control time interval \mathbf{T}_c , linear combination of costs J_{comf} and J_{power} . J_{comf} is the quadratic cost of the zones' temperature error relatively to temperature setpoints during occupancy periods (\mathbf{o}_c is a Boolean vector function representing the presence or absence of inhabitants). J_{power} is a quadratic cost on the instant power $\mathbf{u}_{heaters}$ consumed in zones. One can notice that J_{power} does not represent the consumed energy in a physical sense. However, such quadratic term still penalizes energy consumption and provides more convexity to the optimization which is convenient for numerical solving. In future studies, one could use linear costs such as energy with appropriate optimization algorithms.

2.3. Application of the adjoint method for MPC

Given the equation (1), one can apply the optimal control theory to find the best command for a setpoint or estimate a given set of parameters. Each optimal command or parameter estimation problem can be formulated as an optimization problem. For an estimation problem, the cost function to minimize will measure the distance between measurements and simulation results. For an optimal control problem, the cost function can be the distance between a setpoint and the simulated room temperature. Such optimization problems can be formulated generically by the following quadratic optimization problem:

$$\begin{cases} \mathbf{w}^\circ = & \underset{\mathbf{w} \in \mathcal{W}}{\operatorname{arg\,min}} J(\mathbf{w}) \\ J = & \|\mathcal{O}f(\mathbf{w}) - \mathbf{m}\|_{\mathcal{M}}^2 + \|\mathcal{T}(\mathbf{w} - \mathbf{w}_0)\|_{\mathcal{V}}^2 \\ & \varphi(\mathcal{O}f(\mathbf{w})) \leq \mathbf{0}, \psi(\mathbf{w}) \leq \mathbf{0} \end{cases} \quad (5)$$

Here f is the building model, $\mathbf{s} \in \mathcal{S}$ the model state vector and $\mathbf{w} \in \mathcal{W} \subset (\mathcal{P} \times \mathcal{V})$ a subset of all model variables (inputs and parameters, both constant and time dependant), such as:

$$\mathbf{s} = f(\mathbf{w}) \quad (6)$$

For our model, spaces \mathcal{W} and \mathcal{S} are square-integrable on the time range $T = [0, t_f]$, with their classical scalar products and norms. For example, $\|\mathbf{s}\|_{\mathcal{S}}^2 = \langle \mathbf{s} | \mathbf{s} \rangle = \sum \int_{t \in T} \mathbf{s}^2(t).dt$ is the L^2 norm of vector \mathbf{s} in \mathcal{S} .

We define similarly the space of setpoints and measurements \mathcal{M} , subspace of \mathcal{S} . J is the cost function to minimize, with constraints φ and ψ on model's response and entries. \mathcal{O} , is the observation operator from \mathcal{S} to \mathcal{M} which models a measure \mathbf{m} on the building. Likewise the vector \mathbf{m} can represent a setpoint. \mathcal{T} is a linear operator applied over model parameters and *a priori* values \mathbf{w}_0 .

Supposing that the problem is well-posed (according to Hadamard's definition), one can efficiently find the solution with the adjoint method coupled with a gradient-based optimization algorithm [8, 26]. Indeed, with the adjoint method, one can compute the gradient with the numerical cost of approximately two

simulations: one for the “direct model” (1) and one for the “adjoint model” derived from the optimization problem. The gradient is then a simple function of both simulation results. Constraints can be ensured
 240 with gradient projection techniques, barrier functions or Uzawa’s method for example [27].

Application example of the Adjoint Method for optimal control of a linear system. To show the application and the interest of the adjoint method, one can apply it on a more specific example. One wants, there, to find an optimal command law over a finite time horizon $[0, t_f]$ for a time-independent linear system. This case matches with our building model as described previously.

245 With null initial conditions, the model is represented by the following equation system:

$$\begin{cases} \frac{d\boldsymbol{\theta}}{dt} = \mathbf{A}\boldsymbol{\theta} + \mathbf{B}\mathbf{u} & t \in [0, t_f] \\ \boldsymbol{\theta}(0) = \mathbf{0} \end{cases} \quad (7)$$

With $\boldsymbol{\theta}$ the temperatures vector, \mathbf{u} the control vector, \mathbf{A} the state matrix and \mathbf{B} the command matrix. One aims to find the command $\mathbf{u}(t)$ over $[0, t_f]$ minimizing the following cost function:

$$J = \frac{1}{2} \int_{t=0}^{t_f} \left((\boldsymbol{\theta} - \mathbf{c})^T \mathbf{P} (\boldsymbol{\theta} - \mathbf{c}) + \mathbf{u}^T \mathbf{Q} \mathbf{u} \right) dt \quad (8)$$

\mathbf{P} and \mathbf{Q} are positive symmetric weighting matrices. With such linear model, the Lagrangian associated with the optimization problem is:

$$\mathcal{L} = J + \int_0^{t_f} \boldsymbol{\theta}^{*T} \left[\frac{d\boldsymbol{\theta}}{dt} - (\mathbf{A}\boldsymbol{\theta} + \mathbf{B}\mathbf{u}) \right] dt \quad (9)$$

250 The Lagrangian is here the sum between the cost function and the scalar product of the differential equation and a Lagrange multiplier $\boldsymbol{\theta}^*$ with the same dimension than $\boldsymbol{\theta}$.

A solution of the optimization problem must fulfill the equality:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}^*} = \frac{\partial \mathcal{L}}{\partial \mathbf{u}} = \mathbf{0} \quad (10)$$

Also, $\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}^*} = \mathbf{0}$ since $\boldsymbol{\theta}$ is a solution of the equation (7). If one rewrite(9) with an integration by parts:

$$\mathcal{L} = J + \int_0^{t_f} \boldsymbol{\theta}^{*T} \left[-\frac{d\boldsymbol{\theta}^*}{dt} - \mathbf{A}^T \boldsymbol{\theta}^* \right] dt + \int_0^{t_f} \boldsymbol{\theta}^{*T} [-\mathbf{B}\mathbf{u}] dt + [\boldsymbol{\theta}^{*T} \boldsymbol{\theta}]_0^{t_f} \quad (11)$$

Then, with the equality $\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \mathbf{0}$ can lead to the variational form (also called the weak formulation) of

255 the adjoint model:

$$\begin{cases} -\frac{d\boldsymbol{\theta}^*}{dt} = \mathbf{A}^T \boldsymbol{\theta}^* - \mathbf{P}(\boldsymbol{\theta} - \mathbf{c}) & t \in [0, t_f] \\ \boldsymbol{\theta}^*(t_f) = \mathbf{0} \end{cases} \quad (12)$$

Since this differential system has final conditions instead of initial conditions, one must solve it numerically backward.

Since $\boldsymbol{\theta}$ is a solution of (7):

$$J(\mathbf{u}) = \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\theta}^*, \mathbf{u}) \quad (13)$$

Then one can write the gradient of the cost function J as a partial derivative of the Lagrangian:

$$\nabla_{\mathbf{u}} J = \frac{\partial \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\theta}^*, \mathbf{u})}{\partial \mathbf{u}} \quad (14)$$

260 this leads to an explicit formulation of the gradient of the cost function as a function of the adjoint state vector $\boldsymbol{\theta}^*$:

$$\nabla_{\mathbf{u}} J(t) = \mathbf{Q}^T \mathbf{u}(t) - \mathbf{B}^T \boldsymbol{\theta}^*(t) \quad (15)$$

From a numerical point of view, one can then compute the gradient with only two consecutive simulations of differential systems, the direct one and the adjoint one, with any temporal horizon and discretization step. If one wanted to compute the gradient with a finite difference approach, he should perform simulations 265 of the direct system for a little variation of \mathbf{u} along each dimension and discrete-time of \mathbf{u} , which is much more costly.

2.4. Software implementation

As we can see, the adjoint method eases the computation and can be used at all steps of a MPC strategy. To test and implement this approach of optimization problems on buildings, our team developed ReTroiT 270 (REal Time eneRgy simulation and Optimization soFtware Toolbox), a software toolbox implemented in Matlab [28].

With this toolbox, we built a program to perform and evaluate our MPC strategy, both in simulation and on a real test case. This toolbox presents the following global architecture:

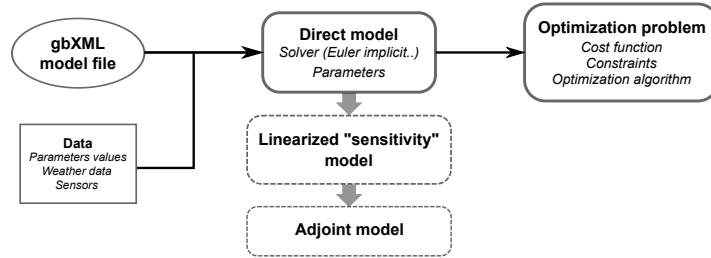


Figure 4: ReTroiT architecture

The toolbox is developed with an Object-Oriented Paradigm. Each box of the diagram (4) is a specific
 275 class.

Then, several steps can be performed sequentially inside a script:

- Data and BIM (Building Information Model) parsing: the software provides tools to parse measurement and weather data (CSV format) as well as BIM in gbXML standard.
- Direct model building: building model objects can be programmatically created, as well as generated
 280 from BIM data. Discretization rules (in walls and space) can then be declared to generate a numerical model and configure the numerical solver.
- Optimization problem definition: an object describing an optimization problem can be defined. This object contains the cost function, the set of parameters to optimize, the set of constraints and the chosen optimization algorithm with associated parameters.
- Adjoint model and linearised models generation: when needed, the optimization algorithm can call
 285 linearised and adjoint models for fast gradient computation.

Simulation implementation details. As seen in 1.1 on page 3, a building thermal model can be written as a linear state space equation (1). This kind of differential equation can be solved easily. In our case, we chose a fixed time-step discretization and implemented an implicit Euler solver. Some specific functions were
 290 developed to handle time vectors as well as input and output vectors. The system matrices are automatically built from the building model defined in a script or generated from a gbXML file.

Optimization implementation details. The adjoint model required for optimization is very similar to the simulation model (the reader can refer to [8] for more theoretical information and in section 2.3 on page 10 for mathematical developments). Its matrices and solution are then obtained with almost the same method,
 295 by compiling the building model and the optimization problem accordingly. One important difference lies

in performing a backward simulation, which is done by changing appropriate signs and flipping time vectors after the Euler implicit solving. The cost function object is linked with simulation and adjoint models to compute gradients efficiently and provide them to the defined optimization algorithm.

3. Results and discussion

300 Alongside the development of ReTrofiT, we also deployed this work on the Model Predictive Control of an experimental building we present in the following section. With this experimental work, on a well known and heavily instrumented building, we faced many difficulties in choosing good sets of sensors and parameters for calibration. These integration difficulties led us to investigate further the methodological need for parameter and sensor selection. Specifically, we present here how sensor and parameter choices
305 impact prediction performance, then how the adjoint method could be used to help this choice.

3.1. Test case

The test case used in this study is the INCAS I-MA house 5, an experimental building of the INES institute, located at Savoie Technolac, Chambéry, France [29]. This building is designed like a classic two-floors domestic dwelling, built with modern construction materials and techniques.



Figure 5: INCAS I-MA house

310 Walls are made of brick blocks with an outside aerogel plaster and a standard gypsum cover inside. This building is provided with numerous temperature sensors: at each material interface within the walls, at the inner and outer surface of the walls and inside each room. A solar sensor provides diffuse and direct solar

radiation. Each room has an electric heater and is connected to a centralized AHU (Air Handling Unit) system.

315 A specific program based on ReTrofiT was hosted on a server exchanging data with the building information system handling both measurements and controls.

3.2. Importance of parameters choice and sensors for the calibration phase

As we saw previously, the calibration problem can be formalized by the equation 2 on page 8. For a given calibration case, we have to choose the set u_i of parameters to calibrate, and the appropriate set of
 320 temperature sensors T_{mi} . The selection of both sets is a combinatorial problem that suffers from the curse of dimensionality. For example, if we limit ourselves to 5 temperature sensors on wall surfaces and zones (55 positions available in our test case), and we fix the set of parameters to estimate, we got 3478761 possible combinations. Since at present the optimization algorithm is quite long to converge (order of magnitude: 1h), it could take more than the impractical time of 397 years to find the best set by brute force on a regular
 325 computer.

One could argue that we can only choose the most unknown parameters, and select the most reliable sensors with the most responsiveness to the building’s thermal dynamics (intuitively, where the temperature is the most likely to change, to best capture the dynamic properties during calibration). We tried this approach on our test case, but it revealed itself cumbersome and with poor results. We had to tune some
 330 parameters manually and empirically to achieve an “acceptable” result. By the way, if some studies were led to evaluate the global uncertainties we can have on each part properties [14, 13, 16], this approach stays quite empirical and hard to adapt on each particular case. Besides, one could say that the more sensors we use, the better the calibration is since we retrieve more information. However, we performed several calibration tests refuting this assertion. Each of those tests is performed according to the diagram figure 6.
 335 Between each test, we modify sets of sensors, calibrated parameters and their first guess error, and compute the calibration quality (quadratic error on parameter estimates and model prediction over a finite horizon).

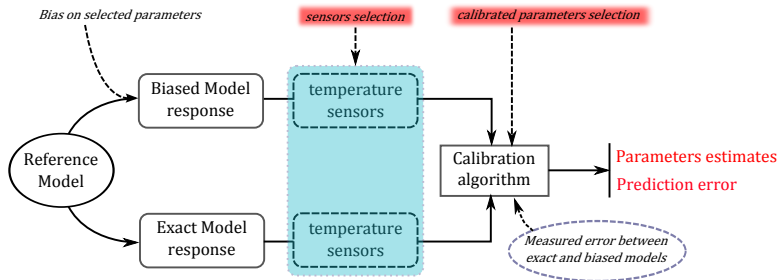


Figure 6: Experimental process of virtual calibration tests

With this experiment scheme, we define three test cases:

Test 1 We impose here an error of -30% on the parietal conductivities. We seek to identify only the conductivity coefficients.

345 **Test 2** The error of -30% is this time imposed on the conductivities and the coefficients h of convective coupling. These are also the parameters we seek to estimate.

Test 3 This test is identical to the previous one, except that only the conductivities are identified. This corresponds to the current case where one seeks to calibrate only a subset of the parameters whose *a priori* is false.

345 For each test case, we vary the set of temperature sensors used for the calibration:

Set ZP Sensors positioned on all areas and surfaces of each wall (indoor and outdoor), for a total of 55 sensors.

Set Z Sensors measuring the temperature of the 5 zones of the building.

Set Z_{1,2} Sensors measuring only the temperature of the two controlled parts.

350 Each calibration is performed by a Levenberg-Marquardt algorithm, with 300 successive linearisations. On all 300 iterations, only the best value is kept (the convergence can stop before reaching the 300th iteration). Each calibration is performed on 7 days of data. It is then tested in prediction over an interval of 7 additional days consecutive to the calibration period.

For each calibration, we can notice the following errors:

355 e_i Response error on the calibration interval, before calibration.

e_c Error on the calibration interval, after calibration.

e_{p1} Consecutive prediction error: The calibrated model response is computed over 14 days (the calibration and prediction interval consecutively). The error is computed on the prediction interval.

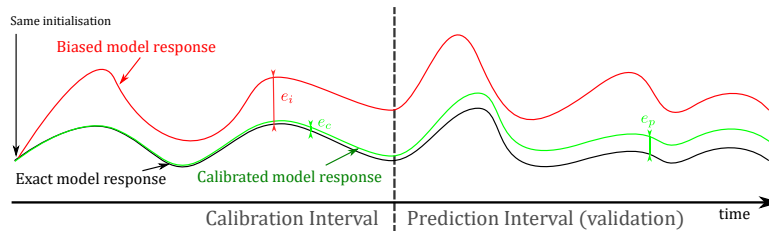


Figure 7: Calibration and prediction intervals (example)

360

In our case, we calibrate the model to decrease the prediction error of temperatures θ_i involved in the MPC cost function, corresponding with sensors $Z_{1,2}$ for instance. We can compute the quadratic prediction error with the following equation(16):

$$e_p = \sqrt{\frac{\int_{t \in \mathbf{T}_e} \left((\theta_1 - \tilde{\theta}_1)^2 + (\theta_2 - \tilde{\theta}_2)^2 \right) dt}{\int_{t \in \mathbf{T}_e} \theta_1^2 + \theta_2^2 dt}} \quad (16)$$

365

Each column of this table corresponds to one of the three test cases and each row to the sensors used for calibration. In each box of the table is represented the evolution of the cost function used for the calibration during the iterations of the optimization algorithm. For each test, we also present the convergence results in table Convergence for each test case / sensor set .

All test results are summarized in the following tables. Each row correspond to a test case and each column to a sensor set used for calibration.

Sensor set for calibration =>		ZP	Z	$Z_{1,2}$
Test case 1	<i>Conductivities</i>	9.28	12.18	25.51
	<i>Conductivities</i>	18.69	24.05	28.19
Test case 2	h_{ext}	5.18	15.48	29.39
	h_{int}	7.03	18.84	29.63
Test case 3	<i>Conductivities</i>	95.92	44.76	31.98

Table 2: Test 1 - Quadratic parameters estimation errors (in percents)

Sensor set for calibration =>		ZP	Z	$Z_{1,2}$
Test case 1		0.0062	0.18	0.32
Test case 2		0.0477	0.25	0.62
Test case 3		2.55	1.94	1.71

Table 3: Test 1 - Quadratic prediction errors e_p on sensors $Z_{1,2}$ (in percents)

370

For the two first tests, the most complete sensor set provided the best calibration results, but increasing the set of parameters to calibrate reduced the calibration performance. However, for the third case, the best calibration result is obtained for the minimal sensor set $Z_{1,2}$. This leads to the following conjectures:

375

- For test cases where parametric errors are only present on calibrated parameters, increasing the number of sensors increases calibration performance.
- When parameters with a bias are not calibrated and when parameters have similar effects on the calibration cost function, increasing the number of sensors decreases the calibration performance.

In a real case, we do not know where are parametric errors, and parametric assumptions errors can compromise calibration results. Plus, we can't calibrate all parameters at once since the problem can become

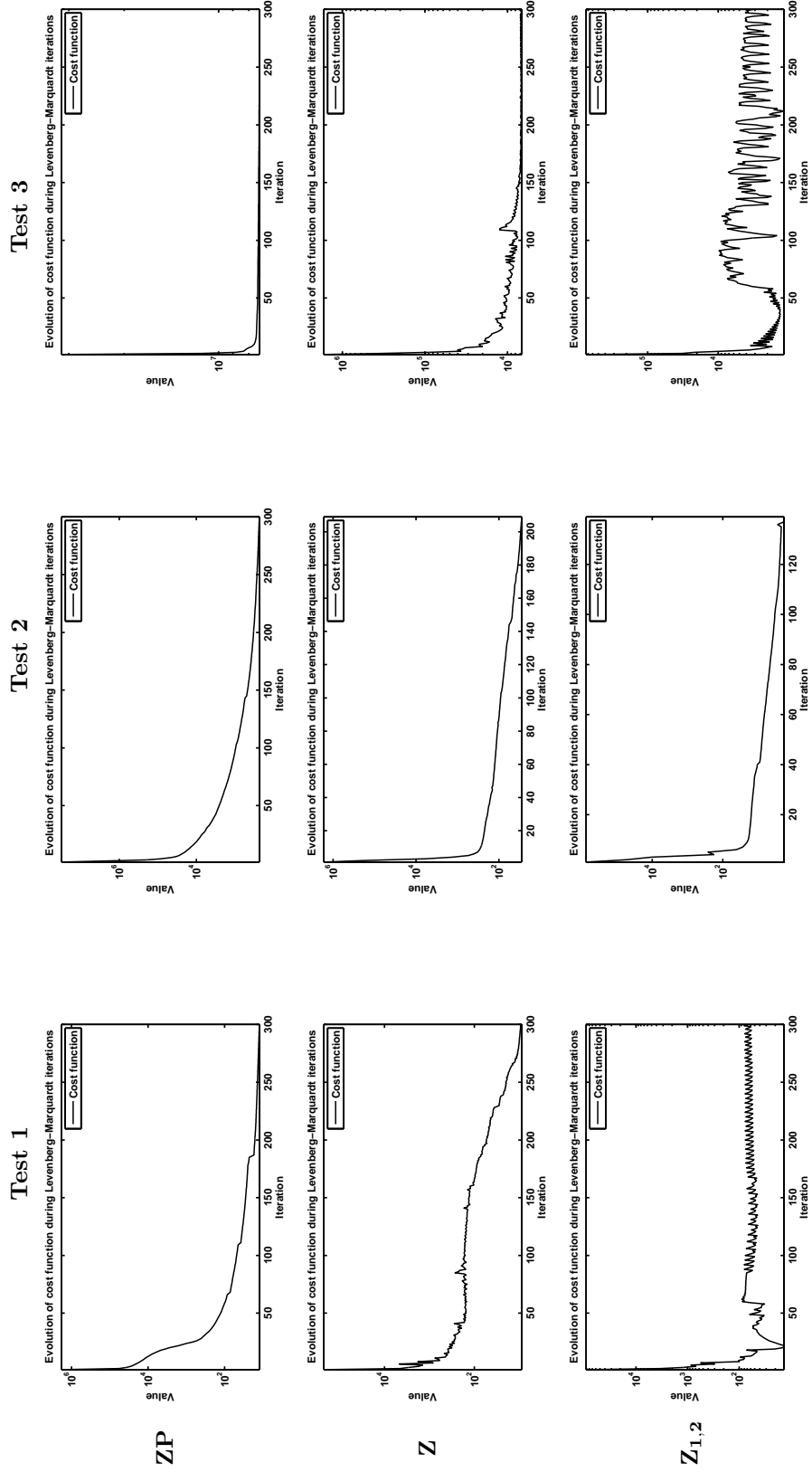


Table 1: Convergence for each test case / sensor set

ill-posed and impossible to solve even with regularization techniques (several parameters have similar influences). Besides, selecting parameters to calibrate using uncertainties on each specific case is not practical.

380 However, sensitivity studies could be used to help to point out the most influential parameters in MPC and calibration processes. Since the adjoint method provides an efficient way to compute gradients and gradients are often used in sensitivity computation techniques, we explored its use in specific sensitivity studies for MPC.

3.3. A sensitivity study for selecting parameters

385 To select a good set of parameters, we have to remind the main objective of model calibration. Here, we want to calibrate the model to get the best predictive performance for MPC. Therefore, the precision in parameter estimation is not mandatory. As we seek here to guarantee optimal control performance, it seems logical to try to select the parameters that have the greatest influence on the latter.

Besides, many sensitivity studies were conducted on buildings' thermal performance or comfort. Three
390 main kind of sensitivity indexes can be identified:

- **Local sensitivity indices (gradient):** Local indices are based on a direct differentiation of the model at a given point. With a gradient calculated by the adjoint method, it is possible to quickly evaluate the local sensitivity of model outputs (eg temperatures) [30]. However, local indices do not take into account model non-linearities and interactions between parameters.

395 • **Qualitative indices based on screening:** This type of index provides an initial (approximate) evaluation of the most influential parameters. The screening method uses a more or less gross discretization of the parameter space. In the Morris [31] method, the individual (finite difference type) effects of each parameter are evaluated on different points of the space by respecting the probability distributions of the parameters (OAT method: One-At-a-Time). The Morris indices are then constructed by evaluating the
400 mean and variance of the individual effects. For the "experimental design" method, we try to approximate the model response by a polynomial function whose coefficients can be seen as sensitivity indices. The identification of the coefficients is done for realizations of the experiment (or simulation of the model) according to well-chosen factorial plans (often a combination of the min and max values of the parameters). These methods are often subject to combinatorial explosion problems. The reader can refer to [32] for a
405 comparison of the screening methods applied to thermal models of the building.

- **Indexes based on an analysis of variance:** Sobol's global sensitivity indices are based on a probabilistic definition of the inputs and outputs of the model and a variance decomposition method (decomposition ANOVA - ANalysis Of VAriance) explaining the impact of each combination of parameters on the output [33]. Their evaluation is generally based on Monte Carlo or quasi-Monte Carlo methods, which

410 is often very computationally expensive.

As the problem of optimal control takes few minutes to be solved here, and we have in our case 750 non-null scalar parameters (more than 1500 parameters in the model), it is unthinkable to use conventional techniques of global sensitivity (computation of Sobol indices, or Morris method).

415 However, it is possible to quickly compute the gradient of the minimum of the cost function in order to deduce sensitivity indices related to optimal control [34]. In fact, let J_c be the cost function of the optimal control, $\mathbf{p} \in \mathcal{P}$ the parameters vector of the building model, \mathbf{c} the control law and \mathbf{c}° the optimal control law. \mathbf{c}° included in the control space $\mathcal{C} \subset \mathcal{U}$ is a function dependent on \mathbf{p} :

$$\mathbf{c}^\circ = \underset{\mathbf{c} \in \mathcal{C}}{\text{arg min}} J_c(\mathbf{p}, \mathbf{c}) \quad (17)$$

The minimum of J_c is:

$$J_{c \text{ min}} = J_c(\mathbf{p}, \mathbf{c}^\circ(\mathbf{p})) \quad (18)$$

After derivation, the gradient $\nabla_{\mathbf{p}} J_{c \text{ min}}$ in a point \mathbf{p}_0 is:

$$\nabla_{\mathbf{p}} J_{c \text{ min}}(\mathbf{p}_0) = \frac{dJ_{c \text{ min}}}{d\mathbf{p}}(\mathbf{p}_0) = \frac{\partial J_c}{\partial \mathbf{p}}(\mathbf{p}_0, \mathbf{c}^\circ(\mathbf{p}_0)) + \frac{\partial J_c}{\partial \mathbf{c}^\circ}(\mathbf{p}_0, \mathbf{c}^\circ) \cdot \frac{\partial \mathbf{c}^\circ}{\partial \mathbf{p}}(\mathbf{p}_0) \quad (19)$$

420 We can then simplify the previous expression:

$$\nabla_{\mathbf{p}} J_{c \text{ min}}(\mathbf{p}_0) = \frac{\partial J_c}{\partial \mathbf{p}}(\mathbf{p}_0, \mathbf{c}^\circ(\mathbf{p}_0)) \quad (20)$$

Indeed, $\frac{\partial J_c}{\partial \mathbf{c}^\circ}(\mathbf{p}_0, \mathbf{c}^\circ) = \frac{\partial J_{c \text{ min}}}{\partial \mathbf{c}^\circ}(\mathbf{p}_0)$ is null if the cost function is convex and continuously differentiable on the \mathcal{C} control space for all \mathbf{p} . In practice, we only have an approximate value of the optimal control: $\frac{\partial J_c}{\partial \mathbf{c}}(\mathbf{p}_0)$ tends to 0 over the iterations of the optimization algorithm. \mathbf{c} being continuous and bounded, $\frac{\partial \mathbf{c}}{\partial \mathbf{p}}(\mathbf{p}_0)$ is also and the term $\frac{\partial J_c}{\partial \mathbf{c}}(\mathbf{p}_0) \cdot \frac{\partial \mathbf{c}}{\partial \mathbf{p}}(\mathbf{p}_0)$ tend to 0. In the presence of constraints on parameters and 425 states, the gradient must be equal to the partial derivative of the augmented Lagrangian taking into account the terms related to the constraints (see Uzawa method [27]), otherwise the cancellation of $\frac{\partial J_{c \text{ min}}}{\partial \mathbf{c}^\circ}(\mathbf{p}_0)$ is not guaranteed (when we take into account the constraints by projection techniques for example).

With a given \mathbf{p}_i (element of the parameters vector \mathbf{p}), we can then use $\nabla_{\mathbf{p}} J_{c \text{ min}}$ to build the local sensitivity index:

$$\Upsilon_i = \nabla_{\mathbf{p}_i} J_{c \text{ min}} \cdot \mathbf{p}_i \quad (21)$$

430 The higher Υ_i , the more the relative variation of p_i will affect the theoretical performance of the optimal control. This index does not give the gradient for a parametric error on the model used for the computation of the optimal command but already makes it possible to build a first approximation of the classification of the influential parameters on the control performance. Such an index would also be of great interest in the design of buildings, by making it possible to locate the walls to better insulate for example. In our case, 435 this index can be evaluated very quickly (computational cost of about two simulations) after an optimal control calculation thanks to the adjoint method, which is a significant advantage.

3.4. Sensitivity study results

After the implementation of this sensitivity computing technique in ReTrofit, we were able to perform first sensitivity comparisons on our test case model.

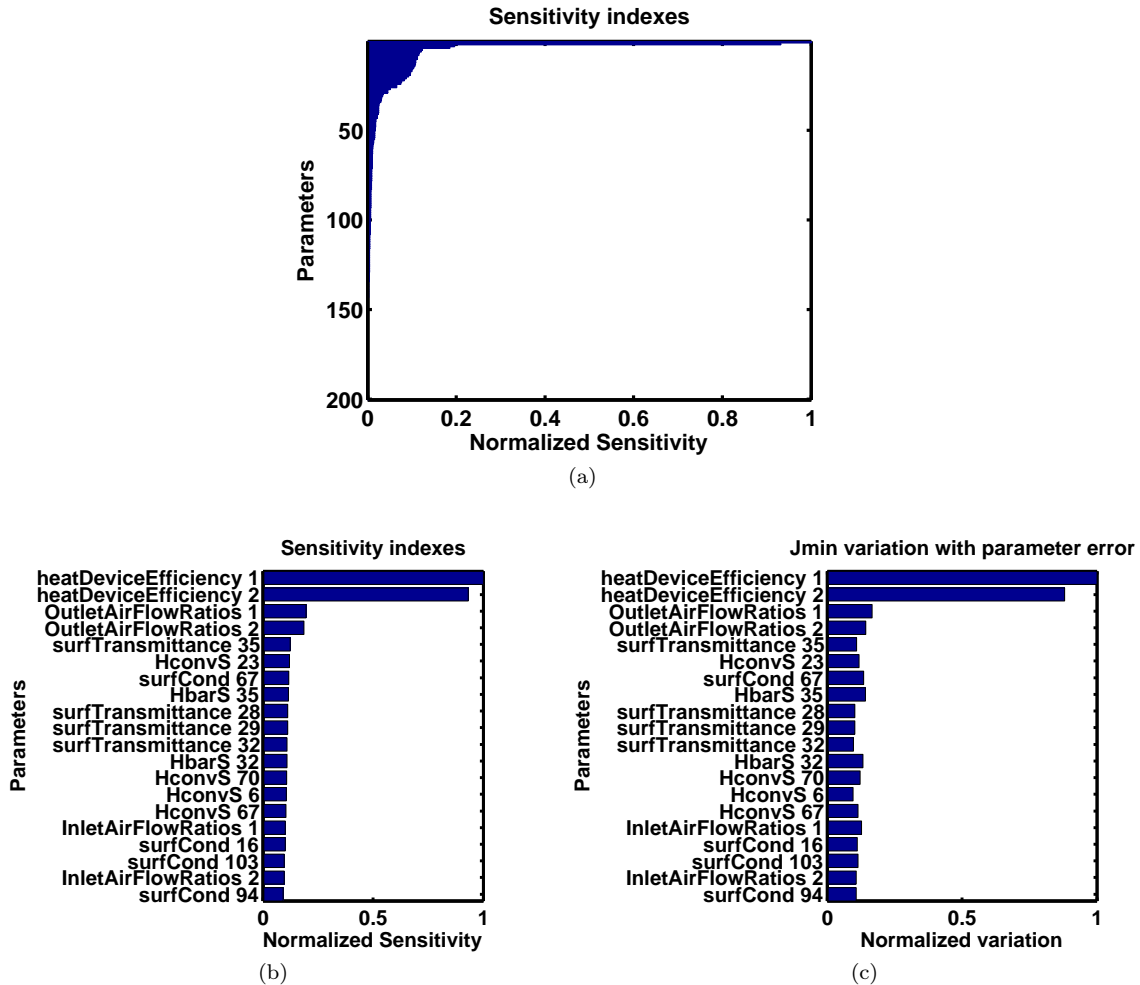


Figure 8: Local sensitivity indexes

440 The figures 8 a and b correspond to the sensitivity indices calculated according to the equations (20) and (21) for the scalar parameters of our model. On the histogram a, only the 200 most influential parameters

are displayed: we note that only 50 parameters stand out from the 735 others. Figure c corresponds to the computation of indices by finite differences. We calculate here the variation of J_{cmin} for a small variation of each parameter (ie. $J_c(\mathbf{p} + \delta\mathbf{p}, \mathbf{c}^\circ(\mathbf{p} + \delta\mathbf{p})) - J_c(\mathbf{p}, \mathbf{c}^\circ(\mathbf{p}))$). This involves recalculating an optimal command for each of them. Despite the errors of approximation, we find the same orders of magnitude for the indices of sensitivity. This finite-difference computation is also much longer, it took indeed more than 15 minutes to calculate the indices of only 20 parameters, against a few seconds for all the parameters of the model with the gradient calculation by adjoint method.

For the 20 most influential parameters according to the histogram b:

- The radiator efficiencies of the two zones are by far the most influential parameters, which is logical because they are directly related to the power injected into the zones.

- Next are the airflow ratios extracted by the AHU (OutletAirFlowRatios). Inbound air ratios are less influential as the air blown in is warmed by the dual flow AHU exchanger.

- Finally, we find the conduction coefficients of the walls (surfCond), indoor and outdoor convection (HconvS and HbarS) window transmittance (SurfTransmittance), relative to or near zones 1 and 2. These coefficients correspond to the insulation of areas and the amount of incoming solar gains.

We have also computed the variation of J_c for a parameter error $\delta\mathbf{p}$ on the optimal command (ie. $J_c(\mathbf{p}, \mathbf{c}^\circ(\mathbf{p} + \delta\mathbf{p})) - J_c(\mathbf{p}, \mathbf{c}^\circ(\mathbf{p}))$) to compare it to the variation of J_{cmin} . In this case, the difference between the two variations is not noticeable, but it can also be obscured by the approximation errors, or even be more present on another model or another cost function.

To evaluate the exact impact of a parameter \mathbf{p}_i on the optimal command, it is necessary to compute $\frac{\partial \mathbf{c}^\circ}{\partial \mathbf{p}_i}$, ie. the sensitivity of the optimal control to a given parameter. It is possible to evaluate such gradient by writing the linearised optimality system at the optimal point. This type of approach has for example been tested on the optimal control of a chemical reaction-diffusion system in a 3D domain [35]. An example using a building model has been tested in [24], but at the moment requires additional developments to be implemented in our simulation tool.

It should also be noted that the sensitivity index (21) is built considering the same percentage of uncertainty on each parameter. The gradient could also be used in an uncertainty propagation calculation (via a sensitivity model), taking into account the real uncertainties of all parameters, including those dependent on time. This would locally quantify the uncertainty of optimal control over the entire prediction interval.

Eventually, the gradients of the minimum of the cost function of the control could be used in the computation of DGSM sensitivity indices (Derivative Global Sensitivity Measure). These global sensitivity indices (in fact, the upper bounds of some Sobol indices) are obtained by applying a Monte-Carlo integration

475 on the gradients calculated according to the probability densities of the parameters and makes it possible to converge more quickly and efficiently than methods of Sobol or Morris [36, 37, 38]. This kind of index could help to better take into account the non-linearities and the uncertainties of the parameters in their classification by order of influence.

4. Conclusion

480 In this paper, we presented a generic strategy for Model Predictive Control in buildings based on standard simulation models and the adjoint method for efficient gradient computations. This approach can use detailed models of buildings and is very flexible concerning choices on parameters to calibrate and estimate (any parameter, constant or time-dependent, can be chosen), as well as control objectives and constraints. A wide variety of gradient-based algorithms can be used since we efficiently compute gradients with the
485 adjoint method. It was also experimented on virtual and a real test case with quite promising results.

Then we used the developed tools to investigate further the case of parameter and sensor selection for MPC problems:

- On numerical calibration experiments using our methodology, we showed on a specific test case that parametric uncertainties can significantly reduce calibration performance and impact sensor choices.
- 490 • Consequently, we investigated a way to select parameters to calibrate using sensitivity indexes and the adjoint approach. This method is based on the gradient computed at the point of optimal control, giving local sensitivity indices for optimal control performance. To complete this work, practical use of the selection methodology must be led on several test cases.

As a general conclusion, the use of adjoint models alongside white-box building models is in our opinion a
495 very promising approach by the methods it brings for MPC and model analysis. Such integration in building simulation software could foster the level of insight and the development of MPC strategies using building energy models.

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