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COMPUTATIONAL DESIGN OPTIMIZATION OF LOW-ENERGY BUILDINGS *

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Abstract. European directives and related national technical standards force the substantial reduction of energy consumption of all types of buildings. This can be done thanks to the massive insulation and the improvement of quality of building enclosures, using the simple evaluation assuming the one-dimensional stationary heat conduction. However, recent applications of advanced materials, structures and technologies force the proper physical, mathematical and computational analysis coming from the thermodynamic principles.

This paper shows the non-expensive evaluation of energy consumption of buildings with controlled indoor temperature, decomposing a building, considered as a thermal system, into particular subsystems and elements, coupled by interface thermal fluxes. We come to a rather large parabolic system of partial differential equations, containing the nonlinearities i) from the surface Stefan-Boltzmann radiation and ii) from the heating control; this can be handled using some properties of semilinear systems. The Fourier multiplicative decomposition together with the finite element technique enables us to derive a sparse system of ordinary differential equations, appropriate for the input of climatic data (temperature, beam and diffuse solar radiation). For the approximate solutions the spectral analysis is helpful; all nonlinearities can be overcome thanks to quasi-Newton iterations.

All above sketched simulations have been implemented in MATLAB. An example shows the validation of this approach, utilizing the time series of measured energy consumption from the real family house in Ostrov u Macochy (30 km northern from Brno). Additional procedures for the support of design of low-energy buildings come namely from the Nelder - Mead optimization algorithm.

Key words. Low-energy buildings, heat transfer, computational modelling, optimization techniques, MATLAB software tools.

AMS subject classifications. 35K05, 35K20, 65K10, 65M60, 65M70, 80A20.

1. Introduction. Knowledge of the position of Sun on the sky, used for natural winter heating and summer shading, dates back to the antique architecture and to the manuscripts by Aischylos and Socrates. However, the modern history of solar, low-energy and similar houses starts from the global economical crisis in the 30ties of 20th century, with the MIT “solar houses” (Massachusetts Institute of Technology, USA), coupling the new trends in architecture and civil engineering with the technological progress oriented to the reduction of energy requirements of buildings, namely of the cost of artificial heating. The actual European concept of passive house, forced by the directive [29] and national technical standards, is connected with the project CEPHEUS (Cost Efficient Passive House as European Standard, 1998–2001), whose ideas are explained in [8] in all details. All energy gains rely on the massive insulation of the building enclosure, together with available technological equipments (heat pumps, air recuperation, etc.) and certain exploitation of solar benefits; this is reflected by the rather simple software tool [9].

The approach of [8] does not handle the thermal accumulation and available climatic data properly, namely in the case of buildings with carefully controlled interior

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temperature in their particular zones and rooms, as in the freezing and cooling plants where the substantial effect of decrease of energy consumption thanks to their optimal design can be expected. Moreover, the inhabitants of family houses or block of flats frequently prefer quite other criteria of well-being than the minimization of energy cost, as reviewed in [4], to suppress (often intuitively) the "sick building syndrom", occurring just in advanced structures minimizing the heat loss without proper ventilation. Also some new experimental research outputs like [25] do not coincide with traditional simplified calculation results. Software simulation packages for building energy performance developed in the last 2 decades, introduced in [5], involve much more physical processes than [9]; however, their complicated "black box" structure with extensive direct computations is not very friendly to the design optimization aims of architects and civil engineers.

In this paper we shall introduce a computational model of a building as a thermal system, whose basic ideas come from [21] and [23]. The decomposition of a building to building parts, as walls, roof, floor, ceilings, etc., as subsystems, with their own interior structure, containing particular constructive, insulation and other layers, as included subsystems, up to particular elements, incorporating selected physical processes with necessary geometric and material characteristics, enables us to obtain a compromise between model complexity and practically reliable, robust and inexpensive computations, supporting the above mentioned optimization of various types. The modular structure of the corresponding software in MATLAB respects such system approach in our practical implementation. Unlike [12], referring to [15] and [24], based on the analogy with the analysis of LC-electric circuits, coupling the finite difference approach with the Euler or similar time integration scheme, we shall work with the finite element technique, the Fourier multiplicative decomposition and the spectral properties of solutions, following some results of [13] (for direct computations) and [14] (for optimization algorithms).

2. Physical and mathematical fundamentals. We shall demonstrate the approach sketched above on the rather simple case of non-stationary heat conduction in the isotropic materials (at least macroscopically, not homogeneous in general), driven by boundary heat transfer from external environment, as studied in [6], including such interface transfer between adjacent subsystems, up to the level of particular elements, occupying a domain Ω in the 3-dimensional Euclidean space R^3. To avoid technical difficulties, we assume certain regularity of Ω, sufficient for the validity of standard Sobolev embedding and trace theorems in the sense of [20], p. 15; for possible generalizations see [18], pp. 69, 160, 512. The development of similar considerations with slightly stronger results in the Euclidean spaces of lower dimensions R^1 and R^2 are left to the patient reader. The following notations hold literally for constructive, insulation, etc. elements of buildings, whereas their modification for empty rooms (representing a majority of volume of a building) needs to set zero values of thermal conductivity; potential generalizations will be mentioned later.

2.1. A simple model problem. Let R^3 be supplied by some Cartesian coordinate system $x = (x_1, x_2, x_3)$. Let the boundary $\partial\Omega$ of Ω in R^3 having a local vector of outward unit normal $\nu(x) = (\nu_1(x), \nu_2(x), \nu_3(x))$ almost everywhere. The usual notation for the Hamilton operators $\nabla = (\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)$ will be used. Moreover, let us consider a time interval $J = [0, T]$ with some real positive T (the limit passage $T \to \infty$ is not prohibited); the upper dot symbol is reserved for partial derivatives with respect to the time $t \in J$. The standard notation of Lebesgue, Sobolev, Bochner, etc. (abstract) function spaces will be utilized in the following considerations, following

[20], pp. 10, 22.

Let us introduce 2 basic material characteristics on Ω: the thermal conductivity $\lambda(x)$ (for the insulation ability) and the thermal capacity $\kappa(x)$ (for the accumulation ability, related to unit volume here). It is natural to suppose that λ and κ are functions from $L^\infty(\Omega)$ (for homogeneous materials only constants), a. e. with values greater than certain positive constant. The weak formulation of a heat transfer equation, using the temperature $\vartheta(x,t)$ on $\Omega \times J$ as the reference variable and working with some volume sources $f(x,t,\vartheta(x,t))$ on $\Omega \times J$ and surface sources $g(x,t,\vartheta(x,t))$ on $\partial\Omega \times J$, reads

$$(v,\kappa\dot{\vartheta}) + (\nabla v, \lambda\nabla\vartheta) = (v,f) + \langle v,g\rangle \quad \text{on } J \tag{2.1}$$

where $(.,.)$ denotes scalar products (for any fixed t) both in $L^2(\Omega)$ and in $L^2(\Omega)^3$, $\langle .,.\rangle$ those in $L^2(\partial\Omega)$, v is an arbitrary test function from V and ϑ must be contained in $L^2(J,V)$, with certain $\dot{\vartheta}$ in $L^2(J,H)$; here we set $H = L^2(\Omega)$, V will be specified later due to the particular choice of f and g, crucial for the implementation of the model. The Cauchy initial condition

$$\vartheta(.,0) = \vartheta_0 \tag{2.2}$$

with a priori known $\vartheta_0 \in V$ then completes the problem definition.

Let us notice that, regardless of (2.2), the formal application of the Green-Ostrogradskij theorem (at least in the sense of distributions – cf. [28], p. 244), using the central dots for the scalar products in R^3, can convert (2.1) to its strong form

$$\dot{\varepsilon} + \nabla\cdot q = f\,, \quad \varepsilon = \kappa\vartheta\,, \quad q = -\lambda\nabla\vartheta \quad \text{on } \Omega\times J\,, \quad q\cdot\nu = g \quad \text{on } \partial\Omega\times J\,, \tag{2.3}$$

compatible with [1], pp. 5, 14: the 1st equation of (2.3) represents the principle of conservation of energy ε related to unit volume, due to some thermal flux q, the 2nd equation quantifies the thermal energy, the 3rd equation is the well-known empirical Fourier constitutive relation between thermal fluxes and temperature gradients, finally the 4th equation represents a general boundary (or interface) condition.

2.2. Fourier multiplicative decomposition. Following the approach of [3], p. 346, let us consider the temperature ϑ on $\Omega \times J$ in the form of multiplicative decomposition

$$\vartheta(x,t) = \phi_i(x)\theta_i(t) \tag{2.4}$$

for any $x \in \Omega$ and $t \in J$ where i denotes the Einstein summation index from $\{1,\dots,n\}$ for certain integer n, with the aim of the limit passage $n \to \infty$, and $\phi_1(x),\dots,\phi_n(x)$ represents a basis of some finite-dimensional approximation V_n of V. For simplicity let us assume $V_n \subset V$; possible "variational crimes" violating such assumptions can be handled by [27]. Consequently in (2.1) we are allowed to consider $v = \phi_j$ for arbitrary $j \in \{1,\dots,n\}$, i. e.

$$(\phi_j,\kappa\phi_i)\dot{\theta}_i + (\nabla\phi_j,\lambda\nabla\phi_i)\theta_i = (\phi_j,f) + \langle\phi_j,g\rangle \quad \text{on } J\,. \tag{2.5}$$

The least squares minimization of $(\theta_k\phi_k - \vartheta_0, \kappa(\theta_i\phi_i - \vartheta_0))$, referring to (2.2), involving also the Einstein summation over $k \in \{1,\dots,n\}$, yields

$$(\phi_j,\kappa\phi_i)\theta_i(0) = (\phi_j,\kappa\vartheta_0)\,. \tag{2.6}$$

The matrix form of (2.5), useful for an efficient software (e. g. MATLAB-based) implementation, is

$$M\dot{\theta} + K\theta = F \quad \text{on } J \tag{2.7}$$

where M and K are positive definite symmetric square matrices from $R^{n\times n}$, $\theta(t) = (\theta_1(t),\dots,\theta_n(t))^{\mathrm{T}}$ is a column vector from R^n for any fixed t, as well as $F(t)$, covering the whole right hand side of (2.5); however, its evaluation is not easy in general. (2.7) forms a system of ordinary differential equations, which should by analysed analytically. Due to practical reasons for m equidistant time steps (where environmental data needed for the composition of F are measured usually) are introduced: $\theta^r = \theta(rh)$ with $r \in \{1,\dots,m\}$, m being en integer number, $h = T/m$; this is compatible with $\theta^0 = \theta(0)$ by (2.6). Also (2.6) can be rewritten as

$$K\theta^0 = \theta_\star\,, \tag{2.8}$$

with $\theta_\star$ (a column vector from R^n again) generated by the right hand side of (2.6).

Finite element approximations by [28], pp. 247, 427, work usually with some continuous functions ϕ_i ($i \in \{1,\dots,n\}$) with values from $[-1,1]$ and small compact support, not orthogonal exactly, unlike classical Fourier analysis. The Lebesgue measure of supports of such functions on Ω is not greater than $c^{-1}n^{-3}$ and their Hausdorff measure on $\partial\Omega$ is not greater than $c^{-1}n^{-2}$ where c is a positive (sufficiently small) constant independent of n. Moreover, we shall consider the integer upper bound N for the number of functions ϕ_i supported on the same part of Ω or $\partial\Omega$ of non-zero relevant measure. It is reasonable to suppose that this choice guarantees also $cn^{-3}|a|^2 \le a\cdot Ma \le c^{-1}n^{-3}|a|^2$, $cn^{-1}|a|^2 \le a\cdot Ka \le c^{-1}n^{-1}|a|^2$, the last couple of inequalities also for K constructed with $\lambda = 1$ everywhere instead of the correct λ formally, for all $a \in R^n$ (considered as column vectors) where $|.|$ denotes the norm in R^n (not only in R^1); the central dots here are used for the scalar products also in R^n (similarly to those in R^3 by (2.3)).

2.3. Existence and uniqueness of solution. Let us start with the purely linear (not very realistic) case $f \in L^2(J,H)$, $g \in L^2(J,X)$ where $X = L^4(\partial\Omega)$, with f and g independent of ϑ; in this case we can take $V = W^{1,2}(\Omega)$. For any fixed $t \in J$ we can rewrite (2.7), supplied by θ^0 from (2.8), as in two different forms as

$$\int_0^t \theta'(\tau)\cdot M\theta'(\tau)\,\mathrm{d}\tau + \frac{1}{2}\theta(t)\cdot K\theta(t) = \frac{1}{2}\theta^0\cdot K\theta^0 + \int_0^t \theta'(\tau)\cdot F(\tau)\,\mathrm{d}\tau\,, \tag{2.9}$$

with the prime symbol replacing the dot one for all time derivatives with respect to τ instead of t. Utilizing the above introduced estimates, (2.9) yields

$$\frac{c}{2n^3}\int_0^t |\theta'(\tau)|^2\,\mathrm{d}\tau + \frac{c}{2n}|\theta(t)|^2 \le \frac{1}{2cn}|\theta^0|^2 + \frac{c}{4n^3}\int_0^t |\theta'(\tau)|^2\,\mathrm{d}\tau + \frac{n^3}{c}\int_0^t |F(\tau)|^2\,\mathrm{d}\tau\,. \tag{2.10}$$

For the last additive term of (2.10) we have

$$\begin{aligned}\int_0^t |F(\tau)|^2\,\mathrm{d}\tau \;&\le \int_0^t\int_\Omega \phi_i(x)f(x,\tau)\cdot\phi_i(x)f(x,\tau)\,dx\,\mathrm{d}\tau \\ &+ \int_0^t\int_{\partial\Omega} \phi_i(x)g(x,\tau)\cdot\phi_i(x)g(x,\tau)\,ds(x)\,\mathrm{d}\tau \le \mu_f\|f\|^2_{L^2(J,H)} + \mu_g\|g\|^2_{L^2(J,X)}\,,\end{aligned} \tag{2.11}$$

utilizing the measures

$$\mu_f = N\left(\left(\frac{1}{cn^3}\right)^{1-1/2}\right)^2 = \frac{N}{cn^3}\,, \qquad \mu_g = N\left(\left(\frac{1}{cn^2}\right)^{1-1/4}\right)^2 = \frac{N}{c^{3/2}n^3}\,. \tag{2.12}$$

Combining (2.10), (2.11) and (2.12), we obtain the brief result

$$\int_0^t |\theta'(\tau)|^2\,\mathrm{d}\tau \le \mathcal{C}n^3\,, \qquad |\theta(t)|^2 \le \mathcal{C}n \tag{2.13}$$

for some positive constant $\mathcal{C}$ independent of n. Thus, inserting (2.13) into (2.4), we get

$$\|\vartheta(.,t)\|^2_H \le \frac{N\mathcal{C}n^3}{cn^3} = \frac{N\mathcal{C}}{c}\,, \qquad \int_0^t \|\nabla\vartheta(.,\tau)\|^2_{H^3}\,\mathrm{d}\tau \le \frac{N\mathcal{C}n}{cn} = \frac{N\mathcal{C}}{c}\,. \tag{2.14}$$

Let us notice that ϑ in (2.14) involves the dependence on n, inherited from (2.4), generating certain sequences $\vartheta^{(n)}$. Due to the reflexivity of both V and $L^2(J,H)$, the Eberlein - Shmul'yan theorem (as introduced in [7], p. 66) yields, up to subsequences, the existence of a weak limit $\vartheta(.,t)$ of $\vartheta^{(n)}(t)$ in V for each $t \in J$, which is strong in H (because of the existence of compact embedding of H into V); simultaneously $\dot{\vartheta}$ is a weak limit of $\dot{\vartheta}^{(n)}$ in $L^2(J,H)$. Such ϑ can be then identified with the solution of (2.1) with (2.2).

Let $\bar{\vartheta}$ be the difference between 2 solutions of (2.1) with (2.2) and t an arbitrary time from J. Then the choice $v = \bar{\vartheta}(.,t)$ gives

$$\frac{1}{2}(\bar{\vartheta}(.,t), \kappa\bar{\vartheta}(.,t)) + \int_0^t (\nabla\bar{\vartheta}(.,\tau), \lambda\nabla\bar{\vartheta}(.,\tau))\,\mathrm{d}\tau = 0\,. \tag{2.15}$$

Thanks to the positive-valued κ and λ, from (2.15) we receive $\bar{\vartheta} = 0$ on J, which implies the uniqueness of ϑ satisfying (2.1) with (2.2).

Similar arguments can be repeated also for the limit case $\lambda \to 0$: this is important for the simplification of temperature development in empty rooms where no more detailed information is available, unlike constructive and insulation building parts. Consequently $\vartheta(.,t)$ is constant for any fixed $t \in J$.

2.4. Realistic classes of thermal sources. More realistic cases for the choice of f and g, needed in computational tools for thermal analysis of buildings, are:

i) $g = \beta(\vartheta_* - \vartheta)$ for the thermal transfer from external environment with some prescribed external temperature $\vartheta_* \in L^2(J,X)$ and some known a. e. positive transfer factor $\beta \in L^\infty(\partial\Omega)$, taking the rigid body − air convection into account, later used also for the thermal transfer between two neighbour domain through their interface analogously,

ii) $f = \alpha(\vartheta_* - \vartheta)$ for the obligatory ventilation by technical standards, similar to i), but applied to the above mentioned case of constant $\vartheta(.,t)$ for a fixed $t \in J$, with some known a. e. positive transfer factor $\alpha \in L^\infty(\Omega)$: such simplified "volumetric convection" is needed to include the heat exchange caused by various installed equipments (without deeper analysis of their performance) between rooms and external environment,

iii) g coming from the beam and diffuse components of solar radiation, occurring just on the building envelope (not on internal interfaces) evaluable from the climatic records of the so-called reference climatic year, due to the day and year quasi-cycles, the mutual position of Sun and Earth, the geographical location of our building object and on the slope and orientation of the relevant building surface, under certain astronomical simplifications presented (including numerous further references) in [13], with the resulting setting of $g \in L^2(J,X)$,

iv) $g = \sigma(\vartheta_*^4 - \vartheta^4)$ for the thermal radiation on the building envelope due to the physical Stefan - Boltzmann law and some known a. e. positive factor $\sigma \in L^\infty(\partial\Omega)$, interpretable as the Stefan - Boltzmann constant (exact for the ideal black body), modified by the empirical surface emissivity, which cannot be incorporated to i) properly because of the presence of ϑ^4,

v) f coming from the artificial heating (or air conditioning, too) in the case similar to ii), but with the requirement of the type $\vartheta \geq \vartheta_\diamond$ for some prescribed indoor temperature $\vartheta_\diamond \in V$ (depending on the room categories by technical standards) at least in the least square sense, due to the real maximal power of heating equipments and to their expected (summer, winter, etc.) different regimes – for more details see [13] again.

All such volume sources f and surface sources g are able to generate additive contributions to the right hand side of (2.1). However, it is useful to incorporate some their parts to the left hand side of (2.1).

Whereas i), ii) and iii) can be handled inside the theory of linear parabolic equations, iv) forces the redefinition of V and the inequalities in v) will be overcome using some facts from the control theory. In i) and ii) g and f force 2 new additive terms $\langle v, \beta\vartheta \rangle$ and $(v, \alpha\vartheta)$ on the left hand side of (2.1); $\beta\vartheta_*$ and $\alpha\vartheta_*$ can be then hidden in g and f on the right hand side as above. Consequently K in (2.7) is replaced by $K + K_f + K_g$ formally with some sparse positive symmetrical matrices K_f from ii) and K_g from i), even with certain regularizing effect. Due to the limited extent of this paper, the detailed analysis can be performed by the patient reader without substantial difficulties. Then iii) brings no new left hand side modification of (2.1) unlike i) and ii); its significance lies in practical long evaluations, accounting for all available environmental data: the temperature θ_*, needed in i) and ii), too, and both relevant components of solar radiation. The repeated application of such data leads to certain quasiperiodicity of the solution of (2.1), suppressing the effect of (2.2) for increasing time.

For iv) the rough heuristic approximation (acceptable for the usual range of temperature) $\vartheta^4 - \vartheta_*^4 = (\vartheta^2 + \vartheta_*^2)(\vartheta + \vartheta_*)(\vartheta - \vartheta_*) \approx 4\vartheta_*^3(\vartheta - \vartheta_*)$ highlights certain quasilinearity of the problem. Using the notation $\langle .,. \rangle$ also for the duality between $L^5(\partial\Omega)$ and $L^{5/4}(\partial\Omega)$, we are able to introduce $V = \{v \in W^{1,2}(\Omega) : v \in L^5(\partial\Omega)\}$ (in the sense of traces), supplied with the norm $\|v\|_{W^{1,2}(\Omega)} + \|v\|_{L^5(\partial\Omega)}$ by [20], pp. 64, 253 (which generates a reflexive Banach space again), and, motivated by i), to add $\langle v, \sigma|\vartheta|^3\vartheta \rangle$ to the left hand side and $\langle v, \sigma|\vartheta_*|^3\vartheta_* \rangle$ to the right hand side of (2.1). Consequently, in addition to the 2nd left-side additive term of (2.9), we have the contribution of the type $\frac{1}{5}|\theta(t)|^{3/2}\theta(t) \cdot S|\theta(t)|^{3/2}\theta(t)$, containing certain sparse positive symmetrical matrix S; the enrichment of the right side of (2.9) is evident. The existence and uniqueness of solution of (2.1) with (2.2) can be then verified as above.

To handle v), the best choice is seemingly to convert (2.1) to the form of a variational inequality. However, the above sketched technical specifications bring serious complications to the design of an efficient computational algorithm, thus another approach, avoiding general optimization strategies, based on the careful control of a heating equipment, is considered: $\vartheta \geq \vartheta_\diamond$ is satisfied in every time step just during the correct (a priori prescribed) heating season, thanks to the controlled heating source f in a corresponding room; the maximum value for the heating power is still considered if this is insufficient.

2.5. Building as a thermal system. All generalizations i) − v) are useful for the development of a model of thermal behaviour of buildings. Understanding Ω as a building element at the lowest (most detailed) level, we are able to compose substructrues at the finite number of levels, using the transfer conditions by i) and ii), up to the whole structure. If ϑ_* and consequently θ_* refer to the external environment, this contributes both to the matrix K in (2.7) (using the matrices K_f and K_g from the preceding discussion) and to the right hand side F. Usually such conditions are applied only in the case when some interface to the room is present, otherwise it is acceptable to take $\alpha \to \infty$, i. e. to force the continuity of temperature on the interface in the normal direction. Clearly iii) and iv) occur only on the external interfaces (building claddings). The existence and uniqueness considerations, handling all possible interface types, can be repeated without substantial difficulties.

Such computational model is open to various generalizations. In particular, let us remind that physical and mathematical homogenization approaches, trying to involve (even incomplete) information on material microstructure, lead to effective anisotropic material characteristics even in the case of composites with isotropic components, due to their location, orientation, etc. (as typically in fibre concrete). Removing the isotropy assumption, we come to the direction-dependent material characteristics λ and κ on Ω and α, β and σ on $\partial\Omega$, generating certain square matrices from $L^\infty(\Omega)^{3\times3}$ or $L^\infty(\partial\Omega)^{3\times3}$ (using the notation from an introductory simple problem for brevity again). At least for the case that all such matrices are a. e. symmetrical and positive definite, the above sketched existence and uniqueness considerations can be repeated with slight technical modifications.

Even more general case with the material characteristics $\lambda(.,\vartheta)$, $\kappa(.,\vartheta)$ on Ω and $\alpha(.,\vartheta,\vartheta_*)$, $\beta(.,\vartheta,\vartheta_*)$ $\sigma(.,\vartheta,\vartheta_*)$ on $\partial\Omega$, important in building practice, can be handled as a quasilinear problem, using selected results on pseudomonotone or weakly continuous mappings by [20], p. 321. However, some additional growth assumptions are needed and all proofs become much more complicated, thus they are not presentable in this short conference paper.

Deeper generalizations cover both the 1st thermodynamic principle of conservation of mass, (linear and angular) momentum and energy (not only of thermal energy as above) and the 2nd thermodynamic principle, handling the irreversibility of some thermal processes, as [22], pp. 145 (for closed systems) and 231 (for open systems). Unfortunately, there is a lot of open questions in the mathematical analysis of corresponding systems of equations of evolutions and related inequalities, as well as in the suggestion of computational algorithms constructing some sequences of reasonable approximate solutions; this is still true even in the particular case of Navier - Stokes equations (cf. the "mysteriously difficult problem" of [20], p. 257).

Fortunately, some simplified approaches for the analysis of parallel physical processes, as heat and moisture transfer in porous media, are available: instead of ϑ we have the couple of unknown variables (ϑ, u) where u evaluates certain moisture content (related to the mass or volume unit), considering the conservation of mass (moisture in pores) and (thermal) energy. The Fick constitutive relation between u and some moisture flux η can be written in the similar way as the Fourier one between ϑ and q in (2.3); however, in the complete system of 2 equations of evolution we need (and must be able to identify in practice) additional material characteristics to handle the Dufour effect (time redistribution of ϑ depends not only on q, but also on η) and the Soret effect (time redistribution of u depends not only on η, but also on q). The proper mathematical and numerical analysis is based on generalization of the results sketched above to the system of 2 equations; practical computations must take the slow moisture transfer in comparison with the thermal one into account.

3. Computational modelling and optimization. Computational tools, at least for direct calculations, including those minimizing the energy consumption, can be based on (2.7) with (2.8). Since some sources are frequently prescribed by their time derivatives in practice, namely those by ii) and v), it is useful to consider the right hand side of (2.7) as $F(t) = \Phi(t) + \dot{\Psi}(t)$ for any $t \in J$, namely for $t \in \{h, 2h, \ldots, mh\}$ where $h = T/m$; the reliable construction of the limit passage $m \to \infty$ depends on the environmental data by iii). To derive the semi-analytic formulae for the evaluation of θ in time, the spectral decomposition $MV\Lambda = KV$ with the generalized real diagonal eigenvalue matrix Λ and the matrix of eigenvectors V is then helpful.

3.1. Direct calculations with heating control. For the brevity, let us consider $\theta^1, \ldots \theta^m$ instead of $\theta(h), \ldots \theta(mh)$ (a priori unknown temperatures) and also $\Phi^1, \ldots, \Phi^m$ and $\Psi^1, \ldots, \Psi^m$ (characterizing all prescribed thermal sources) in the similar sense. For the beginning, let us neglect all nonlinear thermal sources by iv) and v). Applying the classical integral calculus, namely the method of variations of constants, for any time step index $s \in \{1,\dots,m\}$ we come to the direct evaluation formula

$$\theta^s - V\exp(-\Lambda h)V^T M\theta^{s-1} = V\Lambda^{-1}V^T\Phi^s - V\Lambda^{-1}\exp(-\Lambda h)V^T\Phi^{s-1} + V(I-\exp(-\Lambda h))\left(\Lambda^{-1}V^T\frac{\Psi^s-\Psi^{s-1}}{h} - \Lambda^{-2}V^T\frac{\Phi^s-\Phi^{s-1}}{h}\right), \tag{3.1}$$

exact for any $\Phi(t)$ and $\Psi(t)$ with $t \in J$ considered as a Lagrangian linear spline using the nodes $\{0,h,2h,\dots,T\}$. This holds for an arbitrary positive h, unlike the Euler explicit or implicit, Crank - Nicholson, etc. discretization schemes.

To adopt (3.1) to handle iv), at least for sufficiently small h, we can add some $|\theta|^{3/2}S|\theta|^{3/2}$ to K, inserting some reasonable estimate of θ, and apply the quasi-Newton iterations inside each s-th time step; the exploitation of the inexact Newton method is expected to reduce the number of algebraic operations. The same is true for v) where, using the least squares approach, some $\mathcal{G}$ must be added to $\dot\Psi$, to minimize (if possible and required, due to technical specifications) $|\theta-\theta_\diamond|^2$; this can be modified by some prescribed weights for particular rooms if needed. Since $\mathcal{G}$ is just a vector of constants $\mathcal{G}^s \in R^n$ for $(s-1)h < t \le sh$, the total consumption of energy for heating can be evaluated easily as

$$Q = h\sum_{s=1}^{m}\mathcal{G}^s\,. \tag{3.2}$$

Fortunately, both corrections iv) and v) can be unified in one iteration procedure; its details (together with the instructive example), distinguishing between 4 typical heating regimes, are discussed in [12].

The validation of this approach here works with the real living house and atelier in Ostrov u Macochy (30 km northern from Brno), presented (as an example of low-energy house from ecological materials) in [11], p. 146. This small experimental house, designed by architect M. Hudec, built from wood and straw balls, contains 2 floors and 4 rooms, whose 26 mutual interfaces, including those to external environment, are assumed to consist of finite numbers of homogeneous isotropic layers. The design temperature for all rooms is $\vartheta_\diamond = 20^{\mathrm{o}}$ C; $\theta_\diamond$ can be then set analogously to θ_0 in (2.8). The annual climatic records for $h = 1$ hour from the international airport Brno - Tuřany need improvements using the incomplete data from the (colder and wetter) Moravian Karst. The original software code implementing (3.1) and its iterative generalizations has been written in MATLAB. Certain type of optimization is built even in the seemingly direct computational algorithm, thanks to the least squares technique in v). The 1st block of results in the following table documents the process of validation of the algorithm; the comparative variable is Q by (3.2) everywhere.

3.2. Selection of design parameters. The work of architects and civil engineers is far from the optimization of one physically transparent goal function under some simple set of additional conditions: it contains aesthetic, artistic, ecological and other criteria, whose deterministic quantification would be very complicated or quite impossible. The resulting project is typically a result of discussion based on comparison of a finite number of variants, supported by some auxiliary calculations.

As an example, we consider the principal motivation by the economy of heating here, e. g. we are seeking for a sub-optimal (sufficiently small) value of Q, corresponding to some of the prepared variants. The 2nd block in the table demonstrates the effect of the installation of particular heating devices on every floor, or even in every room, instead of one central device, as well as the effect of 2 types of possible replacement of materials in walls. The computation works just with $h = 1$ hour, assuming $\vartheta_0 = 20^{\mathrm{o}}$ C everywhere, repeating the same climatic data for all considered years; it finishes in the case of quasi-periodicity of results, here after 3 years in all cases.

TABLE 3.1
Consumption of energy for heating by various methods including design optimization.

Q [MWh]	evaluation method
1.881	new software, correction for building location
1.419	new software, original climatic data from Brno - Tuřany
1.897	software Energie 2009 (related to Czech technical specifications)
1.710	qualified estimate from time series of user payments for energy
1.915	heating on both floors: 2 devices, total power preserved
1.900	heating in all rooms: 4 devices, total power preserved
1.849	partial replacement of glass garden frontage by non-transparent one
3.039	replacement of straw balls in walls by clay blocks
1.841	Nelder - Mead optimization, 1 parameter: vertical rotation 20.81°
1.769	Nelder - Mead optimization, 2 parameters: vertical rotation 21.37°, glass transparency factor 0.1

3.3. Nelder - Mead simplex algorithm. In the case of proper mathematical optimization, no simple numerical evaluation of gradients like [2] is available, which justifies the choice of the Nelder - Mead downhill simplex method, coming from [19] originally. In the formulation of [26] this method works, in general, with the 5-step algorithm, involving (after sorting simplex vertices) 1) reflection, 2) expansion, 3) outer contraction, 4) inner contraction and 5) shrinkage. Theoretical convergence results for this method are not quite satisfactory: namely by [16], assuming Q (in our notation) as a strictly convex function of 1 or 2 parameters with bounded level sets, the convergence is guaranteed just for 1 parameter, whereas for 2 parameters only the simplex diameter tends to 0 (but need not converge to any minimizer); [17] presents the computer-supported 25-page convergence proof for 2 parameters by contradiction, but only for the restricted algorithm with missing step 2). However, some unpleasant cases of total divergence or numerical stagnation of the algorithm, even for more parameters, can be overcome using some ad hoc adaptive strategies, following [10].

The 3rd block in the table shows the application of this method, making use of the MATLAB function *fminsearch* from the *optimization* toolbox (in addition to the above sketched software code for direct calculations) for 1 and 2 parameters with respect to their lower and upper bounds, included via simple penalty functions: the 1st parameter is the hypothetical vertical rotation of the house, the 2nd one is certain glass transparency factor. More practical considerations and recommendations of this type, including graphs, figures and further references, have been recently published in [14].

4. Conclusion. The computer-supported design of high-performance buildings, accenting their thermal behaviour, motivated by the development of new structures, materials and technologies, as well as by the requirements of sustainable environmental solutions for buildings, contributing to the health and well-being of their inhabitants, reflected by [29], brings new challenges also for physicists, mathematicians, hardware and software developers and other experts. Existing modelling and simulation tools, even those declared as multi-physical, frequently predict other results then those observed in situ; to identify all substantial sources of such differences is not easy.

The system approach, presented in this paper, can be helpful to meet the requirements of reliable and robust optimization with the work style of architects and civil engineers, as well as with investors' money, time and patience. Nevertheless, the need of deeper interdisciplinary discussion is evident.

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