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COMPUTATIONAL APPROACHES TO SOME INVERSE PROBLEMS FROM ENGINEERING PRACTICE

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Abstract

Development of engineering structures and technologies frequently works with advanced materials, whose properties, because of their complicated microstructure, cannot be predicted from experience, unlike traditional materials. The quality of computational modelling of relevant physical processes, based mostly on the principles of classical thermomechanics, is conditioned by the reliability of constitutive relations, coming from simplified experiments. The paper demonstrates some possibilities of computational identification of such relations, namely for heat and mass transfer, coming from original experimental and numerical results obtained at the Brno University of Technology, in selected engineering applications.

1. Introduction

The analysis of inverse problems is a relatively new interdisciplinary field of knowledge, connecting several theoretical and experimental branches: i) theory of ordinary and partial differential equations, ii) development of robust and effective computational algorithms, coming from the least squares, conjugate gradients, etc. approaches – cf. [8], iii) handling unstable and ill-posed problems, needing construction of artificial regularizers, as discussed in [15], p. 26, iv) transparent physical analysis, taking into account the most significant processes in engineering problems, namely those motivated by the development of structures and technologies, working with advanced materials, whose properties, because of their complicated microstructure, cannot be predicted from experience, unlike traditional materials, v) design of experiments for reliable identification of mechanical, thermal, moisture, etc. characteristics of such materials.

However, the general conception of inverse problems covers problems in nondestructive testing, seismic exploration, remote sensing, radio- and tomography, discussed in [15], p. 192, as well as the determination of an unknown source in the heat equation thanks to some overdetermined values of temperature and heat fluxes like [36]. In this paper we shall pay attention to the shorter list of inverse problems:

from certain balance laws from classical thermomechanics, supplied by constitutive relations, we shall try to determine the unknown or uncertain values of engineering macroscopic characteristics occurring in such relations, thanks to some overdetermined data, obtained by some well-advised experiments.

2. Physical and engineering considerations

Respecting the standard notation of Lebesgue, Sobolev, Bochner, etc. (abstract) function spaces by [25], p. 14, we shall start with a model problem from classical thermomechanics: the conservation of a scalar quantity $u \in L^2(I,V)$ with $V = W^{1,2}(\Omega)$ on certain domain Ω in the Euclidean space R^3 with the boundary Γ supplied by the Cartesian coordinates $x = (x_1, x_2, x_3)$, and on some finite time interval $I = [0, \varsigma]$, bounded by a constant ς, can be expressed, following [4], p. 9, in the form

$$\dot{\varepsilon}(u) + \nabla \cdot \eta(u) = f \qquad \text{on } I \times \Omega\,; \tag{1}$$

dot symbols (here and later everywhere) refer to derivatives with respect to $t \in I$, $f \in L^2(I,H)$ with $H = L^2(\Omega)$ refers to some volume source and $\eta : L^2(I,V) \to L^2(I,V)$ and $\varepsilon : W^{1,2}(I,H) \to W^{1,2}(I,H)$ are certain material-dependent mappings; for the example of conservation of energy with u taken as (absolute) temperature, thermal fluxes $\eta(u)$ and enthalpic (evolutionary) terms $\varepsilon(u)$ see [25], p. 252. Let us assume that Ω is sufficiently smooth to guarantee the validity of Sobolev imbedding, trace and similar theorems by [25], p. 16, needed also in the Gelfand triple by [25], p. 190; more general geometrical configurations could be studied (overcoming a lot of technical difficulties) following [21], p. 62, 222 and 385. Let Γ be decomposed to some disjoint parts Γ_c and Γ_i; consequently we are able to formulate the boundary conditions of the Neumann type

$$\eta(u) \cdot \nu = g \qquad \text{on } I \times \Gamma_c \tag{2}$$

utilizing the (formally) outward unit normal $\nu(x) = (\nu_1(x), \nu_2(x), \nu_3(x))$ on Γ, and those of the Robin type

$$\eta(u) \cdot \nu = \psi(u, u_a) \qquad \text{on } I \times \Gamma_i\,; \tag{3}$$

here we need to know some ambient values $u_a \in L^2((I, L^4(\Gamma_c))$, together with a new (material) interface-dependent mapping $\psi : L^2(I, V \times L^4(\Gamma_c)) \to L^2(I, L^2(\Gamma_i))$. We shall consider the initial $u(.,0) = 0$ on Ω here only; it can be verified that any equilibrium initial condition can be converted to this form.

The much-favoured engineering linearizations of mappings included in (1), (2) and (3) (prime symbols refer to derivatives by the following variables) are $\dot{\varepsilon}(u) = \varepsilon'(u)\dot{u} \approx \kappa\dot{u}$ with some $\kappa \in L^\infty(\Omega)$, $\eta(u) = -\nabla\beta(u) = -\beta'(u)\nabla(u) \approx -\lambda\nabla u$ (in the Fourier, Fick, ... "laws") with some $\lambda \in L^\infty(\Omega)$ and $\psi(u, u_a) \approx \gamma(u - u_a)$ with some $\psi : L^2(I, V \times L^4(\Gamma_c)) \to L^2(I, L^2(\Gamma_i))$. Let us notice that even the existence of some $\beta(u)$ represents an additional assumption: it forces the zero rotation

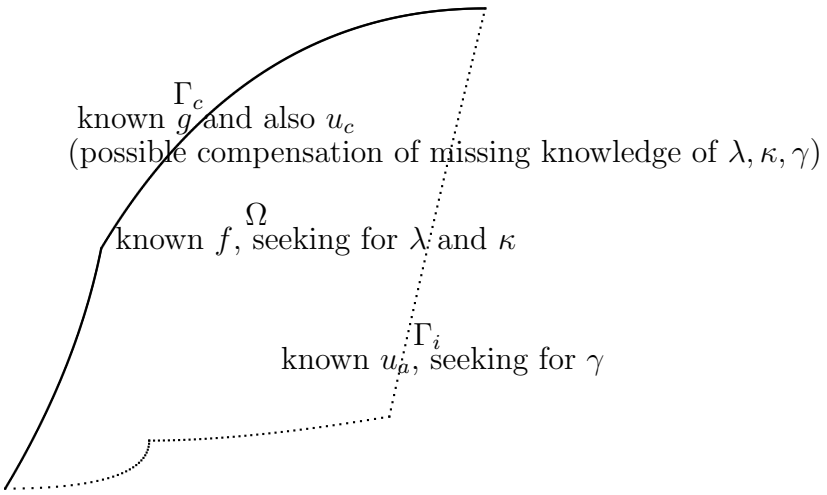

Figure 1: A simplified scheme of geometrical configuration for a model problem.

of $\eta(u)$. Moreover, such scalar characteristics are admissible just for (macroscopically) isotropic media; in more general cases matrix characteristics are necessary.

Fig. 1 shows the above sketched geometrical configuration. To enable the effective analysis with some unknown or uncertain characteristics, some $u_c \in L^2(I, L^2(\Gamma_c))$ is prescribed, too, considered to coincide with the traces of u.

For simplicity, we shall introduce the following notation of scalar products in $L^2(I, X)$, with (generalized) functions ϕ and $\widetilde{\phi}$ from corresponding spaces, i. e. $X = L^2(\Omega)$, $X = L^2(\Omega)^3$, $X = L^2(\Gamma)$,

$$(\phi, \widetilde{\phi}) = \int_I \int_\Omega \phi(x)\widetilde{\phi}(x)\,\mathrm{d}x\,\mathrm{d}t\,, (\nabla\phi, \nabla\widetilde{\phi}) = \int_I \int_\Omega \nabla\phi(x) \cdot \nabla\widetilde{\phi}(x)\,\mathrm{d}x\,\mathrm{d}t\,,$$

$$\langle \phi, \widetilde{\phi} \rangle = \int_I \int_\Gamma \phi(x)\widetilde{\phi}(x)\,\mathrm{d}s(x)\,\mathrm{d}t\,,$$

with $s(x)$ in the sense of Hausdorff measure on Γ; $\langle \phi, \widetilde{\phi} \rangle_i$, $\langle \phi, \widetilde{\phi} \rangle_c$ will denote the same as $\langle \phi, \widetilde{\phi} \rangle$, with Γ_i, Γ_c instead of Γ. Such scalar products are available because X are still Hilbert spaces; some appropriate dualities can be considered instead of them in more general considerations.

The significance of particular physical (and chemical and other) processes depends on engineering applications. In particular, in civil engineering the following processes come into consideration: i) heat transfer (conduction, convection, radiation), ii) air flow, iii) moisture redistribution in porous media, iv) salt and contaminant transport, v) chemical reactions (maturing silicate mixtures, carbonation, ...), vi) phase changes (including those in advanced phase change materials), vii) mechanical deformation (elasticity, plasticity, creep, damage, ...). The above sketched thermomechanical approach generates the balance conditions for a) mass (continuity equations) - with variable density, b) (linear and angular) momentum (Navier - Stokes equations, formulated for various continuum models: by Boltzmann, Cosserat, etc.)

- with variable velocity components (in some reference geometrical configuration), c) energy (Fourier equation) - with variable temperature, d) (semi-)empirical constitutive laws for remaining quantities, separately for particular phases. Bridging between micro- and macrostructure could be performed using some periodic homogenization approach, e. g. the two-scale convergence by [7], or its non-periodic (much more complicated) generalization by [12]; nevertheless, most engineering approaches rely on the mixture theory. Such "multiphysical" analysis dates back to the simple Luikov model, presented in [20], of the simultaneuos heat and moisture transfer, coming to the system of 2 equations of evolution

$$\dot{\tau} = \Delta\tau + \mathcal{K}\dot{\omega}\,, \qquad \dot{\omega} = \mathcal{L}\Delta\omega + \mathcal{L}\mathcal{P}\Delta\tau$$

for 2 unknown functions: the temperature $\tau(x,t)$ and the moisture content $\omega(x,t)$; 3 material characteristics (positive constants) $\mathcal{L}$, $\mathcal{P}$, $\mathcal{K}$ are well-known as Luikov, Posnov and Kossovich numbers. Its slight generalization works with the corresponding fluxes

$$\eta_\tau = (.)\nabla\tau + (.)\nabla\omega\,, \qquad \eta_\omega = (.)\nabla\tau + (.)\nabla\omega$$

and the deeper analysis of material characteristics in all (.) positions; then the first equations handles the so-called Dufour effect, the second equation the so-called Soret one. Much more generalized computational models have been supported by the computer hardware and software development in the last decades: e. g. the model of maturing concrete mixture from [33], referring to the approach of [14], contains 20 equations of evolution, coming from the conservation of mass, momentum and energy related to 4 phases, supplied by appropriate algebraic constitutive relations; the hydration degree, driving the fraction of particular phases must be evaluated from an auxiliary ordinary differential equation.

3. Experimental settings

Unlike complicated advanced "multiphysical" models for direct deterministic calculations, all identification procedures try to arrange necessary measurements under very special conditions, i) to remove or suppress most other influences disturbing a separate physical process by (1), ii) to simplify the geometrical configuration to reduce the complexity of the mathematical and computational analysis, e. g. by the reduction of dimension, thanks to various symmetries, iii) to have a chance to perform some reasonable a posteriori uncertainty analysis. An example of such simple inexpensive measurement equipment for the identification of the thermal conductivity λ and of the thermal capacity (related to unit volume) κ, assuming $\gamma = 0$, is shown on Fig. 2. The controlled heat flux, accompanied by the temperature recorder, supplies all information, needed by Fig. 1. Moreover, for sufficiently large plates the one-dimensional simplification (at least for the first estimate of λ and κ) by [27] is available. However, the proper analysis in R^3 leads to rather complicated relations: even in the case of exploitation of analytic integrals by [3], p. 193, their numerical evaluation may be not quite easy.

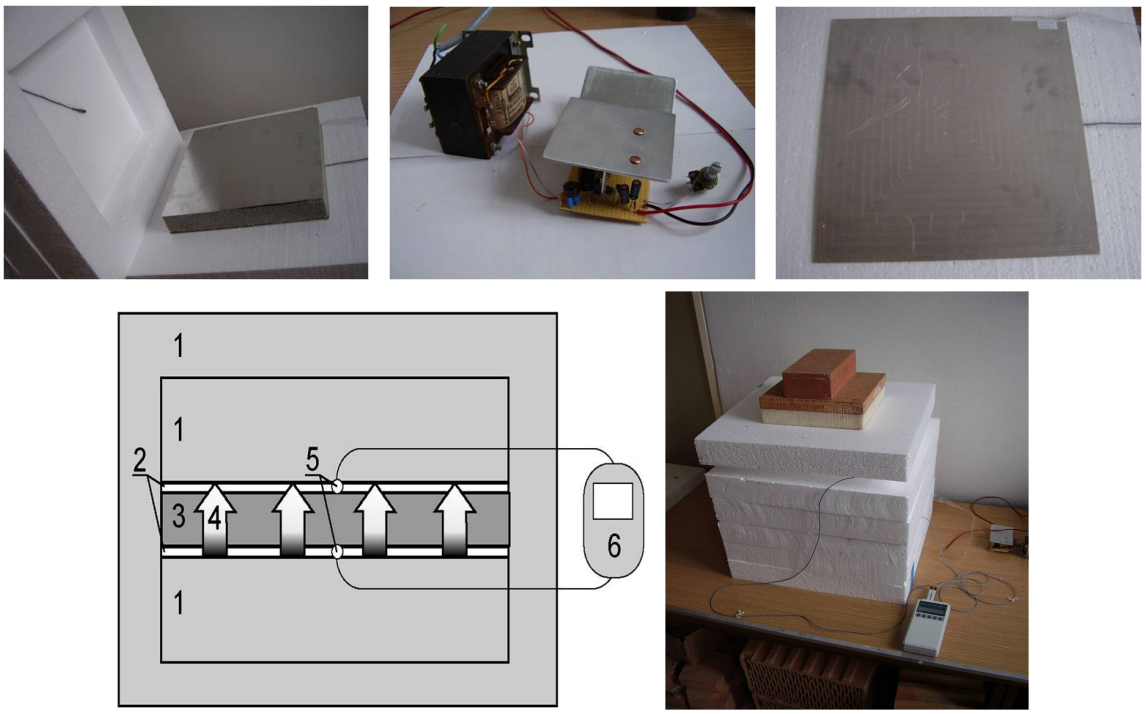

Figure 2: Measurement equipment of the hot-plate type: 1 massive polystyrene insulation layer, 2 couple of aluminium plates: lower heated, upper cold, 3 sample with unknown λ and κ, 4 direction of controlled heat fluxes, 5 temperature sensor(s), 6 temperature recorder.

Other technical solutions of measurement systems than the just presented hot-plate one are known as the hot-ball and hot-wire ones – see [1]. The hot-ball approach works with a sufficiently small heated metal ball, utilizing the spherical coordinates for all computational evaluations, the hot-wire one with a very thin and long heated metal wire, utilizing the cylindric coordinates. In some laboratory settings, namely under hard conditions, as for the testing of fire-clay brickworks, or for the alternative design of powdery insulation materials at high temperature and in vacuum, as an important component of certain heat production and storage system based on sunlight and optical fibers, some modifications are needed, in particular the (nearly) ideal thin hot wire has to be replaced by some massive hollow (ceramic or metal) cylinder, as shown on Fig. 3; for more details see [16].

Especially in the case of elevated or high temperature, in maturing concrete mixtures, during the fire simulation, etc., the factors λ and κ are not constant; as an illustrative example, the lower part of Fig. 3 shows λ for selected powdery insulations (aerogel, perlite, crashed fire clay and certain experimental nano-particles-based material) as a (not very rapidly) increasing function of temperature. Relevant experiments can be organized in several steps at some discrete environmental temperature levels; the contribution of additional thermal fluxes generated by the measurement equipment can be considered as negligible. However, such approach is not practicable in the case of the capillary transfer coefficient λ where (1) describes the conservation

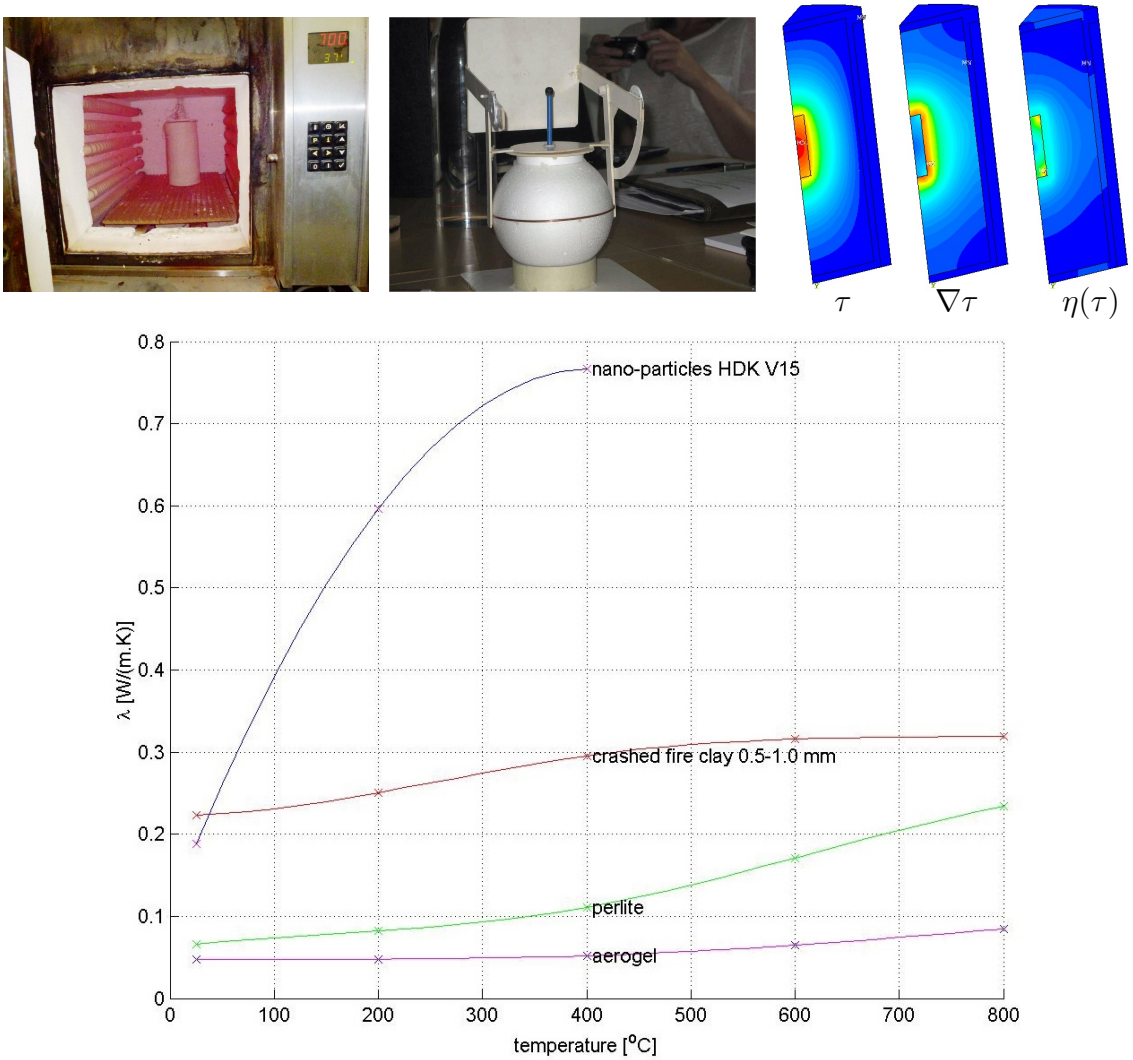

Figure 3: From the left: i) high-temperature cylindric measurement equipment, ii) small model of the thermal accumulator, iii) results of supporting ANSYS-based computations for the evaluation procedure on a cylindric segment, due to service wires. Lower graph: temperature dependence of the thermal conductivity for selected types of powdery insulations.

of moisture mass in some porous material structure ($\kappa = 1$ can be set without loss of generalization) because all experiments show strong dependence of such coefficient on the moisture volume fraction u, thus the tricks with simple functions (like the preceding case) are not adequate. Moreover, to prevent the lack of input data for the identification procedure, the knowledge of values u is needed on Ω or its substantial part, not only on its boundary. Consequently no direct and nondestructive measurements are available; a reasonable compromise may be the indirect measurement exploiting the microwave technique, based on the difference between (relative) electric permittivity and/or magnetic permeability of water and air in pores, as sketched on Fig. 4; for more details on laboratory measurements including calibration techniques see [26].

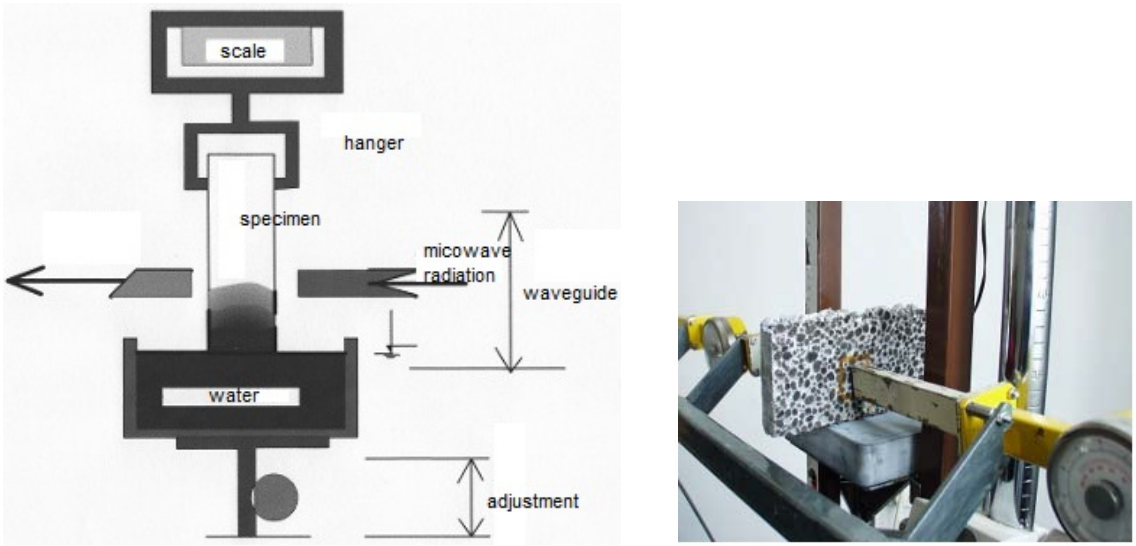

Figure 4: Indirect nondestructive microwave measurement of water content in porous material structure for the identification of the capillary transfer coefficient.

4. Linear and quasilinear problems

As evident from the previous section, we shall work with the set of (in general a priori unknown) characteristics $\vartheta = (\gamma, \lambda, \kappa)$ in appropriate admissible sets of (usually positive) functions.

Following [35] and [17], according to [5], p. 135, let us introduce two functionals

$$F(\vartheta, u, v) = (\kappa \dot{u}, v) + (\lambda \nabla u, \nabla v) + \langle \gamma, uv \rangle_i - (f, v) - \langle g, v \rangle_c - \langle \gamma, u_a v \rangle_i \,,$$

$$G(u) = \frac{1}{2} \langle w, (u - u_c)^2 \rangle_c \,,$$

supplied by certain weight $w \in L^2(\Gamma_c)$, defined for arbitrary $t \in I$, for $u, v \in L^2(I, V)$; consequently $u, v \in L^2(I, L^4(\Gamma))$ and $uv \in L^2(I, L^2(\Gamma))$. This requires the application of the trace theorem; moreover the Sobolev theorem on (compact) imbedding, the Friedrichs - Poincaré inequality, the Lax - Milgram theorem (and its generalizations), the properties of Rothe sequences of abstract functions (continuous and discrete Gronwall lemma, Gelfand imbedding, ...), the Aubin - Lions lemma for abstract functions, etc. (cf. [25] and [13]), are needed in the complete proofs of the following propositions.

Now we are ready to formulate a) a direct model problem, b) a sensitivity one and c) an adjoint one, useful namely in linearized considerations, including those with slightly variable material characteristics (due to the motivation from the preceding section). Such formulations will be useful for the design of a general algorithm for the analysis of an inverse problem, i. e. the problem of identification of $\vartheta = (\gamma, \lambda, \kappa)$ here. Some particular cases may occur in the literature typically: e. g. [17] takes variable γ only, moreover in the steady-state case.

4.1. A direct problem

The weak formulation of a direct problem reads: for some fixed β and $u_0 = 0$ find u such that $F(\vartheta, u, v) = 0$ for any v, i. e.

$$(\kappa \dot{u}, v) + (\lambda \nabla u, \nabla v) + \langle \gamma, (u - u_a)v \rangle_i = (f, v) + \langle g, v \rangle_c \,,$$

valid for any $t \in I$ (here and in all analogous situations). Its strong formulation comes from the obvious application of the Green - Ostrogradskiĭ theorem

$$(\kappa \dot{u} - \nabla \cdot (\lambda \nabla u) - f, v) = \langle \gamma(u_a - u) - \lambda \nabla u \cdot \nu, v \rangle_i + \langle g - \lambda \nabla u \cdot \nu, v \rangle_c \,.$$

However, the reverse application of the same theorem is possible, too; e. g. for the fundamental solution $v_*(x, y) = -1/(4\pi|x-y|)$ of the equation $\Delta v_*(x, y) = 4\pi\delta(x-y)$ locally for $y \in \Omega$ instead of $v(x, t)$ with fixed $t \in I$ we obtain

$$(\kappa \dot{u}, v) - (\beta(u), \Delta v) = (f, v) + \langle \gamma, (u - u_a)v \rangle_i + \langle g, v \rangle_c - \langle \beta(u), \nabla v \cdot \nu \rangle$$

Let us remind that generalized initial conditions are also available: there is sufficient to take $f - f_0$, $g - g_0$, $u_a - u_{a0}$ and $u - u_0$ instead f, g, u_a and u where all zero indices refer to values in $t = 0$; the same could be done for sensitivity and adjoint problems, too.

4.2. A sensitivity problem

The weak formulation of a sensitivity problem reads: for some fixed ϑ, $\widetilde{\vartheta}$ (expressing some change of ϑ) and $u_0 = 0$ find $\widetilde{u}$ such that $DF(\vartheta, u, v, \widetilde{\vartheta}, \widetilde{u}, o) = 0$, with o referring to zero-valued functions, for any v, i. e.

$$(\kappa \dot{\widetilde{u}}, v) + (\lambda \nabla \widetilde{u}, \nabla v) + \langle \gamma, \widetilde{u} v \rangle_i = \langle \widetilde{\gamma}, (u_a - u)v \rangle_i - (\widetilde{\lambda} \nabla u, \nabla v) - (\widetilde{\kappa} \dot{u}, v) \,.$$

Its strong formulation comes from the obvious application of the Green - Ostrogradskiĭ theorem

$$(\kappa \dot{\widetilde{u}} - \nabla \cdot (\lambda \nabla \widetilde{u}) - \nabla \cdot (\widetilde{\lambda} \nabla u), v)$$

$$= \langle \widetilde{\gamma}(u_a - u) - \gamma \widetilde{u} - \lambda \nabla \widetilde{u} \cdot \nu - \widetilde{\lambda} \nabla u \cdot \nu, v \rangle_i - \langle \lambda \nabla \widetilde{u} \cdot \nu + \widetilde{\lambda} \nabla u \cdot \nu, v \rangle_c \,.$$

The reverse application of the Green - Ostrogradskiĭ theorem gives here

$$(\kappa \dot{\widetilde{u}}, v) - (\beta(\widetilde{u}) + \widetilde{\beta}(u), \Delta v) + \langle \gamma, \widetilde{u} v \rangle_i = \langle \widetilde{\gamma}, (u_a - u)v \rangle_i - \langle \widetilde{\kappa} \dot{u}, v \rangle - \langle \beta(\widetilde{u}) + \widetilde{\beta}(u), \nabla v \cdot \nu \rangle \,.$$

4.3. An adjoint problem

The weak formulation of an adjoint reads: for some fixed ϑ and $u_\varsigma = 0$ find v such that $DF(\vartheta, u, v, o, \widetilde{u}, o) = DG(u, \widetilde{u})$ for u coming from a direct problem and for any $\widetilde{u}$, i. e.

$$-(\kappa \widetilde{u}, \dot{v}) + (\lambda \nabla \widetilde{u}, \nabla v) + \langle \gamma, \widetilde{u} v \rangle_i$$

Its strong formulation comes from the obvious application of the Green - Ostrogradskiĭ theorem

$$-(\widetilde{u}, \kappa\dot{v} + \nabla\cdot(\lambda\nabla v)) = \langle\widetilde{u}, w(u-u_c) - \lambda\nabla v\cdot\nu,\rangle_c - \langle\widetilde{u}, \gamma v + \lambda\nabla v\cdot\nu\rangle_i\,.$$

The reverse application of the Green - Ostrogradskiĭ theorem gives here

$$-(\widetilde{u}, \kappa\dot{v}) - (\Delta\beta(\widetilde{u}), v) + \langle\gamma, \widetilde{u}v\rangle_i = \langle w, (u-u_c)\widetilde{u}\rangle_c - \langle\nabla\beta(\widetilde{u})\cdot\nu, v\rangle\,.$$

Combining $\widetilde{u}$ from a sensitivity and v from an adjoint problem, we receive

$$\langle w, (u-u_c)\widetilde{u}\rangle_c = \langle\widetilde{\gamma}, (u_a-u)v\rangle_i - (\widetilde{\lambda}\nabla u, \nabla v) - (\widetilde{\kappa}\dot{u}, v)\,;$$

thus it is natural to introduce a new functional

$$J(\vartheta) = \int_I G(u)\mathrm{d}t\,.$$

4.4. Computational algorithms

For simplicity of notation, let us set $J_*(\gamma) = J(\vartheta)$ here, in particular with $\vartheta = (\gamma, o, o)$; the analogous derivation of the general case is left to the (very patient) reader. Then we shall need some reasonable estimate γ^0 for the construction of iterations γ^k with $k \in \{1, 2, \ldots\}$, the evaluation of gradients $\mathcal{G}^k = (u^k(\gamma^k) - u_a)v^k$ and differentials $DJ_*(\gamma^k, \widetilde{\gamma}^k) = \langle\widetilde{\gamma}^k, \mathcal{G}^k\rangle_i$, $D^2J_*(\gamma^k, \widetilde{\gamma}^k, \widetilde{\gamma}^k) = \langle w, \widetilde{u}(\gamma^k, \widetilde{\gamma}^k)^2\rangle_c$. The conjugate gradient algorithm, following [2], can be expressed in the form

$$\gamma^{k+1} = \gamma^k + a^k\widetilde{\gamma}^k\,,$$

$$\widetilde{\gamma}^k = b^k\widetilde{\gamma}^{k-1} - \mathcal{G}^k\,, \quad \text{in particular } \widetilde{\gamma}^0 = 0 \;\; (b^1 \text{ is not needed})\,;$$

a^k come from the minimum line search with the result

$$a^k = -DJ_*(\gamma^k, \widetilde{\gamma}^k)/D^2J_*(\gamma^k; \widetilde{\gamma}^k; \widetilde{\gamma}^k)\,,$$

whereas b^k are generated by the Fletcher - Reeves formula

$$b^k = \langle\mathcal{G}^k, \mathcal{G}^k\rangle_i/\langle\mathcal{G}^{k-1}, \mathcal{G}^{k-1}\rangle_i\,,$$

the Dai - Yuan formula

$$b^k = \langle\mathcal{G}^k, \mathcal{G}^k\rangle_i/\langle\widetilde{\gamma}^{k-1}, \mathcal{G}^k - \mathcal{G}^{k-1}\rangle_i\,,$$

or some similar one; for the discussion of suitable choice of such formulae see [23] and [29]. Especially for an assumed constant γ on Γ_i this degenerates to the classical Newton algorithm.

Now the complete computational strategy depends on the choice of number of iterations for γ^k, λ^k and κ^k separately. However, λ^k and κ^k, defined on Ω, may suffer from the lack of data, namely in the case of their rather rich admissible sets; therefore some modification of this approach could be needed. Certain remedy will be recommended in the sixth section.

5. Stochastic generalizations

To obtain $J(\vartheta) \approx 0$ in the previous section is quite not realistic; this depends not only on the quality, efficiency and robustness of the above presented purely deterministic algorithm, but also on the stochastic character of data, influence of disturbing physical processes and measurement imprecisions. However, sources of such errors cannot be distinguished, which restrains the validity of identification results; moreover, most technical standards on the laboratory testing require to submit some uncertainty analysis. Thus it could be useful to generalize all deterministic formulations to stochastic ones, although a lot of difficulties, including that in the mathematical verification (as the absence of simple imbedding and similar theorems for proofs), must be expected.

In general, instead of the spaces of abstract functions of the type $L^2(I, \mathcal{S})$ with S taken as V, $L^2(\Omega)$, etc., we are able, following [35], to define the spaces $L^2(\Theta, I, \mathcal{S})$ where Θ refers to a space of elementary events, supplied with some σ-algebra and some probability measure P. Our optimization functional then obtains a new parameter $\theta \in \Theta$, i. e.

$$J_*(\gamma) = \frac{1}{2} \int_\Theta \int_I \int_{\Gamma_c} w(x,\theta)(u(x,t,\theta) - u_c(x,t,\theta))^2 \,\mathrm{d}s(x)\,\mathrm{d}t\,\mathrm{d}P\,.$$

Various approaches to the mimimization of such (or similar) functional can be then found in the literature, e. g. i) [22] applies the Karhunen - Loève spectral expansion, or, alternatively, the expansion based on the Hermitean polynomial chaos, which leads to the stochastic finite element technique, ii) [34] prefers the Bayesian approach, with Markov chains and Monte Carlo simulations, iii) a quite different algorithm comes from the Sobol sensitivity analysis by [19], relying on Monte Carlo simulations again. Nevertheless, the common drawbacks of such analysis, in addition to the above mentioned difficulties in functional and numerical analysis, are numerous artificial regularization tricks, as the Tikhonov regularization by [36], absence of appropriate software tools oriented to engineering applications and exceedingly time-consuming and expensive computations.

6. Nonlinear problems

Regardless of the formal similarity of mass and energy balance equaitions, as well as of the linearized Fourier and Fick constitutive equations, typical material characteristics for diffusion of liquid water, water vapour and various contaminants are much more complicated than those from the heat transfer with dominated conduction, discussed in [31] – all results depend on material microstructure (not only on such macroscopic characteristics as volume fraction of pores) significantly, diffusion is typically not quite reversible, etc. Consequently the approach from the fourth section do not lead to any credible results for engineering simulations. As a motivation from an useful modification of such approach, we shall come from the experimental tool sketched on Fig. 4.

Let us start, following [25], p. 253, with some useful transforms and substitutions, namely with the enthalpic and Kirchhoff transformations by [31] (for various right-hand sides)

$$\kappa(u)\dot{u} - \nabla \cdot (\lambda(u)\nabla u) = \dots$$

$$\hat{\kappa}(u(r)) = \int_0^r \kappa(\rho)\,\mathrm{d}\rho\,, \qquad \hat{\lambda}(u(r)) = \int_0^r \lambda(\rho)\,\mathrm{d}\rho\,, \qquad \beta(u) = \hat{\lambda}(\hat{\kappa}^{-1}(u))\,,$$

consequently

$$\dot{U} - \Delta\beta(U) = \dots$$

for the (adroitly defined) enthalpy $U = \widehat{\kappa}(u)$. For simplicity, in all remaining considerations we shall take only $\kappa(u) = 1$, zero f and empty Γ_i.

For an effective computation, the natural requirements are: i) $u \approx u_*$ on some set $\Omega_* \subseteq \Omega$ with $\mathrm{meas}(\Omega_*) > 0$, with measured u_*-values, to avoid lack of data, ii) introduction of

$$G(u) = \frac{1}{2}(u - u_*, w(u - u_*))$$

with some weight $w \in L^\infty(\Omega_*)$, zero-valued outside Ω_* iii) local estimates of $\beta(.)$ or $\lambda(.)$, coming from the direct formulation. For sufficiently smooth $\beta(.)$ we are then able to perform obvious conversions

$$\nabla\beta(u) = \beta'(u)\nabla(u) = \lambda(u)\nabla u\,,$$

$$\Delta\beta(u) = \nabla \cdot \nabla\beta(u) = \nabla \cdot (\lambda(u)\nabla u) = \lambda'(u)\nabla u \cdot \nabla u + \lambda(u)\Delta u\,.$$

The weak formulation of a direct problem reads: for some fixed ϑ and $u_0 = 0$ find u such that $F(\beta, u, v) = 0$ for any v, i. e.

$$(\dot{u}, v) + (\nabla\beta(u), \nabla v) = \langle g, v\rangle\,.$$

Its strong formulation comes from the obvious application of the Green - Ostrogradskiĭ theorem

$$(\dot{u} - \Delta\beta(u), v) = \langle g - \nabla\beta(u) \cdot \nu, v\rangle\,, \tag{4}$$

or from its alternative form (with λ instead of β)

$$(\dot{u} - \lambda'(u)\nabla u \cdot \nabla u - \lambda(u)\Delta u, v) = \langle g - \nabla\beta(u) \cdot \nu, v\rangle\,. \tag{5}$$

The analysis of solvability of (4) can be done by [25], p. 239. The analogous (not quite general) analysis of (5) in [24] needs non-trivial regularity results from [13] and auxiliary lemmas from [10]. The reverse application of the Green - Ostrogradskiĭ theorem gives here

$$(\dot{u}, v) - (\beta(u), \Delta v) = \langle g, v\rangle - \langle \beta(u), \nabla v \cdot \nu\rangle\,.$$

Most authors do not distinguish between u and u_* at all, inserting u_* (if available) instead of u into all calculations. To identify a function $\beta(u)$, some decomposition (finite-dimensional in practical calculations) is needed. The standard one is $\beta(u) = c_i\beta_i(u)$ where the sum over $i \in \{1, 2, \ldots\}$ (due to the Einstein summation rule) is considered for prescribed functions $\beta_i(u)$ and unknown real coefficients c_i. However, [6], p. 62, develops another approximate method where $M_i = \{(x,t) \in \Omega \times I : \overline{\lambda}_{i-1} \leq \lambda(u(x,t)) \leq \overline{\lambda}_i\}$, $\lambda_i(u) = (\overline{\lambda}_{i-1} + \overline{\lambda}_i)/2$ and $c_i = \mathrm{meas}(M_i)$, utilizing a priori given constants $\overline{\lambda}_0, \overline{\lambda}_1, \ldots$, as a basis for the *double integration method* by [9].

Some explicit formulae for the evaluation of $\lambda(u)$ can be found in the literature, coming from the one-dimensional simplification on a half-line (for a theoretically infinite sample). The most celebrated result, based on the Boltzmann - Matano transformation $y = x/(2\sqrt{t})$ (generating an ordinary differential problem in y), is

$$\lambda(u(x,t)) = \frac{1}{2tu'_x(x,t)} \int_x^\infty \xi u'_\xi(\xi,t)\,\mathrm{d}\xi\,; \tag{6}$$

for various modifications of this formula and for the historical remarks see [18]. As shown in [32] (including an original software code in MATLAB), infinite integrals in (6) can be removed for the prescribed boundary flux g (from direct measurements) with the result

$$\lambda(u(x,t)) = \frac{1}{u'_x(x,t)} \left(\int_0^x \dot{u}(\xi,t)\,\mathrm{d}\xi - g(t) \right) .$$

Another modification of (6)

$$\lambda(u(x,t)) = -\frac{1}{u'_x(x,t)} \int_x^\infty \dot{u}(\xi,t)\,\mathrm{d}\xi$$

is presented as the *third integration method* in [28].

General estimates of $\beta(.)$ or $\lambda(.)$ from three-dimensional experimental data are more delicate, utilizing some (numerically unpleasant) Dirac distributions $\delta(.)$ in most cases. The *second integration method* by [28] comes from the equation of type

$$(\dot{u} - \lambda'(u)\nabla u \cdot \nabla u - \lambda(u)\Delta u, v) = \ldots$$

for $v = \delta(x - \xi)\delta(t - \iota)$, $\xi \in \Omega$ and $\iota \in I$. Consequently

$$\lambda'(u)\nabla u \cdot \nabla u + \lambda(u)\Delta u = \dot{u}$$

remains on $\Omega \times I$; this can be solved (unlike a direct nonlinear problem) as one linear ordinary differential equation. The *first integration method* by [28] considers

$$(\dot{u}, v) - (\beta(u), \Delta v) = \ldots$$

for $v(x,t) = v_*(x,\xi)\delta(t - \iota)$; the integration then gives

$$\beta(u(x,t)) = -\frac{1}{4\pi} \int_\Omega \frac{\dot{u}(\xi,t)}{|x - \xi|}\,\mathrm{d}\xi$$

locally. In the above announced *double integration method* it is sufficient to choose $v = \delta(x-\xi)\delta(t-\iota)$ with $\xi \in \Omega$ and $\iota \in I$ in

$$(\dot{u} - \nabla \cdot (\lambda(u)\nabla(u)), v) = \dots ;$$

however, M_i for $i \in \{1, 2, \dots\}$ must be (approximately) detected from the analysis of isohypersufaces $u(x,t)$, consequently the integration over $\Omega \times I$ is needed to determine c_i (which is extremely expensive for any two- ore more-dimensional case). An alternative approach of [6], p. 67, then relies on some special genetic algorithms; for still other alternative optimization approaches cf. [8].

Let us consider $c = (c_1, c_2, \dots)$ (and later also $\widetilde{c} = (\widetilde{c}_1, \widetilde{c}_2, \dots)$). A direct, sensitivity and adjoint problem can be now formulated similarly to the fourth section here; we shall present the weak formulations only. For a direct problem this reads: for some fixed $c = (c_1, c_2, \dots)$ and for $u_0 = 0$ find u such that $F(c, u, v) = 0$ for any v, i. e.

$$(\dot{u}, v) + (\nabla \beta_i(u), \nabla v) c_i = \langle g, v \rangle .$$

For a sensitivity problem this reads: for some fixed c and $\widetilde{c}$ and for $u_0 = 0$ find $\widetilde{u}$ such that $DF(c, u, v, \widetilde{c}, \widetilde{u}, o) = 0$ for any v, i. e.

$$(\dot{\widetilde{u}}, v) + (\nabla \beta_i(\widetilde{u}), \nabla v) c_i = (\nabla \beta_i(u), \nabla v) \widetilde{c}_i .$$

For an adjoint problem this reads: for some fixed c and for $u_\varsigma = 0$ find v such that $DF(c, u, v, o, \widetilde{u}, o) = DG(u, \widetilde{u})$ for u from a direct problem and for any $\widetilde{u}$, i. e.

$$-(\widetilde{u}, \dot{v}) + (\nabla \beta_i(\widetilde{u}), \nabla v) c_i = (w(u - u_*), \widetilde{u}) .$$

Combining $\widetilde{u}$ from a sensitivity and v from an adjoint problem, we receive

$$(\nabla \beta_i(u), \nabla v) \widetilde{c}_i = (w(u - u_*), \widetilde{u}) ;$$

$J(c) = G(u)$ can be introduced.

The conjugate gradient algorithm, starting from certain initial estimate c^0 of c, works with iterations c^k for $k \in \{1, 2, \dots\}$, gradients $\mathcal{G}^k = (u^k(c^k) - u_*) v^k$ and differentials $DJ_*(c^k, \widetilde{c}^k) = (\widetilde{c}^k, \mathcal{G}^k)$, $D^2 J_*(c^k, \widetilde{c}^k, \widetilde{c}^k) = (w\widetilde{u}(c^k, \widetilde{c}^k), \widetilde{u}(c^k, \widetilde{c}^k))$. This leads to the algorithm

$$c^{k+1} = c^k + a^k \widetilde{c}^k ,$$

$$\widetilde{c}^k = b^k \widetilde{c}^{k-1} - \mathcal{G}^k , \quad \text{in particular } \widetilde{c}^0 = 0 \ \ (b^1 \text{ is not needed})$$

again; here

$$a^k = -DJ_*(c^k, \widetilde{c}^k) / D^2 J_*(c^k; \widetilde{c}^k; \widetilde{c}^k) , \qquad b^k = (w\mathcal{G}^k, \mathcal{G}^k) / (w\mathcal{G}^{k-1}, \mathcal{G}^{k-1}),$$

with possible alternatives for the evaluation of b^k again.

7. Conclusion

The increase of requirements from engineering practice to reliable analysis of inverse problems, namely on identification of material characteristics in thermodynamical applications, discussed in this paper, due to advanced materials, structures and technologies, seem to be faster than the progress in analysis of existence of their (unique) solutions, of (global) convergence of sequences of approximate solutions in finite-dimensional spaces, etc. Even the variety of (often ad hoc) computational algorithms documents the absence of a general, inexpensive and robust one, working for a large class of experimental settings. Clearly this is a strong motivation for further research – maybe following the way predicted by [11]: i) overreaction to immature technology (naive euphoria), ii) frustration (cynicism), iii) true user benefits (realistic expectation), with certain asymptote of reality.

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