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Solution of Identification Problems in Computational Mechanics – Parallel Processing Aspects

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Abstract Problems of identification of material parameters (mostly parameters appearing in constitutive relations) have applications in many fields of engineering including investigation of processes in a rock mass. This paper outlines the structure of parameter identification problems, methods for their solution and describes an identification (calibration) problem from geotechnics, which will serve as a realistic benchmark problem for illustration of the behaviour of selected parameter identification methods.

Keywords inverse problems, identification of material parameters, Nelder-Mead method, genetic algorithms, rock mechanics

1 Introduction

Generally, the identification problems appear in investigation of physical processes in material environment. The processes are described by the state variables u and driven by the control variables f. The material is characterized by parameters $\kappa \in \mathscr{K} \subset R^p$.

Direct problems focus on computation of $u = u_h(\kappa) = u_h(\kappa, x, t)$, where (x, t) gives space and time localization, if f and κ are known. On the opposite, identification problems use the knowledge of f and some partial apriori knowledge on the state variable u for (partial or full) determination of κ.

If the apriori information about the state variable u is given by the vector $d = (d_i) \in R^m$ of measured values, then the search for the unknown material parameters can be formulated as the following minimization problem

$$F(\kappa) = \| \mathscr{M} u_h(\kappa) - d \| \longrightarrow \min_{\kappa \in \mathscr{K}} . \qquad (1)$$

Above, $\mathscr{M}$ is an observation operator, which computes from u_h values corresponding to the measured data from d. In the simplest case, it just select the values $u(x_i, t_i)$ corresponding to d_i.

In contrary to direct problems, it is known that some identification problems are not well posed [4], which means that some of the following properties can be violated:

- there exists a solution of the problem,
- the solution is unique,
- the solution is stable under small changes of input data.

Although the properties of the minimization problems can be difficult to analyse, a lot of different iterative techniques can be used for the minimization (1) (mostly without theoretical proof of convergence). The range of applicable methods includes

- gradient methods, e.g. Gauss-Newton, Levenberg-Marquardt, conjugate gradients, see [3], [4], [6], [7],
- gradient-free direct method, e.g. Nelder-Mead simplex method [3],
- stochastic methods e.g. [5], genetic algorithms e.g. [6], [9] and [8].

In this paper, we discuss the use of these methods also from the point of view of parallelization. Some of the approaches are illustrated by numerical experiments, implementation of the other methods is in progress.

Note also that the identification problem is very close to the calibration of a mathematical model. The difference is if we stress the computed material parameters or coincidence of values predicted by the model with measured data.

2 A Benchmark Problem

The in-situ Äspö Pillar Stability Experiment (APSE) has been performed at SKBs Äspö Hard Rock Laboratory in south eastern Sweden with the aid of investigation of granite mass damage due to mechanical and thermal loading. The measured data are now used for validation of mathematical models within the DECOVALEX 2011 international project. APSE used electrical heaters to increase temperatures and induce stresses in a rock pillar between deposition holes (Fig. 1) until its partial failure. To determine accurately the temperature changes, a heat flow model is formulated and monitored temperatures are used for identification of heat flow parameters (heat capacity, heat conduction coefficient, heat convection into the

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holes). The identification should provide parameters taking into account water bearing fractures and water flow and calibrate the model. More details and another approach to the model calibration can be found in [1].

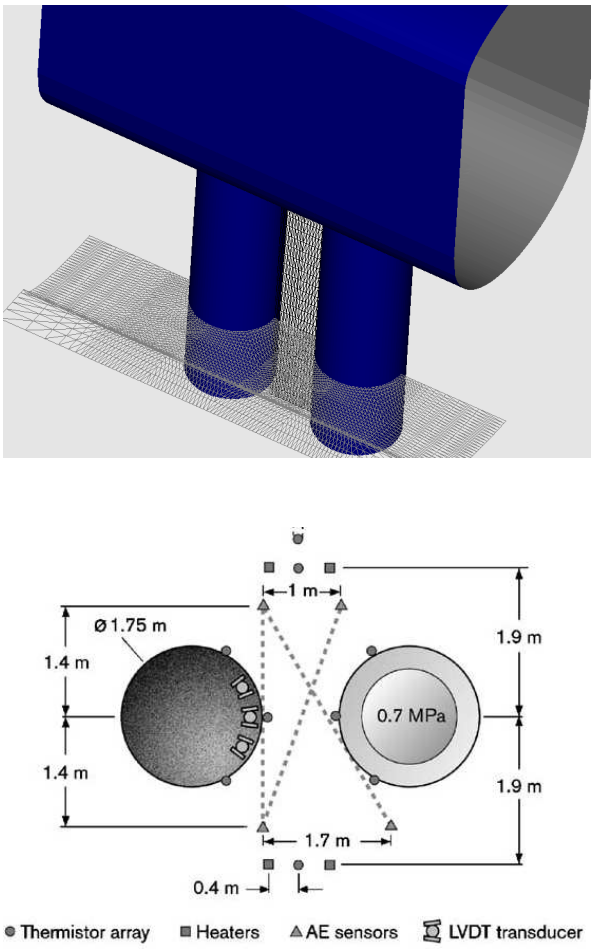

Figure 1: The APSE model - detail of the FE grid around the pillar (GEM software [2]) and plan view on the pillar, holes, location of heaters and points of temperature measurement

The exploited APSE model, realized by GEM software [2], considers domain of $105 \times 125 \times 118$ m and $99 \times 105 \times 59$ nodes. The grid is refined around the pillar, see Fig. 1. The heaters are producing heat which varies in time. The model assumes original temperature 14.5°C on the outer boundaries, zero flux onto the tunnel and nonzero flux given the convection onto the holes. The initial condition is given again by the temperature 14.5°C.

Monitoring of the temperatures during two month heating phase of APSE is essential for calibration of the thermal model. There are 14 temperature monitoring positions and temperatures are measured in 12 time moments. Altogether 168 values of temperature measurement (vector d) are used for parameter identification, which according to (1) can be written as follows

$$F = F(\lambda_1, c_1, \lambda_2, c_2, \lambda_3, c_3, H_1, H_2, H_3)$$
$$= (\sum_i [u_h(x_i, t_i) - d_i]^2)^{0.5} \longrightarrow \min. \qquad (2)$$

The material parameters represent different conductivity λ and heat capacity c for dry and wet side of model (according to Fig. 1). The rock in the right hole had yielded from a depth of approximately 0.5 m down to 3 m which motivates to introduce a third type of material with different λ and c for the damaged part of the pillar. We supposed heat conduction between rock and air in excavated holes determined by different values of the heat conduction coefficient H for individual holes with third coefficient corresponding to surface for the above mentioned damaged part of the pillar. It gives 9 material parameters of the cost functional F in (2).

3 Nelder-Mead Optimization

The first optimization algorithm, which we describe in this paper, is the Nelder-Mead algorithm, which maintains a simplex $S^{(k)}$ in the space of parameter vectors. This simplex locally approximates the objective function F and serves for getting information about its behaviour and getting approximation to the optimal point. If $F = F(\kappa)$ and $\kappa \in R^p$ then the k-th step simplex $S^{(k)}$ is determined by $p+1$ vectors of parameters (vertices) $\kappa^{(k,1)}, \ldots, \kappa^{(k,p+1)}$. We assume that the object function values are evaluated and vertices are sorted, so that

$$F(\kappa^{(k,1)}) \leq F(\kappa^{(k,2)}) \leq \ldots \leq F(\kappa^{(k,p+1)}).$$

The k-th step then continues by evaluation of the stop criterion and if the approximation is not found to be satisfactory, then the worst vertex $\kappa^{(k,p+1)}$ is replaced by a new one or, in a specific case, the whole simplex is shrunk.

In any case, first, the new vertex is sought in the form

$$\kappa(\mu) = (1+\mu)\bar{\kappa} - \mu\kappa^{(k,p+1)},$$

where $\bar{\kappa} = \left((\kappa^{(k,1)} + \ldots + \kappa^{(k,m+1)})/m\right)$ is the barycentre and μ is equal to $\mu_r = 1$ for reflection, $\mu_e = 2$ for extension, $\mu_{oc} = 1/2$ for outer contraction and $\mu_{ic} = -1/2$ for inner contraction.

The k-th step always begins with evaluation of $F_r = F(\kappa(\mu_r))$. If $F(\kappa^{(k,1)}) \leq F_r < F(\kappa^{(k,m)})$ then we take $\kappa(\mu_r)$ as the new point, otherwise we gradually test for the expansion, outside and inside contraction and take the selected case. It means that the k-th step typically contains one or two evaluations of the object functions. In the case of contractions, we can also decide for shrinking the simplex, which is more expensive and costs p evaluations of the object function. The details can be found in [3].

The optimization is stopped when both decrease of the cost functional F is small (below ε_f) and changes of parameters are small (below ε_p) or if too many evaluations of the cost function are required.

Our experience with the Nelder-Mead method is described in the next Section.

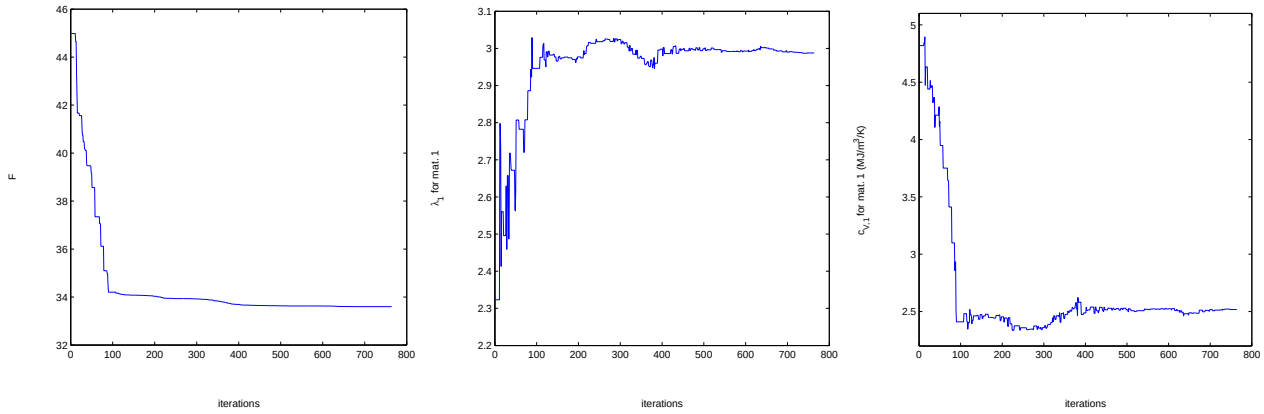

Figure 2: The convergence of the cost functional F (left), parameter λ_1 (center) and c_1 (right)

As concerns the parallelization, the Nelder-Mead method is in principle sequential, which means that parallelization can be involved only in evaluation of the cost function and eventually in realization of the shrinking of simplex in some steps.

4 Numerical Results

Let us consider numerical solution of the benchmark problem from Section 2, i.e. finding of various heat transfer coefficients, by the Nelder-Mead method. Note that we use method of unconstrained optimization, but to guarantee the positivity of the parameters, we use exponential transformation, i.e. finding x such that $\kappa = e^x$ is the required parameter. As the parameters have quite different orders, we scale the heat capacity c for having all parameters in order of units.

The Nelder-Mead iterations are stopped when both decrease of the cost functional F is small (below ε_F) and changes of parameters are small (below ε_p). To find very accurate approximation of the parameters, we stop iterations with $\varepsilon_F = 0.001$ and $\varepsilon_p = 0.01$. With a physical initial guess, the stop occurred after 764 iterations, for a non physical initial guess surprisingly less iterations were required. The convergence behaviour is illustrated in Fig. 2. But the stopping test could be fulfilled much earlier (say after 100 iterations) if we weaken the requirement on small changes in all parameters. This is also due to the fact that the objective function depends only mildly on some of the parameters, see [11].

Note also that computation of $u = u(\kappa, x, t)$ represents here the solution of an evolution parabolic heat transfer problem, which is solved by linear finite element discretization in space and backward Euler method in time. Linear systems appearing in each time step are solved iteratively by conjugate gradient method preconditioned by one-level additive Schwarz method, which is efficient it this case, see [10]. Of course the parallel computing can be also used for assembling the finite element matrices.

5 Stochastic and Evolution Methods

To get a larger space for parallelization we shall consider stochastic and evolution methods for optimization. In this section, we shall consider a constrained search space for parameters, i.e. $\kappa \in \mathscr{K} = \prod_1^p \langle \kappa_{i,\min}, \kappa_{i,\max} \rangle$. The the simplest stochastic (Monte Carlo) algorithm is then as follows

MC algorithm with $N = N_{MC}$ individuals

(1) generate N random vectors $\kappa^{(i)} \in \mathscr{K}$, $i = 1, \ldots, N$,
(2) evaluate (in parallel) $F(\kappa^{(i)})$, $i = 1, \ldots, N$,
(3) select $\kappa = \mathrm{argmin}_i F(\kappa^{(i)})$.

Genetic algorithms (GA) enrich the selection by operations of crossing and mutation. It provides the following algorithm

GA with $N = N_{GA}$ individuals

(1) generate N random vectors $\kappa^{(i)} \in \mathscr{K}$, $i = 1, \ldots, N$
(2) for given generation, evaluate (in parallel) $F_i = F(\kappa^{(i)})$, if F_i is not known yet,
(3) select τN parameter vectors $\kappa^{(i)}$ with smallest values F_i; so called parents. Then create $(1-\tau)N$ new vectors (childrens) by crossing randomly selected parents,
(4) create a new generation by taking the selected parents and created childrens with mutating some of them,
(5) evaluate stopping test and GOTO (2) if results are still not satisfactory.

In our case, the crossing and mutation acts on parameter vectors and can be described as algebraic (not binary) rule, see e.g. [8], [9]. For example:

Crossing of vectors x and y is a new vector z, which can be given by

$$z_i = x_i + \alpha_i (y_i - x_i),$$

where for discrete crossing α_i is selected from $\{0, 1\}$ with probability 1/2, but also α_i can be selected randomly in the range $\langle -\delta, 1+\delta \rangle$ for e.g. $\delta = 0.25$,

Mutation of the vector x concerns its components x_i. Each component is mutated with probability, which is usually $1/p$. Mutation uses a range Δ_i, for $x_i \in \langle \kappa_{i,\min}, \kappa_{i,\max} \rangle$

it is typically $\Delta_i = 0.1(\kappa_{i,\max} - \kappa_{i,\min})$. Mutation of x then gives a new vector z, e.g.

$$z_i = x_i \pm \Delta_i 2^{-k\alpha},$$

where α is choosen uniformly in $\langle 0, 1\rangle$ and k is so called precision constant depending on the problem.

For more details on GA, we refer to [9] and [8]. The method is attractive for a large space for parallelization and still reasonable efficiency, see [6].

6 Conclusions

The paper describes the philosophy of the solution of the identification problems and numerical realization of the method. Optimization with the Nelder-Mead and genetic algorithms are discussed in more detail. At present, we have experience with numerical behaviour of the Nelder-Mead optimization. The efficiency is increased by parallelization of the solution of the embedded direct method as well as by the gradual improvement of the discretization accuracy during optimization. Implementation and testing of the genetic methods are in progress now. We suppose that parallel computations based on GA will be efficient even on parallel systems with larger number of processing elements.

In this paper, we omit the discussion on the gradient algorithms, which can be efficient and involving some parallelism for computing the Jacobian by either finite differences or a semianalytic approach.

For the future, similar identification problems will be applied to another geotechnical problems including the development of in-situ rock mass tests and testing samples of geocomposites in the laboratory scale. There are also another aspects, which will be considered, such as selection of parameters, regularization of the cost function, application to nonlinear problems and automatic problem and computer oriented choice of the optimization method.

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