Derivative-Free Local Search in Hybrid Algorithms for Hydromechanical System Model Updating

V. D. Sulimov P. M. Shkapov
spm@bmstu.ru

Abstract

Multitudinous practical studies related to the safety and early diagnostics of significant objects in the nuclear power industry are based on reliable mathematical modeling in hydromechanical system dynamics. Procedures of model updating are powerful tools for producing adequate models. Consideration is being given to problems of building accurate mathematical models for detecting anomalies in the phase constitution of the coolant flowing throw the reactor primary circuit. Main dynamical characteristics of the object under diagnosing are considered as continuous functions of the bounded set of control variables. Possible occurrence of anomalies in the phase constitution of the coolant can be found out owing to changes in dynamical characteristics of the two-phase gas-liquid flow. Computational model updating techniques are used for adjusting selected parameters of hydrosystem models in order to make the models compatible with measured experimental data. This is performed by minimizing the differences of analytical and measured data with the use of numerical optimization methods. Incompleteness of measured spectral data and presence of multiple frequencies result in the error function of the extremal problem being non-convex and non-differentiable. Two novel hybrid algorithms with derivative-free local search for solving the corresponding global minimization problem are proposed. The first algorithm M-PCASFC combines the stochastic Multi-Particle Collision Algorithm (scanning the search space) and deterministic Space Filling Curve method (local search). The second algorithm M-PCAMNM implements the Modified Nelder-Mead simplex method for local minimization. Results of successful computational experiments are presented to show the efficiency of the approach.

1 Introduction

Present-day nuclear power industries have increasing interest in using fault detection and diagnosis methods to ensure safety and reliability of nuclear power plants [1]. The methods are classified into model-based methods, data-driven methods and signal-based methods. Development and operational processes for nuclear power systems impose heavy demands on the accuracy and computational reliability of appropriate mathematical models. Thus a number of recent papers are devoted to modelling and simulation problems in connection with finite element model updating for in-core components of nuclear reactors, construction of a simulation framework for technical systems life cycle cost analysis, investigation of a chattering problem which arises in a dynamic mathematical two-phase gas-liquid flow model [2, 3, 4]. Development and updating sets of computational models representing the physical behaviour of the object under consideration make up an actual problem. One of the most severe accidents in nuclear power generation is loss of coolant, where the recirculating coolant of the pressurized water reactor may flash into steam [5]. It should be noted that methods of computational modelling and experimental investigations of two-phase flows have received much attention [6, 7, 8]. The standard reactor instrumentation can register signals caused by pressure fluctuation of a coolant. The problem at hand is an interpretation of the registered spectra and useful data extraction for computational model updating. As to actual practice in the field of two-phase flow dynamics, numerical estimates generally do not sufficiently match the measured data obtained from experiments. The modern methodology to reduce the above discrepancies is to update the assumptions made for physical idealizations and parameters of the computational model until the agreement between numerical predictions and experimental results satisfy practical requirements. In particular, appreciable effort has been made in the development of special-purpose procedures for updating parameters of computational models using data extracted from vibration tests. The much used approach to computational model updating is the inverse sensitivity technique where residuals between numerical and measured eigenvalues and/or mode shapes are minimized in order to improve user-selected parameters. The finite element model updating method has been proved to be a reliable approach for practical problems [9].

In the gradient-based inverse sensitivity methods of the model updating is critically important to define an appropriate error function between the computed and measured modal data. The estimated parameters can be obtained by minimizing the error function, which is generally a non-linear function of the updating parameters. Moreover, in defining the error function the correct pairing of computed modal data with the measured modal data is essential. The reason is that the pairing of computed and experimental modal data based on the sequential order of mode numbers may not be correct at all times. With the aim of establishing the correct modal correspondence the modal assurance criterion is generally used. One further important stage in model updating is the selection of the parameters to be updated. In particular, the computed natural frequencies and corresponding mode shapes of the computational model should be sensitive to the selected updating parameters. Quite often only the measured eigenvalues are used for model updating. This is because firstly the measured mode shapes contain more noise than the natural frequencies and secondly the mode shapes are not very sensitive to parameter changes. Nevertheless, the mode shapes are necessary to ensure that the modes under consideration are paired correctly. The objective function in the minimization problem is the weighted sum of squares of the error in the eigenvalues. The problem is non-linear and requires an appropriate iterative solution, and in turn this requires the formulation and computation of the sensitivity matrix of the function to be minimized with respect to the updating parameters. Possible availability of repeated or very close eigenvalues one should take into account. As the minimization problem is usually ill-conditioned, then various regularization techniques should be applied [10].

The inverse problems under study are solved for perfect but incomplete spectral data. The results of corresponding direct problem solutions have been confirmed by using the finite-element code ANSYS. Incompleteness of the experimental spectral data and presence of repeated eigenvalues result in the error function being non-convex and non-differentiable. So there is a need to use nonsmooth or derivative-free optimization methods. Since the error function has numerous local minima, it is necessary to use global optimization methods. Properties of deterministic global optimization algorithms are well-studied. Thus a modified tunnelling algorithm had been used for the diagnostic problem of the nuclear reactor primary circuit [11]. It is common knowledge that the performance of deterministic algorithms essentially depends on the problem dimension. New hybrid global optimization algorithms have been proposed recently [12, 13]. Both of them combine the stochastic

Particle Collision Algorithm (PCA) [14] (scanning the solution space) with deterministic methods (local search). Another global optimization software tool MEMPSODE that integrates stochastic algorithms (Particle Swarm Optimization and Differential Evolution) with efficient local search procedures is presented in [15]. Further implementation of two novel hybrid algorithms is discussed. The first algorithm implements the Multi-Particle Collision Algorithm (M-PCA) [16] for scanning the solution space of the problem in combination with the deterministic space-filling curve method [17]. In the second hybrid algorithm the modified Nelder-Mead Simplex method for local search is used [18]. A good collection of derivative-free methods for nonlinear programming is presented in [19, 20, 21].

The remainder of the paper is organized as follows. The next section contains statement of the computational model updating problem. Section 3 provides brief description of hybrid global optimization algorithms. In section 4 successful computational experiments for two model updating problems are presented to illustrate peculiarities of the proposed approach. Section 5 gives conclusions and discussion on further work.

2 Formulation of the problem

It is supposed that a set of performance index values associated with a computational model to be updated is defined by a set of controlling variables. Experimental spectral data registered by permanent instrumentation may be incomplete. So the goal is to determine vectors of controlling variables using only measured data on natural frequencies of the object. The standard approach is to set the inverse spectral problem and then to solve the corresponding least squares problem

$$\min_{x \in X \subset \mathbb{R}^n} f(x)\,, \tag{1}$$

where $f(x) = \sum_{i=1}^{N} w_i(\zeta_i(x) - \zeta_i^*)^2$; x, X — the vector of controlling variables and its feasible domain of the error function $f(x)$ respectively; the w_i stand for weighting factors that reflect the confidence level in the measurements; N is the number of eigenvalues under consideration; $\zeta_i(x)$ and ζ_i^* denote the eigenvalues that correspond to computed (solutions of the direct problem) and to measured natural frequencies respectively;

$$X = \{x_i \,|\, x_i^L \le x_i \le x_i^U\,;\, i = \overline{1,\, n}\}\,; \tag{2}$$

here x_i^L, x_i^U — the lower and upper bounds on the i th controlling variable.

As practical observations show, the error function in the considered problem is often multiextremal. Therefore, it is necessary to turn to methods of global optimization. It is clear that if the measured spectral data exactly match to the computational model then the solution of the minimization problem will cause error function to take its global minimum value of zero. Let us suppose that there is a unique solution of the ill-posed inverse spectral problem and that this corresponds to the global minimum of the error function. However, the fact is that the theoretical question of the uniqueness of solutions of the problem may not be relevant to practical applications in which there is the additional complication of accuracy of experimental measurements. Furthermore, some complications may arise due to incompleteness of measured spectral data, influence of the two-phase interference on the flow dynamics, the presence of noise, etc. Within the scope of this work we take it as a convenient and reasonable assumption that global minimization of the error function in the above inverse problem will yield correct model updating for objects under consideration.

3 Hybrid global optimization algorithms

3.1 The M-PCASFC algorithm using the Space-Filling Curve Method

The modern Multi-Particle Collision Algorithm [16] has some essential advantages in relation to well known stochastic global optimization algorithms such as the Genetic Algorithms, Simulated Annealing, Fast Simulated Annealing, etc. Specifically, the M-PCA does not require any additional parameters other than the number of iterations; the algorithm is extremely easy to implement and can be applied to both continuous and discrete optimization problems. The original PCA [14] works as follows. First an initial configuration is chosen, then a modification of the old configuration into a new one is implemented. The qualities of the two configurations are compared. A decision then is made on whether the new configuration is acceptable. If it is, the current configuration acts as the old configuration for the next step. If it is not acceptable, the algorithm proceeds with a new change of the old configuration. It is pertinent to note that acceptance of current trial solution with certain probability may avoid the convergence to local optima. However, the PCA is in its early stages. In spite of its advantages over Genetic Algorithm and Simulated Annealing in solving test problems, practical application of the PCA is restricted because of solutions remain too expensive. As possible development, the local search procedure in the algorithm could be improved.

The modern Multi-Particle Collision Algorithm is based on the canonical PCA, but a new characteristic is introduced: the use of several particles, instead of only one particle to act over the search space. So, the new outer loop for the particle control has been added to the basic global optimization algorithm. Thanks to use of several particles the M-PCA can better explore the search space, avoiding convergence to a local minimum. Coordination between the particles was achieved throw a blackboard strategy, where the *Best_Fitness* information is shared among all the particles in the process. Similar to PCA, M-PCA also has only one parameter to be determined, the number of iterations. But in this case, the total number of iterations is divided by the number of particles which will be used in the process. The division of the task is the great distinction of the M-PCA, which leads to a great reduction of required computing time.

Some powerful algorithms for multi-extremal non-convex optimization problem are based on reducing the initial multi-dimensional problem to the equivalent problem of one dimension. This reduction can be executed by applying Peano-type space-filling curves mapping a unit interval on the real axis onto a multi-dimensional hypercube [17]. The Peano curve development maps the segment $[0\,,\;1]$ of the real axis $\mathbb{R}^1$ into the hypercube $x \in \mathbb{R}^1$ determined in (2). Actually, this is the case of continuous single-valued mapping that offers finding point $x(z) = (x_1(z)\,, \ldots\,, x_n(z))^T \in X$ for each point $z \in [0\,,\;1]$:

$$\min_{x \in X} f(x_1\,, \ldots\,, x_n) = \min_{0 \le z \le 1} \phi(z)\,. \tag{3}$$

So, the initial multi-dimensional minimization problem (1) is equivalent to the above one-dimensional problem of finding the global minima of the discontinuous multi-extremal function $\phi(z)$. The Hilbert technique is used here for building the development of the Peano space-filling curve depending on parameter m that stands for the number of subdivision levels.

The approach needs not any derivatives of the function to be minimized with updating parameters. Some disadvantage of this approach is in the fact that one-dimensional problem obtained by the above reduction leaks some information on the closeness of iteration points in the initial multi-dimensional space. The pseudo code brief description of the PCASFC algorithm that combines the PCA and the deterministic space-filling curve method is presented in [22]. The novel global optimization algorithm M-PCASFC on base of the M-PCA and SFC algorithms is constructed in analogous manner.

3.2 The M-PCAMNM algorithm using the modified Nelder-Mead Simplex Method

As an alternative to the hybrid algorithm NMPCA [12] a novel hybrid algorithm PCALMS was presented in [22]. In this new version of the global optimization algorithm the local search mechanism is a standard deterministic linearization method. Inverse problems are considered to be substantially difficult because of the kinks connected with presence of the repeated or very close frequencies in registered spectra for the computational model under updating. The difficulty motivated the development of algorithms for the solution of the minimization problem via some smooth approximation, which could be minimized by using any of the efficient classical approaches for smooth optimization. It is clear that the approach makes it possible to implement efficient gradient techniques in the solution process. In general case the error function is not differentiable everywhere, so the implementation of the smoothing technique may be quite pertinent. Computational experiments show the principal applicability of the proposed hybrid algorithm PCALMS for solving the inverse spectral problems.

Returning to derivative-free algorithms mention may be maid of the convergent variant of the Nelder-Mead algorithm. The algorithm is often claimed to be robust for problems with presence of discontinuities or where the criterion function values are noisy. When an iteration of the Nelder-Mead algorithm does not yield sufficient descent, then a fragment of a grid called a frame is completed, thereby guaranteeing convergence. Frames are defined in terms of positive bases. Full description of the modified Nelder-Mead algorithm is presented in [18]. So this converged version of the algorithm may be used for local search in the hybrid global optimization algorithm. It should be noted that multi-direction-based version of the Nelder-Mead simplex method for solving computationally expensive optimization problems was proposed in [23]. Description and comparison of different nonsmooth minimization methods and corresponding software was presented in [24]. It should be mentioned that in solving highly complicated optimization problems it is necessary to implement parallel methods [25].

The pseudo code brief description of the ultimate hybrid algorithm that combines the M-PCA and the deterministic derivative-free local search procedure is as follows.

```
0. Generate an initial solution Old_Config
   Best_Fitness = Fitness (Old_Config)
   Update Blackboard
   For n = 0 to # of particles
     For n = 0 to # of iterations
       Update Blackboard
       Perturbation ( )
       If Fitness (New_Config) > Fitness (Old_Config)
         If Fitness (New_Config) > Best_Fitness
           Best_Fitness := Fitness (New_Config)
         End If
         Old_Config := New_Config
         Exploration ( )
       Else
```

```
      Scattering ( )
    End If
  End For
End For

2. Exploration ( )
  For n = 0 to # of iterations
    Small_Perturbation ( )
      Local search
      Using deterministic Derivative-Free Procedure
      Check stopping criterion:
      Find global solution Best Fitness
      Else continue
      If Fitness (New_Config) > Best_Fitness
        Best_Fitness := Fitness(New_Config)
      End If
      Old_Config := New_Config
    End For
Return

3. Scattering ( )
  p_scatt = 1 - (Fitness (New_Config)) / (Best_Fitness)
  If p_scatt > random(0, 1)
    Old_Config := random solution
  Else
    Exploration ( )
  End If
Return

4. Perturbation ( )
  For i = 0 to (Dimension-1)
    Upper = Superior_Limit[i]
    Lower = Inferior_Limit[i]
    Rand = Random(0, 1)
    New_Config[i] = Old_Config[i] -
      ((Upper - Old_Config[i]) * Rand) -
      ((Old_Config[i] - Lower) * (1-Rand))
    If (New_Config[i] > Upper)
      New_Config[i] = Superior_Limit[i]
    Else
      If (New_Config[i] < Lower)
        New_Config[i] = Inferior_Limit[i]
      End If
    End If
  End For
Return

5. Small_Perturbation ( )
  For i = 0 to (Dimension-1)
```

```
    Upper = Random(1.0, 1.2) - Old_Config[i]
    If (Upper > Superior_Limit[i])
      Upper = Superior_Limit[i]
    End If
    Lower = Random(0.8, 1.0) - Old_Config[i]
    If (Lower > Inferior_Limit[i])
      Lower = Inferior_Limit[i]
    End If
    Rand = Random(0, 1)
    New_Config[i] = Old_Config[i]−
      ((Upper − Old_Config[i]) ∗ Rand) −
      ((Old_Config[i] − Lower) ∗ (1 − Rand))
  End For
Return
```

4 Computational results

In this section two numerical examples of the novel hybrid derivative-free algorithm M-PCAMNM applications to inverse spectral problems for VVER-1000 nuclear reactor equipment are presented. In the examples the updating of the computational model of the coolant two-phase flow dynamics in the primary circuit is carried out.

Example 1. The computations were performed in connection with the problem of identification of the coolant phase constitution in the VVER-1000 primary circuit. Appearance of the second phase is possible: in a coolant heating zone (pressure tank of the pressurizer), in an exit volume of the reactor pressure vessel (RPV), in a core barrel of the RPV, in exit volumes of main circulating pumps. In order to formulate the inverse problems two vectors of relative acoustic velocities in a coolant flowing throw the specified zones are introduced. Let the anomalous coolant state constitution be characterized by second vector of controlling variables: $x_1^* = 100.0\%$; $x_2^* = 80.5\%$; $x_3^* = 73.0\%$; $x_4^* = 100.0\%$. The error function is determined using ten lower spectral components. Table 1 displays the known spectral data for the considered model updating problem. Here we have: i — mode number; ω_i — natural i th frequency of the coolant oscillation under normal conditions (without appearance of the second phase in the coolant); ω_i^* natural i th frequency of the coolant oscillation with the availability of anomalies in coolant phase constitution.

Table 21: Given spectral data for Example 1

i	1	2	3	4	5	6	7	8	9	10
ω_i, Hz	0.89	6.77	9.82	15.44	15.96	18.94	24.57	26.69	27.07	30.52
ω_i^*, Hz	0.87	6.77	9.06	15.26	15.96	18.93	24.57	26.67	26.85	28.60

The approximate solution reached by using the hybrid algorithm with derivative-free local search is: $x_2^* = 79.93\%$; $x_3^* \approx 74.82\%$; $x_1^* = x_4^* = 100.0\%$. Fig. 1 displays the solution history (Niter stands for the number of final iterations of the hybrid algorithm; $F(x)$ stands for the normalized error function $f(x)$). The inaccuracy of the relative acoustical velocity computing is about 2.5%. As follows from the results obtained in this example the coolant phase constitution anomalies are conditioned by boiling process in the in the exit volume of the reactor pressure vessel and in the core barrel of the RPV.

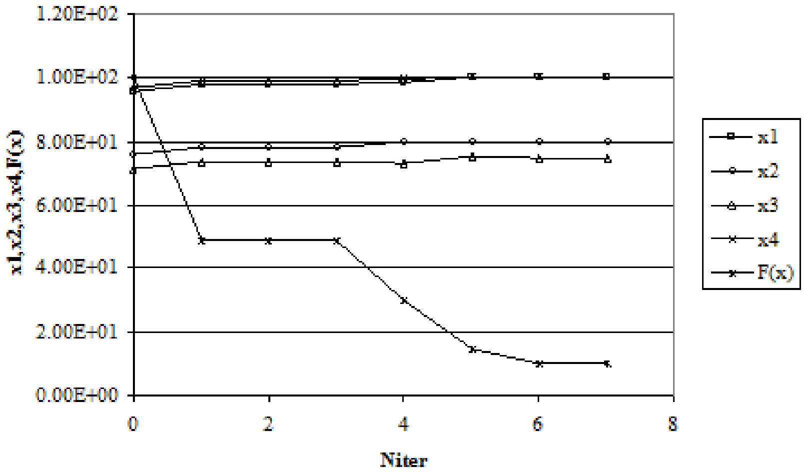

Figure 1: Number of final iterations of the M-PCAMNM vs. relative velocities (Example 1)

Example 2. Let now the anomalous coolant state constitution be characterized by second vector of controlling variables: $x_1^* \approx 76.77\%$; $x_2^* \approx 86.15\%$; $x_3^* \approx 83.23\%$; $x_4^* = 100.0\%$. The error function is determined using ten lower spectral components. Table 2 displays the known spectral data for the considered model diagnostic problem.

Table 22: Given spectral data for Example 2

i	1	2	3	4	5	6	7	8	9	10
ω_i, Hz	0.89	6.77	9.82	15.44	15.96	18.94	24.57	26.69	27.07	30.52
ω_i^*, Hz	0.81	6.77	9.34	15.32	15.96	18.85	21.07	26.67	26.92	29.38

The approximate solution reached by using the hybrid algorithm M-PCAMNM is: $x_1^* \approx 76.77\%$; $x_2^* \approx 86.15\%$; $x_3^* \approx 83.23\%$; $x_4^* = 100.0\%$. Fig. 2 and Fig. 3 illus-trate the solution history (final iterations of the hybrid algorithm). The inaccuracy of the relative acoustical velocity computing is about 2.5%. As follows from the results obtained in this example the coolant phase constitution anomalies are conditioned by boiling process in the coolant heating zone, in the exit volume of the reactor pressure vessel and in the core barrel of the RPV.

5 Conclusions

Two novel hybrid global optimization algorithms combining Metropolis-based algorithm M-PCA with the deterministic derivative-free methods for local search are presented. The first local search method implements the space filling curve algorithm. The second local search method is the provably convergent variant of the modified Nelder-Mead simplex method. The resulting hybrid algorithms M-PCASFC and M-PCAMNM belong to a class of algorithms which do not require derivatives. Both the algorithms were used for solving inverse spectral problems in connection with computational model updating for the two-phase gas-liquid coolant flow in the nuclear reactor primary circuit. Numerical experiments show the principal applicability of the proposed hybrid algorithms for solving the above model updating problems. The future work will be devoted to increasing the computational efficiency of tools for solution the model updating problems with regard to noisy data.

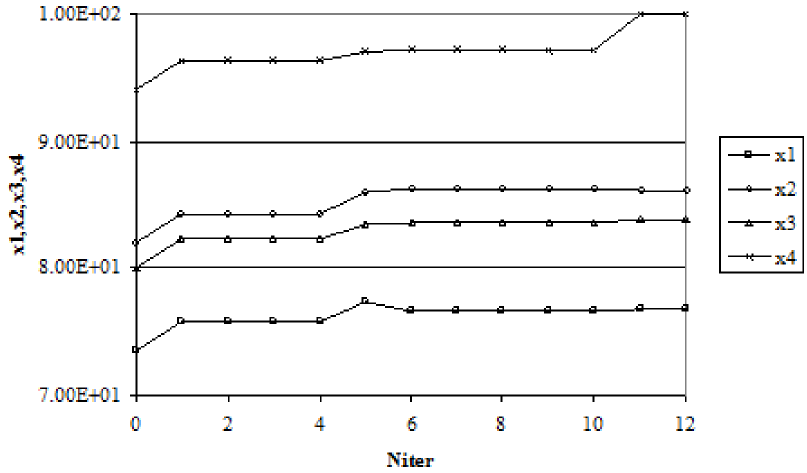

Figure 2: Number of final iterations of the M-PCAMNM vs. relative velocities (Example 2)

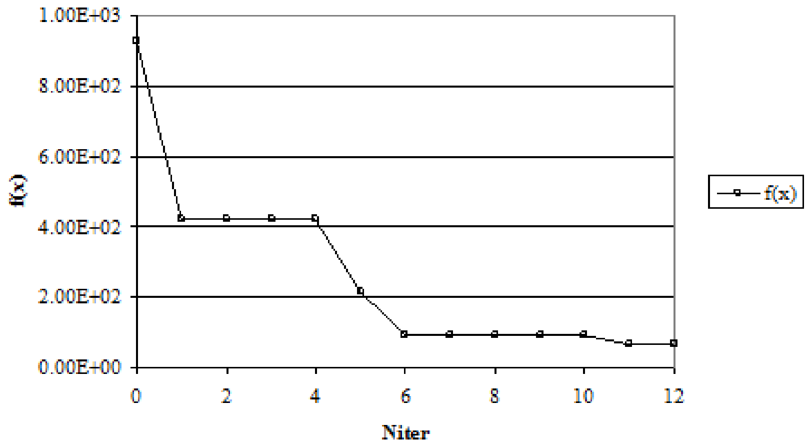

Figure 3: Number of final iterations of the M-PCAMNM vs. error function (Example 2)

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V.D. Sulimov, Baumanskaya 2nd str. 5, Moscow, 105005, Russia.
P.M. Shkapov, Baumanskaya 2nd str. 5, Moscow, 105005, Russia.