Hybrid algorithms for optimization and diagnostics of hydromechanical systems used in food production biotechnology

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Abstract. Reliable computer modelling in hydromechanical system dynamics is very important for studies related to optimizing food manufacturing and biotechnology processes. Searching best parameters of a computational model of a system and its diagnosing are formulated as inverse problems. The current error function is built on base of comparison of corresponding parts of the computed eigenspectrum and the measured one. The incompleteness of the registered data and the presence of multiple eigenfrequencies lead to the fact that the error function to be minimized is nonconvex and not everywhere differentiable. Since the function has many local minima, it is necessary to use global optimization methods. Two novel hybrid global optimization algorithms for solving the inverse problems are described. The hybrid algorithms combine the up-to-date stochastic algorithm for scanning the search space and deterministic derivative-free procedures for local descent. Numerical results on benchmarking the hybrid algorithm are presented to illustrate the efficiency of the approach.

1. Introduction

Profitable and safe operation of the technological equipment in contemporary food production biotechnology is highly related to problems of ensuring the stability of hydromechanical systems used and their individual circuits as coupled dynamic systems. Relevance of these problems has recently been acquired in connection with the following factors: the growth of the energy intensity of the equipment; the supercritical regimes of processing food masses; the inclusion of new, autonomously processing and independently operating systems and assemblies into existing technological schemes and production infrastructure; the introduction of innovative technologies using equipment vibrations and flow pulsations; the formation of two-phase gas-liquid mixtures; the application of automated control systems, regulation and production management. For these reasons, one should take into account the following important characteristics of the hydromechanical system: spectra of natural frequencies, vibration modes, amplitude and phase characteristics, a stability margin and a quality of transient processes [1]. When solving the above issues, information technologies for investigations of hydromechanical systems used in food production are fully utilized [2, 3]. The product properties are sufficiently dependent on process variables and operating conditions. Usually the following two types of optimization problems are under consideration. Namely, designing the integrated biotechnology process (finding the process variables, the operating conditions, etc.) and updating parameters of the mathematical model of the hydrosystem (the inverse problem: searching the parameters of the nonlinear dynamic model giving the best fitness to a given set of measured data). On the basis of the
The same approach, the problems of diagnosing the operating hydrosystem or identifying the properties of the flow of food masses and detecting anomalies in equipment units with parameters directly determining the dynamic characteristics, as well as optimizing the spectrum of natural frequencies of the hydromechanical system can be solved.

Numerical analysis of the hydromechanical system requires adequate computational models representing the physical behaviour of the system. In actual practice in the field of developing dynamic models, numerical estimates generally do not sufficiently match the measured data obtained from vibration experiments. The up-to-date methodology on reducing 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, substantial effort has been made in the development of special-purpose procedures for updating parameters of computational models using data extracted from vibration tests. The most 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. In the gradient-based inverse sensitivity methods of the model updating it 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 error function in the minimization problem is the weighted sum of squares of the differences in the eigenvalues. Generally 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. The eigenvalue derivatives with respect to the updating parameters can be evaluated by the differentiation of the characteristic dynamic equation. Possible availability of repeated or very close eigenvalues one should take into account.

As the minimization problem is usually ill-posed, then various regularization techniques should be applied [4]. It is common practice to reformulate the above problems to nonlinear programming problems subject to preset constraints. In the framework of the implicit methodology the inverse problem is formulated as an optimization problem on minimizing a criterion (error) function. Incompleteness of the experimental data and presence of repeated eigenvalues result in the error function being non-convex and non-differentiable. 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. It is common knowledge that the performance of deterministic algorithms essentially depends on the problem dimensionality. Alternatively, stochastic algorithms are capable of scanning efficiently the search space, but they are computationally expensive and their convergence properties are not guaranteed [5]. Developing hybrid global optimization algorithms, which combine both stochastic and deterministic techniques, is represented the promising approach in reactor equipment diagnostics and optimizing food production and bioengineering processes [6–8]. In the subsequent text certain of the subjects concerning structures of hybrid algorithms are discussed.

The plan of the remainder of this paper is as follows. The section 2 contains statement of the inverse eigenvalue problem under consideration. Section 3 provides brief description of hybrid global optimization algorithms. In section 4 some results of successful computational experiments on benchmarking the hybrid algorithm 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 control variables. Experimental spectral data registered by permanent instrumentation may be incomplete. So the goal is to determine vectors of control 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

$$\min_{x \in X \subseteq \mathbb{R}^n} F(x).$$

where \(F(x) = \sum_{i=1}^{N} w_i (\zeta_i(x) - \zeta_i^*)^2\); \(x, X\) — the vector of control 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 \(\zeta_i^*\) denote the eigenvalues that correspond to computed (from solutions of the direct problem) and to measured natural frequencies respectively.

As practical observations show, the error function in the considered regularized 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 and sufficiently accurate model updating for objects under consideration.

In generalization of the statements of extremal problems the following global optimization problem is formulated: to find

$$f(x^*) = \min_{x \in X \subseteq \mathbb{R}^n} f(x),$$

where

$$X = \{x \in \mathbb{R}^n : a_j \leq x_j \leq b_j, j \in J\},$$

\(f(x)\) is the criterion function; \(J = \{1, \ldots, n\}\) is the bounded set of indexes; \(x^*\) is the global solution. The criterion function \(f(x)\) of the problem (1)–(2) is supposed to be continuous Lipschitzian function. Also it is supposed that the real-valued function \(f : \mathbb{R}^n \rightarrow \mathbb{R}\) is multiextremal, not everywhere differentiable, and there is a numerical procedure for calculating values of the function in points of the supposed area.

3. Hybrid algorithms

The problem at hand is to find global extrema of not everywhere differentiable criterion function. When the number of variables is large they use stochastic global optimization algorithms. Two currently available powerful stochastic algorithms PCA (Particle Collision Algorithm) and M-PCA (Multi-Particle Collision Algorithm) were introduced in [9] and [10] respectively. The PCA algorithm is inspired by the physics of a nuclear particle traveling inside a nuclear reactor (the scattering and the
absorption phenomena). The original (canonical) PCA has some essential advantages in relation to well-known heuristic global optimization algorithms such as the Genetic Algorithms, Simulated Annealing, Fast Simulated Annealing, etc. Specifically, the 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 algorithm 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. The acceptance of current trial solution with certain probability makes it possible to avoid the convergence to local optima. In spite of its advantages over well-known meta-heuristics 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 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 variable space, avoiding convergence to a local solution. Coordination between the particles was achieved through a blackboard strategy, where the current information is shared among all the particles in the process [10]. The M-PCA (similar to the PCA) also has only one parameter to be determined, the number of iterations. The algorithms are claimed to be robust for problems with presence of discontinuities or where the criterion function values are noisy. Usually stochastic algorithms yield too computationally expensive solutions, so this drawback restricts their applications. However, the PCA and the M-PCA are in their early stages. In spite of its advantages over Genetic Algorithms 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. Developing hybrid algorithms that combine a robust stochastic algorithm for scanning the variable space with deterministic local search method is a promising way [11, 12]. A hybridization of the PCA and the deterministic (standard) Nelder-Mead simplex algorithm was introduced in [13]. The Nelder-Mead simplex method belongs to the class of derivative-free methods, so it is relatively insensitive to numerical noise and does not depend on convexity or smoothness of the criterion function. In practical cases, when highly accurate solutions of optimization problems may not be required due to inaccurate computational modelling, the method is an applicable tool. The hybrid algorithm (named NMPCA) was successfully applied to a nuclear reactor core design optimization problem. During processing two procedures are performing: a wide search in the solution space using the stochastic PCA and a local search in the promising areas with the deterministic simplex algorithm. The algorithm works well with irregular criterion functions and it can overcome kinks, local solutions, and discontinuities in functions being minimized. The local search procedure is performed iteratively until a certain number of fitness function evaluations being reached. It was established that the NMPCA performs better than the Metropolis PCA and such well-known metaheuristics as Genetic Algorithms and Particle Swarm Optimization. Nevertheless, a standard implementation of the Nelder-Mead Simplex algorithm during the local search can be expensive for problems with a large number of variables or with costly criterion functions. It is pertinent to note that the convergence theory for Nelder-Mead simplex method is rather far from completion; so the method can fail to converge or converge to non-stationary points [14]. By this is meant that the question of reliability of the algorithm as a whole is an open question. Another hybrid algorithm HJPCA that integrates the PCA based on the Metropolis algorithm and the popular deterministic Hooke–Jeeves method for the local search was proposed in [15]. The HJPCA implements a wide search in the space of variables using the stochastic algorithm and then perform the local search by the derivative-free method. The Hooke–Jeeves derivative-free algorithm performs two types of search: an exploratory search and a pattern search. A simple search strategy and small volume of memory required are the advantages of the method. In implementation of the hybrid HJPCA the local search procedure is performed until a predetermined stopping criterion (a sufficiently small step size) is reached.
Two novel hybrid global optimization algorithms combining the Metropolis-based stochastic algorithm M-PCA with the deterministic derivative-free methods for local search are presented in [16, 17]. The first local search method implements a variant of the modified Nelder-Mead Simplex algorithm [18]. The second approach to the local search is the Hooke–Jeeves method. The resulting hybrid algorithms M-PCAMNM and M-PCAHH JK belong to a class of algorithms which do not require derivatives. Moreover, the hybrid algorithm M-PCAHH JK may be considered as a modification of the earlier algorithm HJPPCA. According to published data on benchmarking, the HJPPCA outperforms two state-of-the-art algorithms C-GRASP and GLOBAL [15]. As the M-PCA is more efficient than canonical PCA, so the more recent hybrid algorithm M-PCAHH JK outperforms the HJPCA.

A new derivative-free stochastic Nelder-Mead (SNM) Simplex algorithm for continuous simulation optimization is proposed in [19]. It is proven that the SNM is a globally convergent algorithm. The essential drawback of the SNM is that its performance can deteriorate as the problem dimensionality is getting large. It is proven that the expansion and contraction steps of the standard Nelder-Mead Simplex algorithm possess a descent property when the criterion function is uniformly convex [20]. This property offers some new insights on the behaviour of the Nelder-Mead algorithm. The adaptive Nelder-Mead Simplex (ANMS) method is proposed whose expansion, contraction and shrink parameters depend on the dimension of the optimization problem. The presented numerical results have shown that the ANMS method outperforms the standard Nelder-Mead method for high dimensional problems.

Recently the substantial progress of parallel computing systems and programming techniques has stimulated the research on parallel global optimization algorithms [21]. The main reason is that solving complex global optimization problems involves intensive computations and evaluation of criterion functions may be rather expensive. Certain of the parallel schemes implementing the Nelder-Mead simplex method were presented in [22]. The advantage of the approach is that the parallel simplexes algorithm is generic and can be applied to any optimization problem to which the Nelder-Mead simplex is applicable. An implementation of the Nelder-Mead simplex method in parallel using a distributed memory is described in [23]. It is pointed out that in simulations the proposed implementation exhibits large speedups and is scalable to large problem sizes. Taking in consideration that parallel versions of the M-PCA were discussed in [10], it may be concluded that developing a parallel hybrid algorithm on base the M-PCA and parallel schemes of the Nelder-Mead simplex method is a promising way.

4. Numerical example

The benchmark is \( n \)-dimensional Levy–Montalvo 1 problem (LM1) [24]

\[
f(x) = \frac{\pi}{n} \left[ k \sin^2(\pi y_i) + \sum_{i=1}^{n-1} \left[ (y_i - A)^2 (1 + k \sin^2(\pi y_{i+1})) \right] + (y_n - A)^2 \right]
\]

where \( x_i = 1 + 0.25(x_i - 1) \), \( -10 \leq x_i \leq 10 \), \( i = 1, 2, \ldots, n \), \( k = 10 \), \( A = 1 \). The global minimum of LM1 is known to be \( f(x^*) = 0 \) with \( x_i^* = 1 \), \( i = 1, 2, \ldots, n \).

The hybrid global optimization algorithm M-PCAHH JK is used. It is supposed \( n = 15 \). The stopping criterion is \( f(x) < \varepsilon = 10^{-6} \). When current scanning the search space is done the set of initial trial points for the local search is determined. The finishing iteration history of the problem variables \( x_i \), \( i = 1, 15 \), versus the number of iterations \( N_{iter} \) is depicted in Figures 1–3. The corresponding history for the criterion function \( f(x) \) is demonstrated in Figure 4. After 20 iteration it have been obtained:

\[ f(x^{20}) \approx 0.6232 \cdot 10^{-6} \]
Figure 1. Number of final iterations $N_{iter}$ of the M-PCAHJ vs. control variables $x_i, i = 1, 5$

Figure 2. Number of final iterations $N_{iter}$ of the M-PCAHJ vs. control variables $x_i, i = 6, 10$
5. Conclusions
Developing hybrid global optimization algorithms that combine stochastic algorithms for scanning the variable space with deterministic local search methods is a promising way. Novel hybrid algorithms M-PCAMNM and M-PCAHJ that integrate the Metropolis-based M-PCA and derivative-free methods for the local search are described. Computational experiments show the principal applicability of the algorithms for solving inverse problems for hydromechanical systems in the field of food production and bioengineering. Some results on benchmarking the M-PCAHJ are presented. The future work will
be devoted to increasing the computational efficiency of the tools with applications to inverse problems.

References

[1] Kostin A M, Yablokov A Ye, Blagoveshchenskaya M M 2015 Perspektivnye metody tekhnicheskoy diagnostiki oborudovaniya pishchevykh proizvodstv Voprosy Nauki [Questions of Science] 7 pp 4-10 (in Russian).

[2] Blagoveshchenskaya M M, Sulimov V D, Shkapov P M 2010 Metodologiya razrabotki osnov modelirovaniya i diagnostiki gidromekhanicheskikh sistem pishchevykh proizvodstv po ikh dinamicheskim kharakteristikam Vysokie intellektual'nye tehnologii i innovatsii v obrazovanii i naute: Materialy XVII Mezhdunarodnoy nauchno-metod. Konf. 11-12 Fevralya 2010 g., S.-Peterburg. (SPb.: Izd-vо Politekhn. Univer.) 2 pp 95-98 (in Russian).

[3] Blagoveshchenskaya M M, Zlobin L A 2005 Informatsionnye tehnologii sistem upravleniya tekhnologicheskimi protsessami (М.: Vyssh. Shk.) (in Russian).

[4] Kirsch A 2011 An Introduction to the Mathematical Theory of Inverse Problems 2nd edition (Springer, New York).

[5] Žilinskas A, Zhigljavsky A 2016 Stochastic global optimization: A review on the occasion of 25 years of Informatica Informatica 27 (2) pp 229-256.

[6] Kinelev V, Shkapov P M, Sulimov V D 2003 Application of global optimization to VVER-1000 reactor diagnostics Progress in Nuclear Energy 43 (1-4) pp 51-56.

[7] Sulimov V D, Shkapov P M 2015 Hybrid methods of computer diagnosis of two-phase flow in the circulation loop Mathematical Modelling and Numerical Methods, 3 pp 68-88 (in Russian).

[8] Tumuluru J S, McCulloch R 2016 Application of hybrid Genetic Algorithm routine in optimizing food and bioengineering processes Foods, 5 (4) pp 76-87.

[9] Sacco W F, de Oliveira C R E 2005 A new stochastic optimization algorithm based on particle collisions Proceedings of the 2005 ANS Annual Meeting. Transactions of the American Nuclear Society, 92 pp 657-659.

[10] Luz E F P, Becceneri J C, de Campos Velho H F 2008 A new multi-particle collision algorithm for optimization in a high performance environment J. of Computational Interdisciplinary Sciences, 1 pp 3-10.

[11] Voglis C, Parsopoulos K E, Papageorgiou D G, Lagaris I E, Vrahatis M N 2012 MEMPSODE: A global optimization software based on hybridization of population-based algorithms and local searches Computer Physics Communications, 183 (2) pp 1139-1154.

[12] Lara P C S, Portugal R, Lavor C 2014 A new hybrid classical-quantum algorithm for continuous global optimization problems J. of Global Optimization, 60 pp 317-331.

[13] Sacco W F, Filho H A, Henderson N, de Oliveira C R E A 2008 Metropolis algorithm combined with Nelder–Mead Simplex applied to nuclear reactor core design Annals of Nuclear Energy, 35 pp 861-867.

[14] McKinnon K I M 1998 Convergence of the Nelder-Mead simplex method to a non-stationary point SIAM J. Optimization, 9 pp 148–158.

[15] Rios-Coelho A C, Sacco W F, Henderson N A 2010 Metropolis algorithm combined with Hooke–Jeeves local search method applied to global optimization Applied Mathematics and Computation 217 (2) pp 843-85.

[16] Sulimov V D, Shkapov P M, Sulimov A V 2017 Jacobi stability and computational diagnostics of dynamical systems using hybrid algorithms Fundamental and Applied Problems of Engineering and Technology, 4-2 (324) pp 61-71 (in Russian).

[17] Sulimov V D, Shkapov P M, Nosachev S K 2014 Hooke–Jeeves Method-based local search in a hybrid global optimization algorithm Science & Education, 6 pp 107-123 (in Russian).

[18] Xiao H F, Duan J A 2014 Multi-direction-based Nelder–Mead method Optimization: A Journal of Mathematical Programming and Operations Research, 63 pp 1005-1026.
[19] Chang K H 2010 Stochastic Nelder-Mead simplex method – a new globally convergent direct search method for simulation optimization SIAM J. Optimization 9 pp 148–158.

[20] Gao F, Han L 2012 Implementing the Nelder–Mead simplex algorithm with adaptive parameters Computational Optimization with Applications 51 (1) pp 259–277.

[21] Voglis C, Hadjidoukas P E, Papageorgiou D G, Lagaris I E 2013 A parallel hybrid optimization algorithm for fitting interatomic potentials Applied Soft Computing 13 pp 4461-4492.

[22] Lee D, Wiswall M 2007 A parallel implementation of the simplex function minimization routine Computational Economics 30 (2) pp 171-187.

[23] Klein K, Neira J 2014 Nelder–Mead simplex optimization routine for large-scale problems: a distributed memory approach Computational Economics, 43 (4) pp 447-461.

[24] Montaz Ali M, Khompatraporn C, Zabinsky Z B 2005 A numerical evaluation of several stochastic algorithms on selected continuous global optimization test problems J. of Global Optimization, 31 (4) pp 635-672.