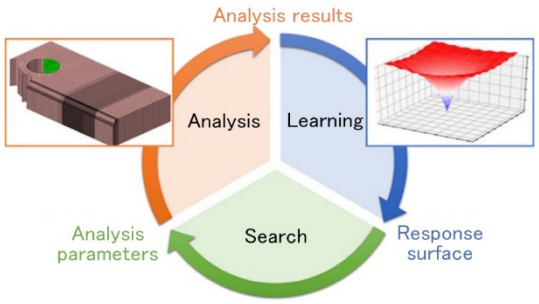
Design Advancement by Applying Bayesian Optimization to Numerical Analysis Techniques



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Mitsubishi Heavy Industries, Ltd. (MHI) applies optimization technology to product design that use numerical analysis techniques such as finite element analysis. However, the optimization calculation requires a considerable number of analysis executions, so there is a problem in that obtaining an optimum solution takes time in the case of a high-cost analysis model that requires several hours for a single analysis. We applied Bayesian optimization, which is an optimization technology, in an effort to solve this problem and made it possible to calibrate the analysis model in a short time. This report presents an outline of these efforts.

1. Introduction

Taking into account the reduction of the cost of trial production and experimentation, MHI has been using numerical analysis techniques such as FEM (finite element method) for event prediction and product design. We have also been calibrating the analysis model with respect to actual equipment based on the test data and adjusting the design parameters using the calibrated analysis model. These require adjustment of the models and the parameters by trial and error, but there is a limit to manual adjustment. Therefore, we carry out rational calibration of analysis model and design parameters using optimization technology(1).

However, optimization based on evolutionary algorithms typified by particle swarm optimization requires hundreds to thousands of analysis executions to obtain an optimum solution, so there is a problem in that applying the optimization to a high-cost analysis model that requires several hours for a single analysis is difficult. For example, in predicting amount of ductile crack growth in plant piping, the finite element analysis model is calibrated with respect to the material test results using small test pieces as shown in **Figure 1**. However, since a single analysis takes several hours, a calibrated analysis model cannot be obtained in a realistic amount of time with optimization technology. Therefore, in the past, the designer had to adjust the model parameters by trial and error and this calibration took about two months. On the other hand, in the field of machine learning, the effectiveness of Bayesian optimization has been confirmed as a method for adjusting hyperparameters of models. We applied multi-task Bayesian optimization, which is an extension of Bayesian optimization, to the calibration of analysis models and attained a significant reduction in the adjustment time. The following chapters introduce an outline of these efforts.

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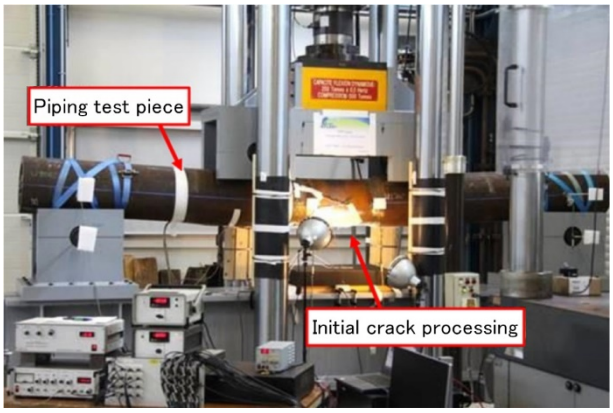

Figure1 Example of material test

2. Optimization technology

This chapter outlines the optimization technology covered in this report.

2.1 Bayesian optimization[(2)]

Bayesian optimization is an optimization technology based on the response surface, and repeatedly executes the three processes of numerical analysis, creation of a response surface, and search for the optimum point candidate using the response surface as shown in **Figure 2**. This response surface is a model that learns the numerical analysis results. Therefore, in the initial stage of optimization calculation where there is little analysis data, the prediction accuracy of the response surface is low and the response surface does not represent the correct solution space, so there is a possibility of falling into an erroneous solution such as a local solution in searching for the optimum solution on the response surface. To solve this problem, Bayesian optimization uses a machine learning model called Gaussian process regression, which can express prediction uncertainty, as the response surface. By calculating the probability that the optimum solution can be obtained based on this prediction uncertainty, searching for the optimum solution while appropriately sampling the unknown region that has not been searched is made possible.

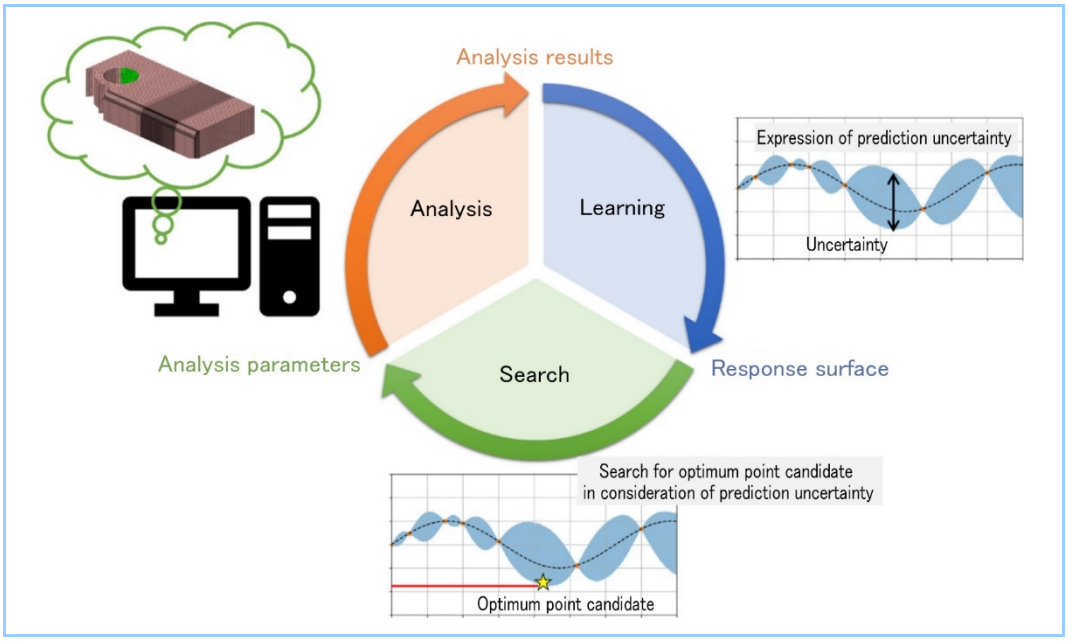

Figure 2 Bayesian optimization

2.2 Multi-task Bayesian optimization[(3)]

Multi-task Bayesian optimization (MTBO) is a Bayesian optimization that aims to solve multiple optimization problems in parallel. MTBO can acquire a highly accurate response surface with a small number of data points by transferring the characteristics of one optimization problem to the characteristics of another optimization problem, and efficiently search for the optimum solution

In the case presented in this report, we applied MTBO to optimization calculation using a numerical analysis model and worked on the realization of efficient optimization calculation. **Figure 3** shows the flow of optimization calculation. In addition to the high-cost numerical analysis model that requires long calculation time, which is the object of optimization, a low-cost numerical analysis model with different analysis conditions for which the required calculation time is short is used. First, the low-cost numerical analysis model was repeatedly analyzed so as to minimize the prediction uncertainty of the response surface model and response surfaces were learned. Next, the learning results were transferred to the response surface model corresponding to the numerical analysis model to be optimized using MTBO and the optimization calculation was performed. This made it possible to generate a highly accurate response surface while reducing the number of high-cost analysis executions and shortened the optimization calculation time.

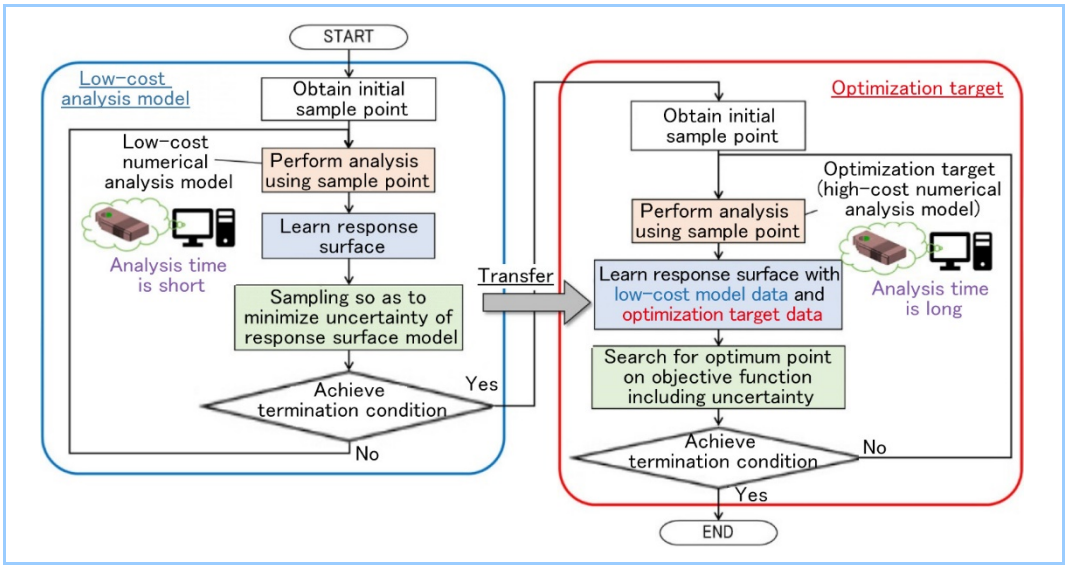

Figure 3 Optimization processing flow using multi-task Bayesian optimization

3. Example of application to crack growth analysis

3.1 Ductile crack growth analysis

In order to predict the ductile crack growth of plant piping, a finite element analysis model of the CT (compact tension) test piece shown in **Figure 4** based on the material constitutive equation called the Gurson-Tvergaard-Needleman (GTN) model was used[(4)]. The GTN model is a model that reproduces the process of void generation, growth, bonding and fracture inside the material by numerical analysis, and the parameters of the constitutive equation need to be adjusted through finite element analysis so that it reproduces the material test results. However, the calibration is difficult due to the strong non-linear characteristics.

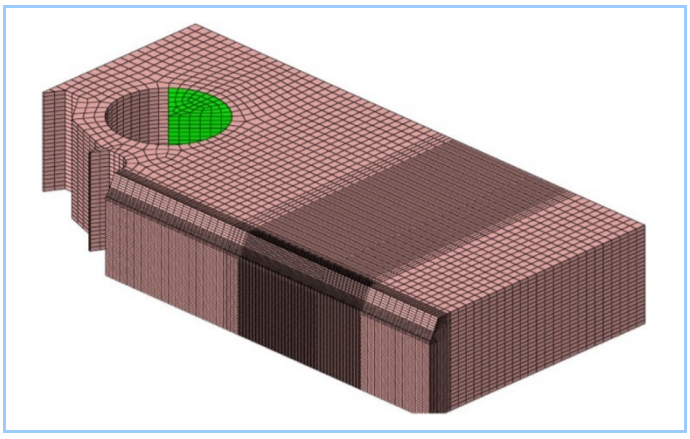

Figure 4 Finite element analysis model of CT test piece

In the case presented in this report, the analysis model was calibrated with respect to (1) load-COD (crack opening displacement) diagram and (2) distribution of ductile crack growth

amount along the thickness shown in **Figure 5** obtained in the material test. Specifically, by optimizing the six GTN model parameters so as to minimize the average relative error between the finite element analysis results and the material test results, we aimed to obtain a numerical analysis model with high reproducibility of the test results. This average relative error is the average value of the relative error between the analysis value and the test results obtained for multiple evaluation points.

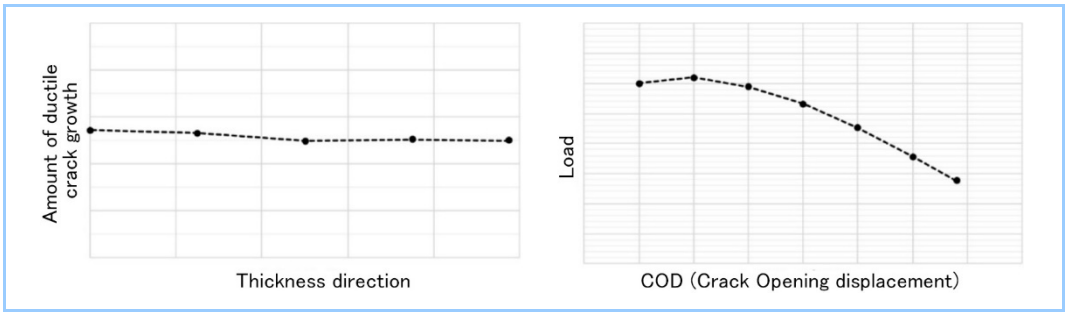

Figure 5 Material test results used for calibration

3.2 Application results

This section describes the results of applying the optimization technology to the calibration of a ductile crack growth analysis model. In addition to the usual finite element analysis model, a low-cost analysis model for which the analysis time was shortened to about 1/3 by increasing the acceleration of the forced displacement was used, and the average relative error between the analysis results and the test results was minimized with MTBO. Since the load-COD diagram and the distribution of ductile crack growth amount have different non-linear characteristics, a strong non-linearity occurs between the GTN model parameters and the average relative error, which is the objective function. Therefore, the optimization calculation takes large iteration when the average relative error is directly expressed by the response surface model. For this reason, in the case presented here, in order to reduce the non-linearity of the response surface model, the objective function value was estimated by creating an individual response surface model presenting the relative error for each evaluation point and performing average value processing on each response surface model estimated value.

Figure 6 shows the results of the optimization calculation using MTBO. When the low-cost analysis was executed 81 times (about 2 days) and then the high-cost analysis was executed 9 times, results satisfying the target error could be obtained. It was confirmed that calibration of the analysis model, which used to take two months, could be achieved in just three days.

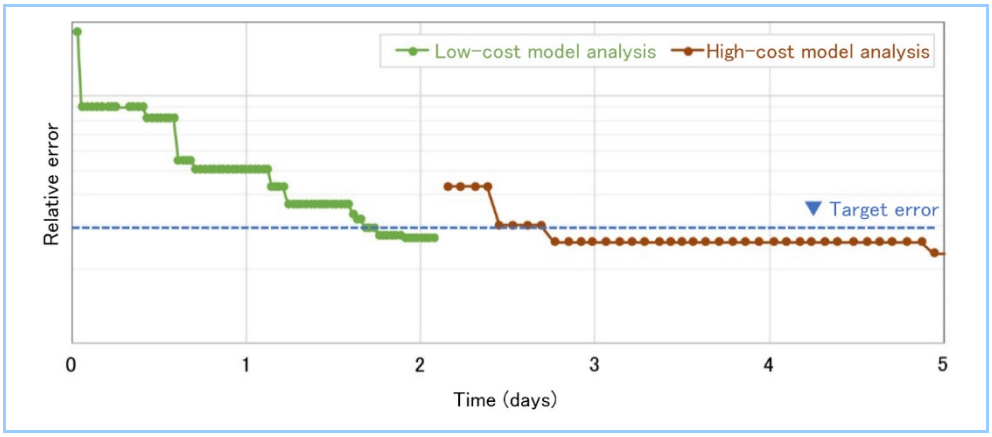

Figure 6 Results of optimization calculation using MTBO

Furthermore, **Figure 7** compares these results with the GTN model parameter calibration results using other methods shown in reference (4). Although the accuracies of the load-COD diagram are the same, the method presented in this report obtained the results of the amount of ductile crack growth with strong non-linearity closest to the test results, so it was confirmed that this method is also effective in terms of accuracy.

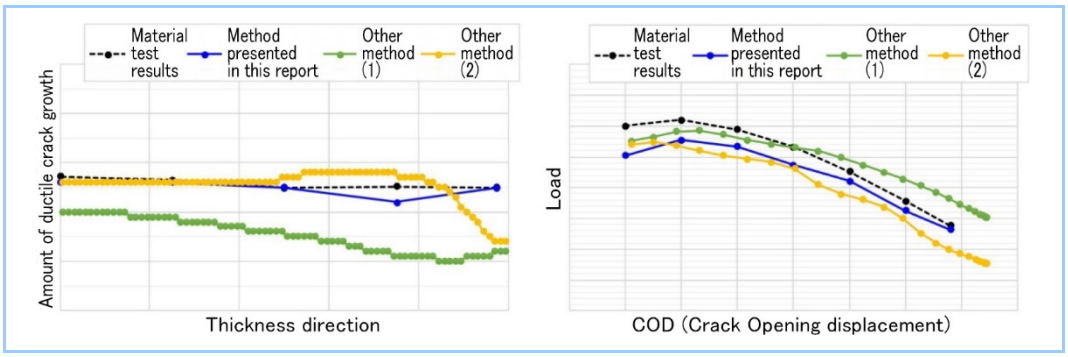

Figure 7 Results of comparison to other methods

4. Conclusion

We have been working on the sophistication of design work by applying optimization technology to numerical analysis techniques. In this report, it was confirmed that by applying multi-task Bayesian optimization technology to calibration of a ductile crack growth analysis model with respect to the test data, the parameter adjustment time of the analysis model, which used to take two months, can be significantly reduced to just three days. In the future, we will promote the development of this technology for our other products. In addition, we plan to verify the applicability of the GTN parameters obtained by optimization to other test pieces in the future.

References

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