COST 526

"Automatic Process Optimization in Materials Technology"

(APOMAT)

Half-Yearly Report

1. Reporting Period	**1.1.2003 – 31.6.2003**
Project title	Numerical Optimization of the Bridgman Casting Process for Stationary Gas Turbine Blades
Project leader Organization	**Dr. J. Jakumeit** ACCESS e.V. Intzestrasse 5, D-52072 Aachen, Germany
Main collaborators involved	Dipl.-Ing. M. Emmerich, ICD, Dortmund, Germany Dr. G. Laschet, ACCESS e.V.

2. Funding Situation	
Amount of money received specifically for COST	80 kEuros
Other resources partially used for the project	40 kEuros

3. International Collaboration (mention group and type of work done in collaboration during the reporting period)
Participation in the Working Group Meeting in Brussels + project progress report X YES ❒ No

4. Industry participation (mention name of companies and work done in collaboration during the whole project)
Alstom Power Ltd, Segelhof 1, CH-5405 Baden-Dättwil, Switzerland Together with our industrial partners we defined one real gas turbine blade and one simplified blade for the application of the optimization strategies. We have the permission to publish results obtained with these test cases.

5. Meetings, visits, exchange of scientists, short-term scientific missions	**Location, date**
EUROTHERM Seminar 69: Heat and Mass Transfer in Solid-Liquid Phase Change Processes	**Ljubljana, 25.-27.6.2003**

COST 526

"Automatic Process Optimization in Materials Technology"

(APOMAT)

Half-Yearly Report

6. Progress within the reporting period

(Not exceeding 3 pages, including tables and figures)

1. Introduction

The highest gas turbine efficiency is achieved today with single-crystal (SX) or directionally solidified (DS) blading material, commonly produced in a Bridgman furnace. The Bridgman process is controlled by time dependent parameters (withdrawal speed, heater temperatures), which are ideal for the application of numerical optimization [1]. In addition the blade casting is the most expensive process during the manufacturing of a turbine making a reduction of the fabrication costs by optimization very interesting for the industry.

In the first year a preliminary optimization loop has been developed based on the validated casting simulation tool CASTS [2]. Goal of the optimization was an improved withdrawal profile for the Bridgman process of a cluster of 3 SX blades. The simulation results were evaluated by 4 criteria:

- the probability of local freckle formation, which is governed, in a first approximation, by the cooling rate at the liquidus isotherm;
- the degree of curvature of the solidification front;
- the ratio G/v (temperature gradient over solidification speed) must be greater than a critical value (~600 K/s), describing the transition from columnar dendritic growth to an equiaxed grain structure;
- the process time.

These criteria where combined to one objective function by a weighted sum of the normalized individual values, integrated over the whole structure. As optimization strategies the Global Convergent Method (GCM) [3] of BOSS Quattro and a Derandomized Evolution Strategy (DES) [4] developed at the Informatic Center Dortmund were used. First results showed, that both GCM and DES lead to improved withdrawal profile in respect to the used optimization criteria [5]. But the best withdrawal profile found by the DES lead to a long process time and a freckle tendency. Thus the objective function did not lead to improvement in respect to all criteria.

In order to achieve a better definition of the optimization goal, a new formulation has been developed for the first three optimization criteria, the freckle probability, the curvature of the solidification front and the G/v ratio. In the new formulation these criteria are evaluated by counting the number of "bad" nodes, i.e. nodes with freckle probability, the curvature of the solidification front is above 20° or the G/v ratio is below 600 K/s. The criteria can be tuned by changing the limits (20°,600 K/s).

2. New metamodel-assisted optimization strategy

Another problem with Evolution Strategies for the optimization of process parameter is the high number of solutions needed to find an optimum. Until now the derandomization was used to reduce this number to a practical size below 100. For a further reduction a metamodel-assisted optimization strategy was developed in the last half year. Figure 1 describes the general scenario.
Leaving away the lower part of the diagram, the standard scenario for automatic optimization can be obtained. An optimization tool (e.g. an evolution strategy) serves as a design scheduler in this scenario. In each of the iterations it samples several input vectors within the search space.
In order to evaluate the response function, these input vectors are passed to the simulator interface. The interface tool integrates the input values into an input file for the simulator and then executes the simulator. After termination of simulator it extracts the response values of interest from the report file

and passes them back to the optimizer. After receiving the response vectors for each input vector, the optimization tool updates internal strategy parameters and generates a new sample of input vectors. This procedure is repeated until a satisfactory solution quality has been obtained or the time budget for the optimization has been exceeded.

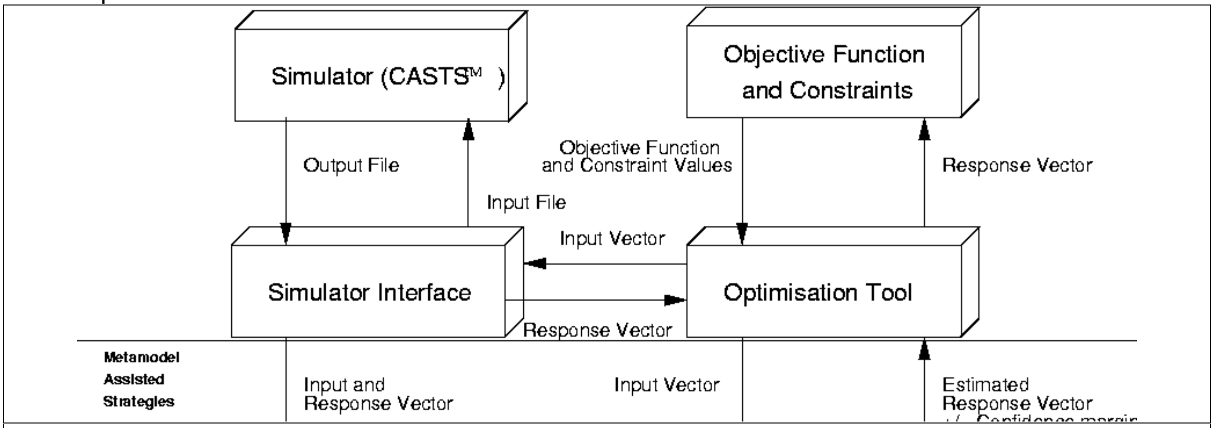

Figure 1: Data flow diagram for a metamodel assisted optimization system

The metamodel assisted optimization approach extends this scenario (c.f. lower part of Figure 1). Each response is stored in an archive (database), where it is attached to the corresponding input vector. The metamodel extracts values from this database in order to predict the response vector for new input vectors that are sampled by the optimization tool. Metamodel assisted optimization tools are able to exploit this information, e.g. in order to skip the evaluation of less promising input vectors within a sample. Advanced metamodelling algorithms also provide a measure of the confidence in an evaluation, which obtained by the local density, correlation and clustering of input vectors in the proximity of the examined input vector. Needless to say that if an input vector fits exactly to a previously evaluated input vector the metamodel returns its true response.

Two metamodelling optimization strategies based on the Kriging algorithm [5,6] were applied. A simple strategy is to initialise the metamodel by a design of experiments (DoE) and then use a numerical optimization strategy to find the optimum of the metamodel. This is done in an iterative way in the iterative *Kriging* method. A more complex strategy is the metamodel assisted evolution strategy (MA-DES). Here the metamodel is consulted during the prescreening of a sample that has been generated within one of the iterations of a derandomized evolution strategy. Then the starting point is set to an input vector from the database. From this starting point 20 variations are generated by adding normal distributed perturbations scaled by an individual step size to each vector position.
Then the algorithm selects the 4 most promising variants out of the 20 variants with a preselection criterion based on the approximation of the response by the metamodel.
The input vectors for the 4 qualified input vectors are then evaluated by the computationally expensive evaluation tool and the archive for the metamodel are updated with the new results.
After adapting the step sizes [7] the next iteration starts. This is repeated until the maximal number of function evaluations has been exceeded.

3. Results

These two metamodel based strategies are compared with the standard downhill simplex algorithm [8] and the derandomised evolution strategy (DES) used so far [7]. The first goal was to obtain as few "bad nodes" as possible with a process time below 5000 s. Only if no "bad nodes" occur should a reduction of the process time become an optimization goal. In figure 2 the convergence dynamics of the four different optimization strategies is displayed. The MA-DES variants clearly outperform the conventional DES and the downhill simplex algorithm. The iterative Kriging finds a rather good solution in the first sampling but no further improvements can be found by the reduction of the sampling range in the following iterations. An objective function value

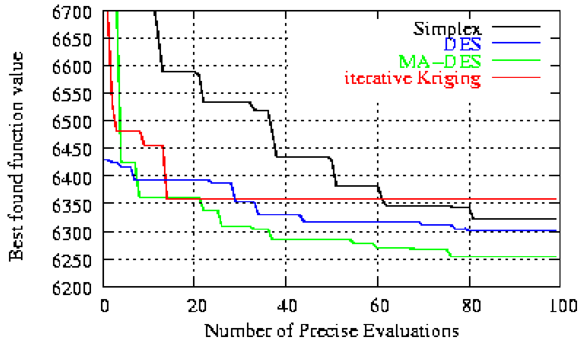

Figure 2: A comparison of different conventional and metamodel-assisted optimization strategies for optimization of the Bridgman casting process. The objective function value is plotted for each of the 100 precise evaluations.

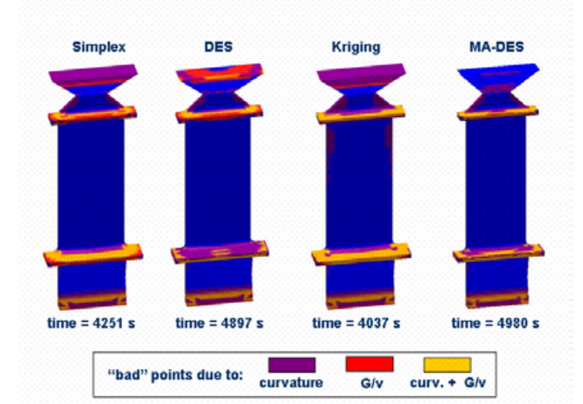

Figure 3: Comparison of the best turbine blades found with the different optimization strategies. The "bad" points are due to a too high curvature, to low G/v value or both are plotted. Freckles are not a problem in this simple turbine blade.

The best solutions found for each strategy are depicted in figure 3 using the new objective function criteria. On each turbine blade casted with the withdrawal profile given by the optimization algorithm the nodes with too high curvature or too low freckel tendency are marked with a specific colour. Freckles cannot be found on this simple turbine blade geometry. Obviously the MA-DES can reduce the size of the regions with bad nodes best, while keeping the process time below 5000 seconds.

4. Conclusion

The results show that the metamodel-assisted evolution strategy MA-DES outperforms classical methods with respect to the results obtained with the same number of precise evaluations. For the next period we plan to apply the new optimization strategy and the new criteria definition to a real turbine blade. In addition "bad nodes" should be weighted by the volume associated to the node in the FE-mesh.

5.References

[1] G. Laschet, M. Schallmö & N. Hofmann: "Optimization tools for Bridgman casting process", Proc. 7th Conf, on Casting, Welding and advanced Solidification, Ed. B. Thomas & C. Beckermann, TMS editions, San Diego, pp 1095-1102, 1998.
[2] G. Laschet, J. Neises and I. Steinbach: « Micro- Macrosimulation of casting processes", 4ième école d'été de "Modélisation numérique en thermique", C8 1-42, Porquerolles, 1998.
[3] BOSS QUATTRO, version 4.2, Samtech S.A., Liège, 2002.
[4] OASIS, optimization toolbox, ICD Dortmund, 2001.
[5] N. Cressie, *Statistics for spatial data*, J. Wiley, N.Y. 1993
[6] J. Sacks, W. J. Welch and E. P. Wynn (1989). *Design and Analysis of computer experiments*, Statistical Science, 4: 409-435
[7] T. Bäck. *An overview of parameter control methods by self-adaptation in evolutionary algorithms*, Fundamenta informaticae 35 (1998), pp. 51-66, IOS Press
[8] H.-P. Schwefel, *Evolution and Optimum Seeking*, Wiley, NY, 1995

7. List of publications

a) Published

R. Laqua, T. Ivas, J. Scheele, J. Jakumeit, M. Braun and M. Pelzer, *Mold Filling and Solidification Simulations of Investment Casting Processes using CASTS-FLUENT,* Proceedings of ERUOTHERM Seminar 69, Ljubljana, 2003
M. Emmerich, ICD and J. Jakumeit, *Metamodel-Assisted optimisation with constraints: A case study in material process design,* Proceedings of EUROGEN 2003, Barcelona

b) Submitted for publications

J. Jakumeit, ACCESS e.V., Aachen, Germany; M. Emmerich, ICD, Dortmund Germany;
G. Laschet, ACCESS e.V., Aachen, Germany; F. Hediger, ACCESS e.V., Aachen, Germany
Optimization of the Bridgman casting process by a Derandomized Evolution Strategy and a mesh

based objective function, submitted to EUROMAT 2003, Lausanne J. Jakumeit, M. Herdy and M. Nitsche *Parameter optimization of the sheet metal forming process using an iterative parallel Kriging algorithm* Submitted to Design Optimization
c) In preparation