



**COST 526:**  
**Automatic Process Optimization in Materials Technology (APOMAT)**

**WG4: Optimization Methodologies**

Final Report

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**Objectives**

COST 526 was promoting interdisciplinary collaboration of material scientist and experts in numerical optimization aimed at designing automatic optimization procedures for material processes. The approach taken was to integrate process simulators for specific material processes with optimization algorithms via quality (cost) functions that relate process parameters with material properties (see Figure 1). The resulting software environments should be capable of finding process parameter values improving the target material properties. In addition, the new values should either contribute to the decrease of experimental or production costs, or increase of productivity or environmental acceptability. There has been no long tradition of collaboration between the two disciplines, hence bridging the gap between them was also a challenge for COST 526.

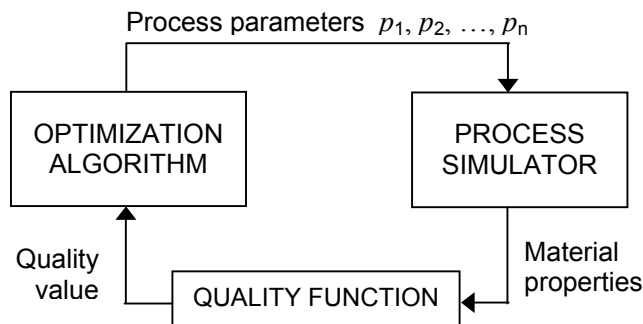


Figure 1: Simulation-based optimization of a material process

**Working group activities**

The role of the Optimization Methodologies Working Group (WG4) was to provide a forum for the exchange of information on optimization techniques and their applications. All COST 526 projects were invited to contribute to the working group activities as well as benefit from them. WG4 sessions held at the COST 526 joint working group meetings consisted of presentations by invited speakers and project members.

During the entire action, six invited talks and 12 talks by the COST 526 participants were given at WG4 sessions. There were presentations of optimization methodology, such as evolutionary strategies for engineering applications (discussed by Thomas Bäck, Michael Emmerich, Dirk Büche, Stefan Kern), multi-objective optimization (Bogdan Filipič), and response surface

optimization (Catherine Knopf-Lenoir). Special approaches useful in time-consuming simulation-based optimization were presented, such as distributed optimization on a network of workstations (Manfred Grauer), and XML communication among applications (Norbert Hofmann). Some speakers presented optimization software packages, for example BOSS Quattro (Patrick Morelle), DesParO (Christof Bäuerle), modeFRONTIER (Jean-Jacques Maisonneuve), and Inverse (Igor Grešovnik). Various case studies from material process optimization were shown, too.

Presentations were followed by discussions on the issues related to material process optimization, such as how to define an appropriate quality function, which optimization method to use, and others. In addition, information on available optimization software was collected, while Dirk Büche contributed a set of downloadable optimization algorithms and test problems. Both materials are accessible from the [project web site](http://www.cost526.de/) (Figure 2).

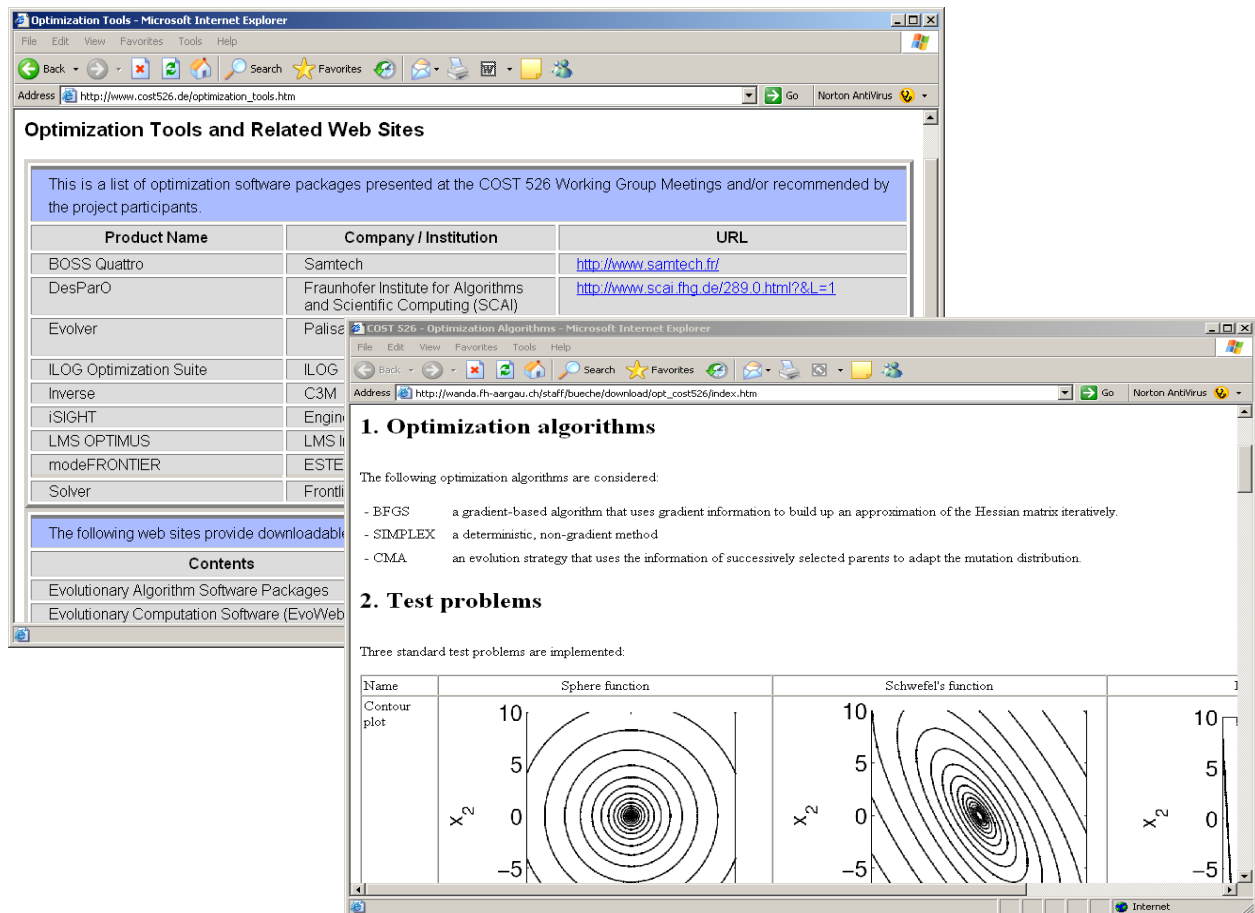


Figure 2: Optimization software pages available at <http://www.cost526.de/>

## Summary of achievements

COST 526 projects were dealing with a variety of material processes and have entered the collaboration at different initial stages. In spite of that, most of them succeeded in establishing an appropriate simulator-optimizer environment for their particular material process, and producing beneficial results either at a laboratory level or even in regular production. Many projects use

commercial simulation programs, such as ANSYS, ABAQUS, FORGE, etc., while the employed optimization software is either commercial or own code.

As a result of interactions in WG4, some common practices were established. For example, to identify relevant parameters for optimization, sensitivity analyses are performed before modeling and optimization takes place if there is not much empirical evidence on the role of parameters. Regarding the quality function design, a common approach is to formulate a measure of unwanted material property, or an error measure, which is to be minimized. However, when multiple criteria need to be taken into account, the predominant approach is calculating the weighted sum of normalized criteria values and performing single-objective optimization.

The optimization method chosen as suitable very much depends on the properties of a particular material process and computational complexity of the employed simulator. Among the participating projects, the selection ranges from traditional numerical methods, such as Nelder-Mead (Downhill Simplex), Levenberg-Marquardt, Quasi-Newton, and BFGS, to advanced stochastic methods, including genetic algorithms, evolution strategies and differential evolution. Figure 3 illustrates a result of modeling and optimization of industrial continuous casting of steel where the task is to tune the secondary coolant flows to achieve the target temperatures. The applied software consists of a 3D finite-element simulation model and gradient-based optimization (steepest descent) procedure.

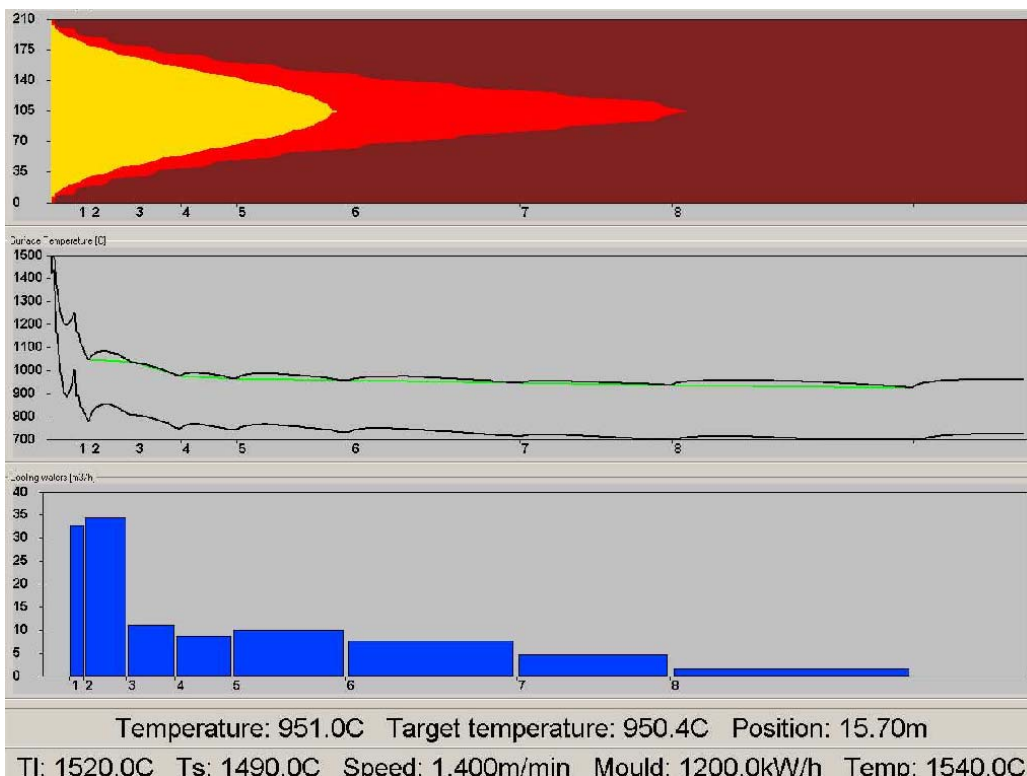


Figure 3: Visualization of industrial continuous casting of steel as modeled and optimized by a program developed at the University of Oulu (Erkki Laitinen)

When computational complexity of process simulation is too high to make iterative optimization feasible, approximations of the parameter search space are constructed and exploited in the optimization process. This has been approached in different ways, e.g. by sequential approximation techniques, with response surface models and meta-model assisted evolution strategies.

In addition, some participants have worked on specific techniques that may utilize complex optimization procedures:

- unified XML communication among applications within the simulator-optimizer environment (Norbert Hofmann),
- parallel/distributed optimization suitable for process simulations of high computational complexity (Manfred Grauer),
- a generic optimization software Inverse (Igor Grešovnik).

## **Conclusion**

In COST 526, WG4 was devoted to providing and exchanging information on optimization methodology and its applications in material processing. Diversity of the considered material processes reflects in a variety of optimization techniques tested and finally accepted into practical use in individual projects. Through contributions of invited experts and optimization specialist participating with their own projects, the awareness of simulation-based optimization potential in material processing increased. Certain common practices were established that helped many projects to accomplish their goals. On the other hand, there are issues that remain to be further explored in a planned follow-up COST action. These include accounting for multi-objective optimization, data visualization for better understanding of results, and practical assessment of the gains resulting from optimized solutions.