

Proposal for a new COST-Action

Automatic Process Optimization in Materials Technology (APOMAT)

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Memorandum of Understanding

for the implementation of a European Concerted Research Action
designated as COST Action 526

Automatic Process Optimization in Materials Technology (APOMAT)

The Signatories to this Memorandum of Understanding, declaring their common intention to participate in the concerted Action referred to above and described in the Technical Annex to the Memorandum of Understanding, have reached the following understanding:

1. The Action will be carried out in accordance with the provisions of the document COST 400/94 „Rules and Procedures for implementing COST Actions“, the contents of which are fully known to Signatories.
2. The main objective of the COST Action is to develop and to apply numerical optimization methodologies for automatic materials process design, based on quantified product quality, relating to process targets and constraints, including economic aspects.
3. The overall costs of the activities to be carried out within this Action were estimated to be ECU 16,5 Million for 4 years.
4. The Memorandum of Understanding will take effect when being signed by at least five Signatories.
5. The Memorandum of Understanding will be in force for a period of 4 years, unless the duration of the Action is extended in accordance with the provisions of Chapter 6, Point 1 of the above cited document.

Technical Annex of the COST Action on 'Automatic Process Optimization in Materials Technology' (APOMAT)

A. Background

A.1. Introduction: Technological approach and methodology

In response to market-driven pressure for reducing time-to-manufacture, numerical analysis has become state-of-the-art in materials sciences and processing. During the past two decades, many virtual process models have been developed world wide and software codes partially commercialized. The basic approach is to integrate material laws with appropriate numerical schemes, e.g. the finite element method, to solve generic equations for heat transfer, fluid flow or stress / strain evolution on both macroscopic and microscopic length scales. For numerous process steps, or even complete manufacturing procedures, these numerical tools have proven to be successful with respect to quality improvement and process design. In particular, this has been demonstrated for some areas in materials sciences and engineering within the frame of the COST 512 action.

Virtual process models (simulation models or simulators) mainly include numerical analysis of a process step which gives insight to the status quo of process evolution. At the same time, they allow execution of virtual experiments, and therefore facilitate systematic process optimization by trial and error methods („manual“ optimization). In short, a virtual process simulation laboratory of this kind can be a helpful tool in

- reducing lead time for process development
- cutting down experimental cost
- improving tailored materials properties
- increasing volume/time yield.

A substantial upgrade of this procedure for materials technology consists in connecting virtual models with numerical optimization techniques. The logical connection is the so-called quality or objective function including its constraints, which allows for automatic quality assessment of the simulation results. Typically, the quality function relates a set of process parameters to some quantitative material laws describing specific material properties and referring to a specific process step (Fig. 1).

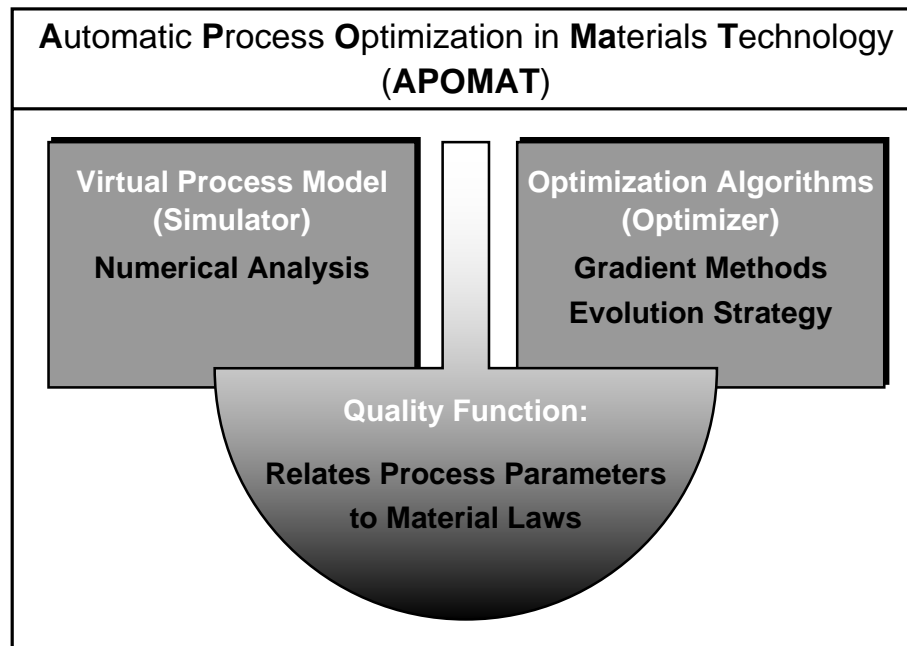


Fig. 1: Connecting virtual process models with numerical optimization techniques: the quality function

A successful application of automatic process optimization has been given recently for cast and directionally solidified large turbine blades. The most expensive production step is the Bridgman casting process. Amongst other parameters, the time dependant withdrawal speed of the solidifying component represents a set of undetermined process parameters strongly linked to material properties and defects like grain structure, stray grain and freckle formation. Typically, casting vendors elaborate the withdrawal procedure by means of expensive and time consuming casting trials, whereas numerical process optimization allows an automatic calculation of these parameters. Optimization is based on both, a numerical analysis of transient temperature evolution (simulator) and a quality function design, incorporating quantified material qualities or defect criterions related to solidification front stability or stray grain formation mechanisms. Using this novel approach it has been validated that overall solidification time could be halved, and at the same time better material qualities were achieved.

A COST Action focused on APOMAT initiates a close cooperation between materials scientists, simulation engineers and optimization experts in order to

- formulate material qualities based on appropriate material laws for quality function design regarding process-inherent constraints
- provide accurate and high-performance process simulation software
- cope with high-dimensional nonlinear optimization problems.

On an organizational level of the new COST Action, this methodology will be developed and demonstrated for a series of technical material processes with a clearly identified optimization potential.

A.2 Current international state of knowledge and the European angle

The method of numerical optimization was originally developed 20 years ago, and has been successfully applied over the last 10 years in mechanical engineering, mainly for optimal shape or structure design of components with respect to their weight, local strength, flow responses or acoustic properties. Developing and implementing this technique into materials technology is a new way of processing, and therefore highly innovative.

Such a concerted COST Action can be considered as a follow-up of the COST 512 program, where a sound basis and broad knowledge in modeling techniques for materials science and engineering was already established. The new COST Action P3 on 'Simulation of Physical Phenomena in Technological Applications' could contribute fundamental knowledge concerning 'ab initio' calculations of material properties and simulation techniques.

European cooperation on this topic is justified by global competition in the marketplace of materials processing. A considerable number of European companies are developing and producing noble materials or noble components, e.g. casting of metals, such as superalloys, TiAl or platinum, remelting processes, production and processing of polymere composites, silicon and metallic or ceramic powders, chemical vapor deposition, laser treatment of materials, etc. The proposed technological approach has a significant potential in making European materials processing more competitive.

Compared with other EU research programs focused on more specifically applied problems and mainly conducted with restriction to a few project partners, COST offers the best open platform for this interdisciplinary research topic and guarantees scientific and technological exchange on a large precompetitive scale.

B. Objectives and benefits

B.1 Main objective

The main objective of the COST Action is to develop and to apply numerical optimization methodologies for automatic materials process design, based on quantified product quality, relating to process targets and constraints, including economic aspects.

This objective constitutes to a high degree an interdisciplinary cooperation between European materials engineers and optimization experts of high reputation. It can be achieved as a compilation of the five sub-topics indicated below.

A given material process can be analyzed in order to determine its response or performance in terms of materials quality for a given number of process parameters. Numerical process optimization works in the opposite way, i. e. for a given desired set of material properties, the task is to find the corresponding best process parameters. In completing analysis of a given process design, each type of analysis can be treated independently, e.g. material property analysis independent of process time analysis etc. However, for process design optimization a change of parameters has an impact on all types of performance or quality, and therefore all process targets have to be considered in parallel, i.e. multidisciplinary optimization.

Today, the learning curve of engineers in materials process design is iterative. The engineer suggests a process layout. The next step is to perform a range of relevant analysis using an initial set of parameters. The results are used to modify the set of parameters, and, in the worst case scenario, to modify process layout. Automatic process optimization is to perform the same procedure but better and faster. Whereas an engineer abandons after a few iterations, process optimization goes further. Each process design step is much more efficient than an engineer can achieve. In short, process design time is much shorter and provides better performance and higher materials quality.

However, numerical optimization is applicable only to processes where accurate analysis can be carried out. This means that existing software for analysis can be used as a black box, for optimization.

B.2 Specific objectives

B.2.1 Construction of quality functions

Provided that research projects are focused on real material processes with significant optimization potential, it is the material engineer who has to construct the process-dependent quality function incorporating materials laws and process constraints. This sub-topic is the most comprehensive task of numerical process optimization, directly linked to both specific objectives described in §2 and 4.

B.2.2. Virtual process model: the Simulator

Initially, the simulation engineer will need to build a physical model which is an approximated mapping of a real material process. A checklist contains crucial questions such as: 'Does the model include all input parameters for material laws and design variables?', 'What is the significant length scale of the model', or 'How is the boundary of the model space defined, e. g. energy and mass balance, nucleation conditions?', etc.

Secondly, the engineer has to evaluate, adapt and calibrate appropriate software (e.g. finite element solver for temperature, stress / strain or fluid flow) for accurate and fast process analysis according to the physical model.

B.2.3. Interactive optimization environment

An essential sub-topic is the implementation of a multidisciplinary interactive optimization system which manages all important tasks of process optimization. This kind of environment can include commercial or in-house program codes, thus ensuring the interface between simulator and optimizer.

B.2.4. Parametric studies and sensitivities

Systematic studies of process parameters are a fundamental task for a process design engineer in order to determine the most relevant process parameters. A finite element simulator can act as a generator of parameter sets, with subsequent repeated process analysis setting parameters to pre-defined values. An alternative approach is the so-called 'design of experiment' method (DOE), a special technique to perform parametric studies.

In addition to revealing 'tendencies', sensitivities are calculated to solve general optimization problems in some cases by explicit approximations. This has proven to be a high-performance approach.

B.2.5. Optimization algorithms

Starting from a given quality function, optimization methods (optimizer) have to be identified and applied. These optimizers must achieve an optimum solution, i. e. a set of process parameters, with

which the quality function reaches an extreme value. Furthermore, the combination of local and global optimization techniques open an innovative road towards finding better solutions of quality function coupled to virtual process models and including higher computing performance.

B.2.6. Assessment of automatic process optimization

This task comprises validating and demonstrating the optimization loop for specific material processes. Documentation of this kind should include 'hard numbers' in terms of process performance and material quality.

C. Scientific program

C.1 General statement

The scientific program is more focused on a pragmatic approach, determined by specific material processing problems, than by a global or universal solution. However, development of a methodology of automatic process optimization includes and combines many cutting-edge research activities:

- Micro and macro models to calculate material properties for metallurgical and chemical processes, including the mathematical formulation of material qualities and quality function design
- Three-dimensional numerical analysis of complex processes, including a high number of variables, and often mathematically-coupled physical phenomena, such as temperature, stress/strain or fluid flow.
- Local and global optimization techniques focused on accuracy and computational workload.

C.2 Specific scientific objectives

The scientific program will include the following specific objectives:

C.2.1 Construction of quality functions

- Formulate, adapt or complete micro or macro models to calculate materials structure properties, e. g. kinetic models for chemical reaction, models calculating morphology of a solidification front or solid state transformation models for ceramics or metals.
- Integrating material models into an optimization problem formulation of real material processes, including definition of process design space and constraints.

C.2.2 Virtual process model: the Simulator

- Provide and adapt high-performance simulation programs (e. g. based on tried-and-tested commercial or in-house software packages) including all relevant features in the calculation of parameters and design variables of a given material process.
- Code optimization and calibration

C.2.3 Interactive optimization environment software

- Coupling of simulator and optimizer
- User interface to define and manage the optimization procedure (input data, data recording and visualization, restart condition, etc.)

C.2.4 Parametric studies and sensitivities

- Methodology of parametric studies, in particular 'design of experiments' (DOE) and 'robust design experiments'
- Stochastic behavior of parameters
- Techniques of sensitivity analysis

C.2.5 Optimization algorithms

- Identification and application of optimization methods (optimizer) in relation to properties such as nonlinearities, discontinuities or noisy process parameters.
- Development of hybrid algorithms including local and global optimization techniques.

- Minimizing computing workload.
- Parallelization of algorithms

C.2.6 Assessment of automatic process optimization

- Quality assurance of the optimization software package
- Validation of results using real process data
- Documentation of performance

D. Organization and timetable

The organization of the COST Action will follow the proposed procedures described in the R&P document. This implies that the Action will be run by a Management Committee (MC). The MC will meet twice a year.

Individual projects will be assigned to working groups (WG) according to the following material classes:

WG 1:metals

WG 2:ceramics

WG 3:polymers

In addition, one working group will be defined to work on a general research topic relating to numerical optimization techniques:

WG 4:numerical optimization: integration and performance

Each working group is coordinated by a competent scientist. The coordinators will keep the MC informed about latest developments in their group and will provide written material for the Action annual progress report. Coordinators are responsible for the organization of regular working group meetings. All processes-oriented working groups 1 to 3 are overlapping with working group 4, responsible for the development of optimization methodologies. This interaction is shown schematically in figure 2. A preliminary organization scheme and time table refers to a 4 year Action period (Fig. 3).

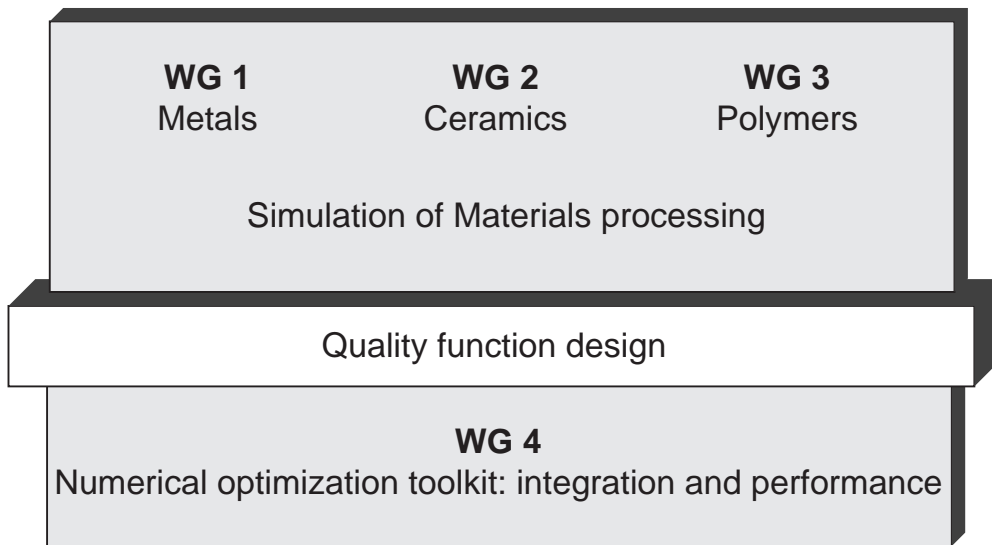


Fig. 2: Preliminary working group scheme.

An evaluation of proposals should be based on the following rules

- Research projects are linked to actual material processes in which a significant optimization potential is to be quantified.
- Each proposal describes material qualities or process parameters to be improved.
- A commercial or in-house software for accurate process analysis has to be identified. The proposed strategy and an assessment of probable technical success for incorporation of process-specific features into this software should be outlined.

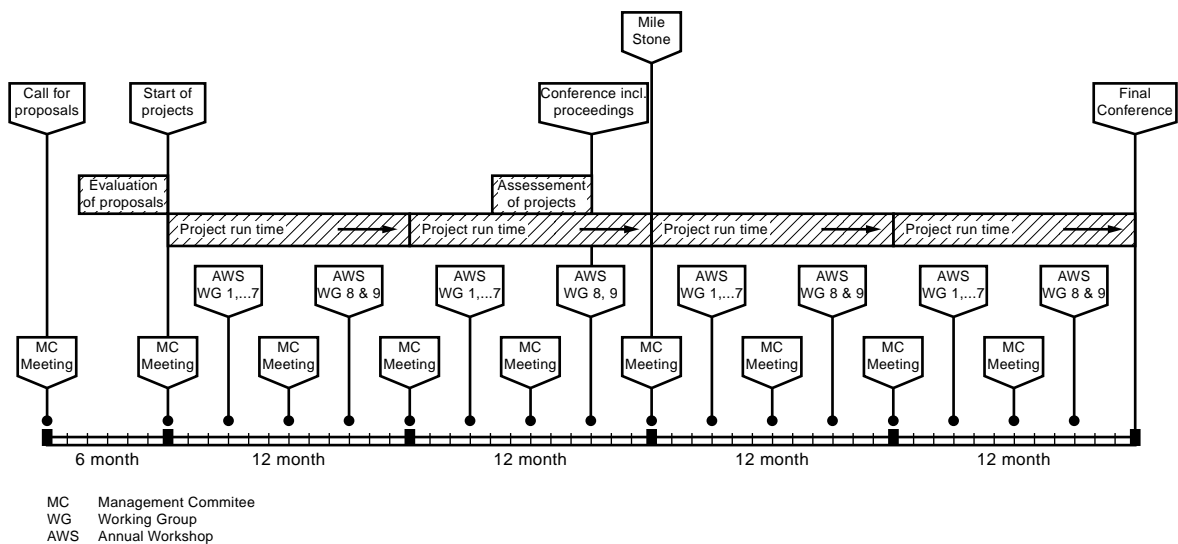


Fig. 3: Preliminary organization scheme and time table for a new COST Action on 'Automatic Process Optimization in Materials Technology' (APOMAT).

Dissemination of scientific results

All publications arising from research carried out under this COST Action will credit COST support, and the Management Committee will encourage and promote all co-authored papers. Results of research carried out by the working groups under this COST Action will be submitted to international scientific journals and reviews.

Joint meetings among different working groups in this COST Action and with relevant working groups from other COST Actions will be organized in such a way as to best promote interdisciplinary communication.

The management Committee of this COST Action will, in conjunction with the different working groups of the Action, meet every year with the main aim of presenting results to the Management Committee as a whole and, where possible, invite potential users and interested parties to this meeting.

The Management Committee will, during the first year of the Action, also set up a workplan for interdisciplinary events for the dissemination of results of the Action.

E. Economic dimension

In the following COST countries, industrial companies or research institutes have indicated their interest in this new action: Belgium, Finland, France, Germany, Sweden, Switzerland and United Kingdom. Assuming a number of approximately 40 research projects approved for funding with an average Budget of ECU 0,4 Millions, including coordination costs of the European Commission, the overall cost of the activities to be carried out under the Action has been estimated at roughly ECU 16,5 Millions. This estimate is valid only under the above assumption and is subject to further change according to both the number of Signatories and the response to an official call for proposals.