

## Adaptive Surrogate Modelling in Unsteady Transport Systems

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In this talk, we will summarize our recent activities in the field of goal-oriented error estimation and model adaptation.

A first aspect is to employ an adaptive multilevel concept to reduce the order of a discrete optimization problem in such a way that most of the optimization iterations are performed on comparably cheap discretizations of the underlying PDEs. To this end, an adaptive multilevel generalized sequential quadratic programming method is applied, which allows the use of independent integration schemes [1, 2]. As the control iterates converge towards the optimum the grids are automatically refined with respect to the ratio of global error estimates and reduced gradient norm. By controlling the accuracy of state and adjoint variables and therefore the consistency between both, we can ensure that the finite dimensional control iterates converge towards the infinite dimensional optimal control.

In a second approach, the concept of goal-oriented adaptivity is used to control discretization errors and a hierarchy of models during the simulation and optimization [4, 5]. Beside refinement in space and variable time stepping, we want to use simplified models in regions with low activity, while sophisticated models are used in regions, where the dynamical behavior has to be resolved in detail. We introduce error estimators for the discretization and the model errors using adjoint techniques and present a strategy to automatically balance those errors with respect to a given tolerance.

The different strategies will be demonstrated for real-life engineering optimization problems including three-dimensional glass cooling processes, two-dimensional steel hardening, and optimal control of water and gas networks.

In the optimization of glass cooling processes, it is important for the quality of the glass that its temperature distribution follows a desired profile to control the chemical reactions in the glass. Typically, time-dependent reference values are provided by engineers for the furnace temperature as well, which should be considered within the objective [1, 2].

The task in steel hardening is to heat the teeth of a steel rack up to a desired temperature profile by induction of a direct current on a part of the boundary. In a second step, the steel rack is cooled immediately such that it gets hardened.

The flow of gas and water through pipelines is of great interest in the engineering community. The aim of operating a transmission network is to minimize the running costs of the compressor or pump stations whereas the contractual demand of the customers has to be met. The enormous size of gas and water networks and their high complexity make the simulation and optimization a difficult computational task [3, 4, 5].

## REFERENCES

- [1] D. Clever, J. Lang, S. Ulbrich, and C. Ziem, Generalized multilevel SQP-methods for PDAE-constrained optimization based on space-time adaptive PDAE solvers, In: G. Leugering, S. Engell, A. Griewank, M. Hinze, R. Rannacher, V. Schulz, M. Ulbrich, and S. Ulbrich (eds.), *Constrained Optimization and Optimal Control for Partial Differential Equations*, Springer Basel AG, International Series of Numerical Mathematics, Vol. **160**, pp. 37-60, 2011.
- [2] D. Clever and J. Lang, Optimal control of radiative heat transfer in glass cooling with restrictions on the temperature gradient, *Optim. Control Appl. Meth.*, Vol. **33**, pp. 157-175, 2012.
- [3] B. Geissler, O. Kolb, J. Lang, G. Leugering, A. Martin, and A. Morsi, Mixed integer linear models for the optimization of dynamic transport networks, *Mathematical Methods of Operations Research*, Vol. **73**, pp. 339-362, 2011.
- [4] P. Domschke, O. Kolb, and J. Lang, An adaptive model switching and discretization algorithm for gas flow on networks, *Procedia Computer Science*, Vol. **1**, pp. 1325-1334, 2010.
- [5] P. Domschke, O. Kolb, and J. Lang, Adjoint-based control of model and discretization errors for gas flow in networks, *Int. J. Mathematical Modelling and Numerical Optimisation*, Vol. **2**, pp. 175-193, 2011.