Master Thesis Proposals
Multiscale Techniques for the Optimal Control of PDEs with Application to the Design of Catalysts

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1 Problem Description and Solution Techniques

Chemical catalysts are essential for the fast and selective transformation of raw materials to end products such as in the production of gasoline, diesel and plastics from crude oil. Discovery of more efficient catalysts therefore has a large economical impact. In this thesis we aim at contributing to this research by developing fast and robust mathematical optimization techniques

The transport of chemical species through a catalyst is modeled by a system of coupled reaction-diffusion equations [3]. Solving these systems via numerical techniques remains to date a computationally challenging task. The straightforward inclusion of these modeling tools in optimization procedures is therefore prohibitevily expensive.

In this thesis we therefore aim at exploiting previously developed expertise in multiscale optimization techniques to the catalyst design problem and to apply space-mapping techniques [2]. The idea here is to consider the PDEs model as a accurate (fine) model and to complement this model with a computationally cheap (coarse) model. A mapping between the models allows to shift the optimization to the coarse model and to correct this model when needed by using the fine model. This approach is expected to result in a considerable speedup of the overall optimization procedure.

In parallel to the application of space-mapping techniques, we will also look into the application of adjoint equation methods to compute the sensitivity of the cost function [1]. It is expected that information on the gradient of the cost function will again allow to speed up the optimization procedure.

References

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