Parameter Estimation for PDE Problems using a Reduced Approach in a Multi-experiment Context

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Abstract: Parameter estimation for PDE models is a recent topic of research. The treatment of this kind of problems with Gauss-Newton-type methods and multiple shooting requires the computation of derivatives of the optimal trajectory with respect to all initial values and parameters. For large-scale PDE problems the number of optimization variables (after discretization) is considerably high and a numerical computation of the parameter estimation problems in a reasonable time is not possible.

One way to reduce the computational cost is to develop methods that lower the number of derivatives significantly. Here we introduce a reduced approach that couples the computation of the Jacobian for the generalized Gauss-Newton method and the subsequent elimination of variables efficiently. By using directional derivatives we are able to reduce the number of derivatives to the number of degrees of freedom while still preserving the convergence properties.

We present an application example from electrochemistry and the solution for the corresponding parameter estimation problem obtained by our methods. These results are compared to ones computed with a conventional multiple shooting method.

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