PDE/ODE-constrained optimization problems and their efficient numerical solution

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Gradient descent methods are a popular tool not only in deep learning, but also in the field of numerical optimization and optimal control. For some constrained optimization problems, they can become very efficient provided that a smart enough method is used for gradient computation. In this lecture, the general optimization problem together with the derivation of the adjoint equation are introduced. Afterward, two particular problems are discussed and the practical issues are pointed out.

The first problem is aimed at determining the correct contributions of different classes of delayed neutrons to the kinetics of the VR-1 experimental nuclear reactor. The facility is installed at the Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague. We consider the system of equations of point kinetics, which is a system of linear ODEs with source terms. We solve the ODE-constrained minimization problem to determine the correct values of the model parameters based on experimental measurement of reactor power output response to the changes in reactivity. The difference between the results of the simulations and the experiments is minimized by several gradient descent techniques. For the computation of the gradient, we employ both the direct method and the adjoint method. We demonstrate the advantages of the adjoint approach, discuss the influence of ODE solver accuracy, properties of the individual gradient descent variants, and the structure of the local minima of the cost functional.

The second problem is to find the Dirichlet boundary condition control for the phase field model describing the solidification of a pure substance from a supercooled melt. In particular, our aim is to control the time evolution of the temperature field on the boundary of the computational domain in order to achieve the prescribed shape of the crystal at the given time. Mathematically, this is a PDE-constrained optimization problem. The adjoint formulation, the numerical solution, and the results obtained in 2D are demonstrated.