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Data Driven PDE Model Discovery: Applications to Surface Erosion Dynamics and Catalytic Reaction Kinetics

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An important application of machine learning algorithms aims to draw conclusions about underlying physical processes from experimental data and to convert this knowledge into a mathematical form. Often this is a model consisting of non-linear coupled partial differential equations, which describe the temporal development of the respective system. Usually, these models contain a large number of coefficients representing different physical processes, which are often difficult to determine ab initio. The methods of datadriven model discovery, however, allow an effective determination of model parameters even for turbulent and highly non-linear dynamics, even with a relatively small amount of experimental data. A brief report is given on the application of model discovery methods in the field of surface science and microkinetic modelling of catalyst surface reactions.