



## Mathematisches Kolloquium

# Duality of estimation and control and its application to rare event simulation

**Prof. Dr. Carsten Hartmann**  
BTU Cottbus-Senftenberg

Abstract:

Many complex systems studied by scientists and engineers are characterised by processes that take place on vastly different time scales. Often the interesting system behaviour, such as phase transitions or regime changes, happens on the longest time scales, and the precise statistical estimation of these slow processes or associated rare events is among the most challenging computational problems in science and engineering. The talk will be devoted to the question of computing the optimal change of measure for certain classes of rare event simulation problems that appear in statistical mechanics, e.g. in molecular dynamics. The method is based on a representation of the rare event sampling problem as an equivalent (or: dual) stochastic optimal control problem, whose value function characterizes the optimal (i.e. minimum variance) change of measure. The specific duality behind the problem is then used to devise numerical algorithms for computing the optimal change of measure where I will describe two approaches in some detail that are built on a semi-parametric representation of the value function: a stochastic gradient descent method and a cross-entropy based stochastic approximation algorithm for the optimal change of measure. I will discuss the general approach, with a particular focus on the choice of the ansatz functions and the solution of high-dimensional problems, and illustrate the numerical method with simple toy examples

**Mittwoch, 18. April 2018, KG I/Bau A 103, 17.00 Uhr s.t.**  
Um 16.30 Uhr werden im selben Raum Kaffee und Tee serviert.