



FACULTY OF
SCIENCE
Charles University

Department of Physical and Macromolecular chemistry

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Department of Physical and Macromolecular Chemistry
invites you to a seminar and a professor lecture

Chemistry by rolling dices

Lecture hall CH3, Faculty of Science, Hlavova 8, Praha 2

on November 29th, 2023 at 14:00

speaker: doc. RNDr. Filip Uhlík, Ph.D.

Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University



Monte Carlo methods can be applied essentially to any problem. For most they would be quite poor, but there are some where they win and sometimes they are the only applicable methods we have. With costs of computing steadily and rapidly decreasing, their embarrassingly parallel nature is another advantage. In this lecture I would like to cover various aspects of the versatile Hamiltonian Monte Carlo method and to give several examples how it can be applied to studying problems of chemical interests.

Organizers: Prof. Tomáš Obšil, Dr. Ondřej Sedláček

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