SIMULATION TOOL COUPLING NON-LINEAR ELECTROPHORESIS
AND REACTION KINETICS FOR DEVELOPMENT AND OPTIMIZATION
OF NEW BIOSENSING ASSAYS

The seminar will be given in English

Electrophoretic separation and concentration techniques are extensively used in a wide
range of chemical and biochemical applications, including drug discovery, genetics, and food
analysis. Recently, there is a growing interest in the use of on-chip electrophoretic techniques for
rapid biosensing and point-of-care diagnostics, requiring not only separation and focusing of
analytes, but also reaction, binding, and hybridization of participating species. Fast computational
tools are an essential part of any such assay development, as they enable insight into physical and
chemical processes and significantly reduce experimental time.

I will present the development, formulation, validation, and demonstration of a fast, generic
and open-source simulation tool, which integrates non-linear electromigration with multispecies
non-equilibrium reaction kinetics. The code is particularly useful for the design and optimization
of new electrophoresis-based bioanalytical assays, in which electrophoretic transport (including
separation and focusing), control analyte spatial concentration and subsequent reactions. The code
can efficiently handle complex electrophoretic setups coupling sharp electric field gradients with
bulk reactions, surface reactions, and competing reactions. In particular, I will demonstrate the
use of the code for investigating accelerated reactions using isotachophoresis (ITP), revealing new
regimes of operation which in turn enable significant improvement of signal to noise ratio of ITP-
based genotyping assays.