# PyURDME, MOLNs and StochSS from new algorithms for spatial stochastic simulation to large-scale distributed computational experiments in "the cloud"

Andreas Hellander

*Uppsala University*
andreas.hellander@it.uu.se

ABSTRACT

this talk I will describe our recent efforts on developing flexible and usable computational science and engineering software ("CSE Software") using modern cloud computing platforms. We will look at the chain from PyURDME, a Python programming API for building and simulating models of biochemical networks, to MOLNs, a cloud orchestration toolkit to create environments that automates the process of scaling e.g. parameter sweeps with PyURDME to large virtual clusters with interactive web-based notebook frontends, to StochSS that exposes our tools (and many others) in easy-to-use software as a service for biologists with no computer science experience.