

Mathematical & Computational Biology Seminar

Organizer: Valerie Hower

Wednesday, 2:00–3:00pm, 939 Evans

Oct. 14 **Vijay Pande**, Stanford University

Folding@home: Pushing the boundaries of molecular simulation orders of magnitude using a combination of Bayesian statistics and large-scale distributed computing

Many key problems involving molecular simulation are fundamentally limited by the timescales they can address (nanoseconds to microseconds), compared to the relevant timescales experimentally (microseconds to milliseconds to seconds). I will describe recent advances that allow for dramatic advances in the capabilities of molecular simulation driven by world-wide distributed computing, i.e. bringing together hundreds of thousands of volunteer computers to tackle problems of interest. The key challenge of such an approach is how one can break a problem into many (10^5 to 10^6) pieces and the use the resulting simulations in an efficient way. The methods I will describe have been demonstrated to not just work efficiently, but are more efficient than the other methods employed. This advance opens the door for new insight from simulation, and I will briefly discuss a few applications of these methods, especially to highlight the methodological challenges.