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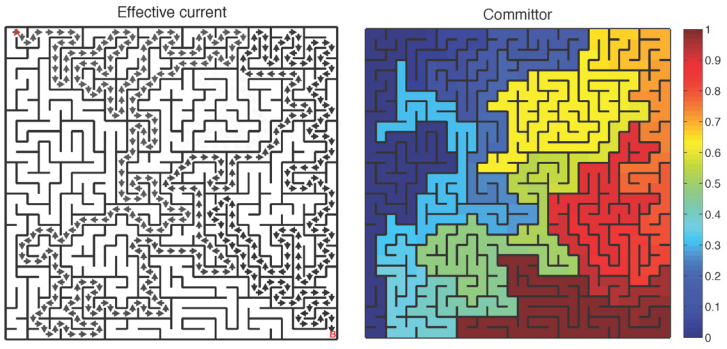
The Fu Foundation School of Engineering and Applied Science

Distinguished Colloquium Series in Interdisciplinary & Applied Mathematics

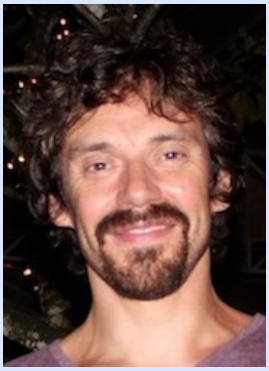
Eric Vanden-Eijnden

Professor of Mathematics, Courant Institute, NYU

Modeling Reactive Events in Complex Systems



Reactive events such as conformation change of macromolecules, chemical reactions in solution, nucleation events during phase transitions, thermally induced magnetization reversal in micromagnets, etc. pose challenges both for computations and modeling. At the simplest level, these events can be characterized as the hopping over a free energy barrier associated with the motion of the system along some reaction coordinate. Indeed, this is the picture underlying classical tools such as transition state theory or Kramers reaction rate theory, and it has been successful to explain reactive events in a wide variety of context. However, this picture presupposes that we know or can guess beforehand what the reaction coordinate of the event is. In many systems of interest - protein folding, enzyme kinetics, protein-protein interactions, etc. - making such educated guesses is hard if not impossible. The question then arises whether we can develop a more general framework to describe reactive events, elucidate their pathway and mechanism, and give a precise meaning to a concept such as the reaction coordinate. In this talk I will discuss such a framework, termed transition path theory (TPT), and indicate how it can be used to develop efficient algorithms to accelerate the calculations and analysis of reactive events. I will also illustrate these concepts on several examples, including the reorganization of Lennard-Jones clusters and the folding of the pinWW domain protein.



Eric Vanden-Eijnden is a professor of mathematics at the Courant Institute of Mathematical Sciences, New York University. Vanden-Eijnden earned his doctorate in 1997 from the Université libre de Bruxelles under the supervision of Radu Bălescu. In 2009, he was awarded the Germund Dahlquist Prize of the Society for Industrial and Applied Mathematics "for his work in developing mathematical tools and numerical methods for the analysis of dynamical systems that are both stochastic and multiscale", and in 2011 he won SIAM's J.D. Crawford Prize for outstanding research in nonlinear science. Vanden-Eijnden's work focuses mainly on the theoretical and computational aspects of Non-Equilibrium Statistical Mechanics and Applied Probability, with applications to biomolecular systems, chemical and biological networks, materials science, atmosphere-ocean science, and fluids dynamics. He has introduced Transition Path Theory (TPT), a general framework to analyze metastability in complex systems. He has developed numerical techniques such as the string methods or temperature-accelerated molecular dynamics to accelerate molecular dynamics simulations. He has also contributed to the development and analysis of multiscale numerical methods for systems whose dynamics span a wide range of spatio-temporal scales.

Thursday, November 12, 2015

4:00pm, 750 Costa Engineering, CEPSR
530 West 120th Street

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