

**Computational Mathematics, Science and Engineering**  
Colleges of Engineering and Natural Science

**Colloquium by Michael Feig**  
**Professor**  
**Michigan State University**

---

**October 14, 2016, 10:30 AM; 1502 Engineering**

**“Exploring the structure and dynamics of biomolecules from molecular to cellular scales via multi-scale computer simulation methods”**

Detailed structural and dynamical formation of how biological macromolecules, in particular proteins and nucleic acids, act and interact within biological environments is key in fully understanding biological processes. While computer simulations of single molecules have become routine, major challenges are still how to connect with biological time scales on one side and embrace the full complexity of cellular environments on the other side. Multi-scale approaches are one strategy to overcome the challenges in expanding both the temporal and spatial domains. A variety of approaches will be discussed, including implicit solvent formalism and coarse-graining strategies. Applications of such methodology to questions of biological relevance are discussed, ranging from membrane-interaction peptides, to models of bacterial cytoplasm and models of bacterial chromosomal DNA structure.

Michael Feig started off early straddling a curiosity for how nature works with a fascination for how computers can contribute to science. He studied physics and computer science at the Technical University of Berlin, Germany, graduating with a Diploma degree in physics in 1994. Inspired by seeing early molecular dynamics simulations and the potential for vast applications in biology, he moved on to graduate school at the University of Houston where Montgomery Pettitt and Andrew McCammon had established a strong program in the simulation of biological systems. He joined the Pettitt group and pioneered simulations of DNA gaining insight into the interplay between the solvent environment and DNA structure. During that time, he started to develop simulation analysis tools and implemented the best parallelized molecular dynamics codes at that time. After graduating with a Ph.D. in 1999, he joined the group of Charles Brooks at The Scripps Research Institute in San Diego where he switched from nucleic acids to proteins, became involved more extensively in computational method development and started to work on multi-scale methods that were applied successfully for protein structure prediction. During this time Michael Feig developed the MMTSB Tool Set that continues to be widely used to run and analyze simulations by many groups. In 2003, he joined Michigan State University as an Assistant Professor in the Departments of Biochemistry & Molecular Biology and Chemistry. He rose through the ranks to become full professor in 2013. At MSU, funded primarily by NIH and NSF, his research has continued to build on the development of multi-scale methods but applications broadened to membrane-bound peptides, large protein-nucleic acid complexes, and more recently, models of bacterial cytoplasm and genomic DNA with the goal of eventually simulating entire cells in molecular detail. The Feig group has also continued to be successful in protein structure prediction, winning the refinement category for the last two rounds of CASP, where such methods are assessed biannually. Michael Feig is a core developer of the widely used CHARMM simulation software led by Martin Karplus (Harvard U.) and he has been collaborating extensively with experimental and computational groups within MSU (Z. Burton, L. Kroos, J. Kaguni, B. Hamberger, B. Hausinger, J. Ohlrogge, G. Wei, S-H. Shiu, C. Hoogstraten, W. Henry, C. Chan, L. Xiao, V. McGuffin), within the United States (U Maryland, U Michigan, Lehigh U.) and internationally (RIKEN, Japan; U. Warsaw, Poland; Bogazici U., Turkey).

Michael Feig currently serves as a managing editor for the Biophysical Journal and Proteins, as the Secretary on the Executive Board of the Telluride Science Research Center, and as co-programming chair for the computational chemistry division of the American Chemical Society."

"Michigan State University is committed to providing equal opportunity for participation in all programs, services and activities. Accommodations for persons with disabilities may be requested by contacting Lisa Roy ([lisaroy@msu.edu](mailto:lisaroy@msu.edu))."

**SPARTANS WILL.**