Short (and non-comprehensive) Description of Research Activities
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In robotics, Kavraki has developed a very successful method for finding collision free paths for complex and highly articulated robots. Path planning is a core problem in robotics. Her method called the Probabilistic Roadmap Method (PRM) caused a paradigm shift in the robotics community. The approach introduced randomization schemes that exploited local geometric properties and produced efficient solutions without fully exploring the underlying search space. Kavraki's work has given rise to the development of sampling-based motion planners that are now ubiquitous in academia and industry. The Open Motion Planning Library that she developed is now part of the Robot Operating System - the Unix of robotics, while a popular robotics textbook that she co-authored covers sampling-based planning algorithms extensively. Departing from purely geometric problems, Kavraki has shown how the foundations of PRM can be exploited and adapted to problems that involve kinematic, dynamic, physics-based constraints, and/or a very high-dimensional solution space. She has the first published results on problems that a few years ago seemed beyond our reach from a computational point of view. These problems range from docking the airspace shuttle to the orbiting space station, to automated manipulation, to planning for flexible objects and tying knots with applications to surgical suturing. Importantly, Kavraki realized early on that the tight coupling of high-dimensional geometry and physics that she achieved in her work paved the way to computational solutions for important bioinformatics problems.

In bioinformatics, Kavraki has studied problems that involve reasoning about the three dimensional structure and flexibility of molecules and their ability to interact with other biomolecules. She has produced computationally efficient representations for molecular motion based on a robotics-engineering approach. Her work includes algorithms for identifying the different shapes that a small molecule can attain, for isolating the spatial common features of molecules that interact with the same target molecule, and for recognizing functional 3D motifs in proteins for automated functional annotation. She uses some of her earlier work and experience (as well as developed libraries) to model interactions of molecules with the goal of producing new therapeutics. In general, biological activity is obtained through the molecular binding of one molecule (the ligand) to the pocket of another, usually larger, molecule (the receptor). In their binding conformations, the molecules exhibit geometric and chemical complementarity, both of which are essential for therapeutic action. Current computational methods for conformational hardly take into account the flexibility of the receptor because of its formidable complexity. Aware of difficulties of solving high-dimensional geometric problems, she has explored dimension reduction techniques for isolating significant receptor motion, a work that has gained a lot of recognition on its own. In her recent work, Kavraki is working on obtaining a mechanistic undertsanding of the possible motions of large macromolecular machines (such as the complement system, chaperonins, phages, and viral shells).