Simulation of Bio-Molecular Microsystems (SIMBIOSYS)

Background: Integrated microsystems offer the potential to significantly improve the speed, sensitivity, efficiency and affordability of chemical processing and analysis. One of the important applications for these systems is chemical/biological sensing and detection. The design of bio-molecular micro/nano-systems requires the development of innovative interfaces between engineering (electronics, optics, mechanics, etc.) and molecular scale processes (chemistry, biology, etc.). The need to produce devices that are highly sensitive (to extremely small sample sizes) and specific (i.e., no false alarms) that perform the detection process quickly and efficiently requires the quantitative understanding and optimization of multi-scale, multi-disciplinary phenomena.

The long-term vision of SIMBIOSYS is to develop and transition technologies to enable the design of multi-functional micro/nano biological devices and systems for civilian and military applications. The program is expected to result in new models/rules for the design community and in new methods/processes for the device community that together will enable the design and development of the next generation of bio-microdevices with enhanced performance and capabilities. SIMBIOSYS hopes to energize multi-disciplinary research by bringing together biologists, chemists, engineers, physicists, computer scientists, etc. to address the hard and pressing challenges in advancing micro and nano-biotechnology.

Objective: The objective of the SIMBIOSYS program is to obtain a quantitative understanding and characterization of bio-molecular processes (such as molecular transport and molecular recognition) and their interface to the engineering world (i.e., transduction of molecular signals to measurable optical/electrical/mechanical signals). Research in these areas will lead to unique multi-disciplinary technologies that enable the design and engineering of integrated bio-molecular systems that have wide applications in the areas of national bio-warfare defense, healthcare and clinical monitoring, drug delivery systems, lab-on-a-chip diagnosis/analysis systems, nanobiotechnology, etc.

One of the important deliverables of SIMBIOSYS is the development and demonstration of advanced computational modeling and simulation tools consisting of scaling rules and phenomenological relationships for the analysis and design of high performance bio-molecular microsystems.

Approach: The projects selected under the program will integrate fundamental experiments and theoretical modeling in a synergistic and complementary manner to enable the characterization, quantification (scaling) and control of bio-molecular phenomena. These research efforts will investigate innovative approaches that enable revolutionary improvements in the sensitivity, specificity, speed, efficiency and affordability of sensing and detection mechanisms relevant to DoD applications. Areas of interest include:

Molecular recognition processes: Most bio-molecular sensing systems rely on molecular recognition processes such as interactions between antibody-antigen, enzyme-substrate, DNA hybridization, ion channels, etc. This area calls for the development of a quantitative description of the chemistry of the (ligand-receptor) recognition process through fundamental experiments and computational models. The objective is to obtain mechanisms and rate constants for recognition processes for various classes of bio-molecules and to explore new methods to improve sensitivity and specificity of these processes.

Transduction of the molecular recognition signal into electrical, optical or mechanical signals: Quantitative characterization of the transduction process is important for performing on-chip detection of the presence and concentration of target bio-molecules. Experimental and theoretical models will be developed to describe innovative transduction methods (including signal amplification) that couple molecular recognition to measurable electrical/optical/mechanical responses.

Fluidic transport phenomena: Fundamental experimental methods as well as computational models will be implemented to describe fluidic and molecular transport at length scales ranging from nanometers to microns. Processes of interest include various fluid pumping and processing (separation, mixing, etc.) methods such as electro-kinetic techniques, surface tension modulated transport, etc. Also of interest is the analysis and characterization of the influence of fluidic transport on molecular recognition and signal transduction. This task will develop a quantitative description of the transport of biological/chemical fluids at the micro/nano scale to enable better control, uniformity, efficiency and speed of the transport process.

Design tools for lab-on-a-chip (LoC) Systems: The prototyping of LoC Systems would benefit significantly from the availability of design tools. This area focuses on integrating models, databases and design rules into a formal design environment/ framework, demonstrating these design tools in prototyping various components of the bio-fluidic chip, and addressing system level design issues, such as optimizing the interaction between the various components on the chip.

The development of data and computational models will form the groundwork for advanced computer aided design (CAD) tools for routine analysis and design of integrated microsystems. CAD tools will enable exploration of novel device concepts and designs, improvements in device performance/reliability and reduction in product time-to-market. These tools will also enable the military to rapidly design novel sensor systems for meeting various mission needs such as biological/chemical threat identification, deployment of countermeasures and monitoring the health of personnel in battlefield as well as urban scenarios.