Organization: **The Johns Hopkins University**

MTO **Simbiosys**

Title: Quantitative Uncertainty Assessment and Numerical Simulation of Microfluid Systems

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Project Goals

1) Construct uncertainty quantification methods that are ideally suited for microfluidic applications involving transport and kinetics; (2) Develop computational solvers and modules that implement these methods; (3) Assemble the uncertainty modules in a computer code that enables simulation of a reacting mixture in pressure- or electrokinetically-driven microchannels; and (4) Demonstrate how the proposed stochastic methods can be used for quantifying model uncertainty, assessing the impact of random variability in operating conditions, evaluating the performance of the microdevices, and assisting in design or deployment strategies.

Technical Approach

Based on incorporating spectral stochastic finite element methods (SSFEM) into direct numerical simulation schemes (DNS) for micro-fluid modeling. Hitherto steps taken towards this objective include (1) the mathematical formulation of uncertainty propagation in an electrokinetically pumped reacting electrolytic solution in a microchannel, allowing for uncertainties in transport properties, chemical rates, and boundary conditions; (2) construction and demonstration of a computational solver for uncertainty propagation in a non-reacting flow in a pressure-pumped microchannel; and (3) construction and demonstration of a computational solver for uncertainty propagation in a 1D electrokinetically pumped reacting flow.

Recent Accomplishments

- Demonstration of stochastic, coupled, transport/finite-rate/equilibrium chemistry formulation in 1D and 2D electrokinetically-driven flow. Tests include pH-dependent protein-labeling reaction including buffer chemistry.
- Application of simplified design code to band crossing simulations. Parameter study in support of experiment design and in preparation for uncertainty/sensitivity study.
- Development of a second-order upwind implementation for stochastic scalar transport.
- Formulation of a specially-tailored stochastic multigrid solver for non-separable, elliptic, electric field equation in slender domains.

Six-Month Milestones

- Couple stochastic electric field module with chemistry and momentum, thus completing the overall code structure.
- Extend study of band-crossing reactions to analyze sensitivity and role of uncertainty.
- Explore adaptive Polynomial Chaos expansions and fractional stepping schemes.

Team Member Organizations

Sandia National Laboratories

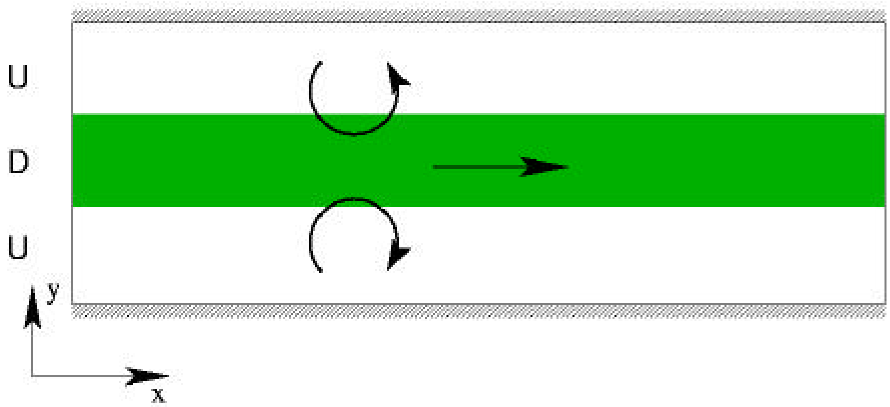

Figure 1: Schematic illustration of 2D electro-kinetically driven flow in a 1cm-long, 100µm-high micro-channel. U refers to the unlabeled protein while D refers to the dye. A potassium phosphate buffer at pH=7.25 is used. Reversal of the ?-potential between 2.5mm < x < 6.5mm creates a recirculation zone, which mixes the dye with the unlabeled protein and facilitates the labeling reaction.

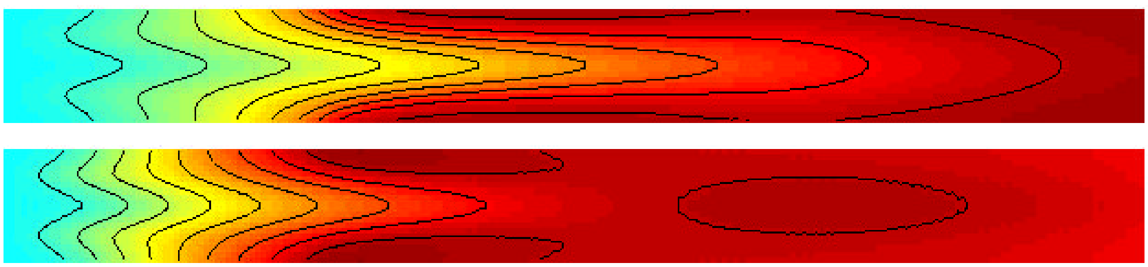

Figure 2: Top: Contours of the mean labeled protein at steady state. Contour minimum at 0.01 mol/l, with increments of 0.02 mol/l. Bottom: Standard deviation of labeled protein concentration at steady state. Contour minimum at 1.4×10^{-4} mol/l with increments of 2.9×10^{-4} mol/l.

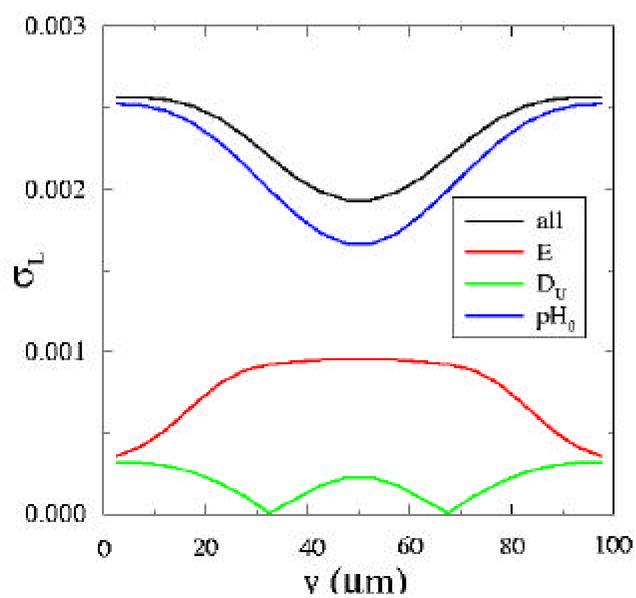

Figure 3: Contribution of specific stochastic input parameters to the standard deviation of the labeled protein concentration. A 1% uncertainty is assumed in the electric field (E), the pH where the reaction peaks (pH_0), and the unlabeled protein diffusivity (D_U).