Organization(s): The Johns Hopkins University
Sandia National Laboratories

MTO **Composite CAD**

Title: Quantitative Uncertainty Assessment and Numerical Simulation of Micro-Fluid Systems

Duration of Effort: June 2000 - June 2003

Principal Investigator(s): Omar M. Knio / Roger G. Ghanem / Habib N. Najm
Phone: (410) 516-7736/(410) 516-7647/(925) 294-2054
Email: knio@jhu.edu/ghanem@jhu.edu /hnnajm@ca.sandia.gov
Web: http://www.me.jhu.edu/people/faculty/knio.html
http://venus.ce.jhu.edu/users/ghanem

Objective

1) Construct uncertainty quantification methods that are ideally-suited for microfluidic applications involving transport and kinetics, (2) Develop computational solvers and flexible modules that implement these methods, (3) Assemble the uncertainty modules in a computer code that enables simulation of a multicomponent 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.

Major Challenges

- Formulation, development and optimization of efficient schemes for the solution of large systems of equations resulting from the spectral stochastic representation of the solution process.
- Development and implementation of efficient integration schemes for applications involving stiff kinetics.
- Construction and optimization of parallel algorithms that implement the stochastic representation methods and the numerical solution schemes.

6th Month Milestones

- Develop a mathematical formulation which accounts for uncertainty representation using the Polynomial Chaos expansions, adapted to microchannel flow of non-reacting isothermal liquid with uncertainty in viscosity. Includes the Navier-Stokes and continuity equations for an inelastic fluid.
- Develop a numerical solution scheme for the non-reacting isothermal liquid. Involves an adaptation of the projection method to the uncertainty formalism.
- Extend the isothermal formulation to include finite-rate and equilibrium kinetics, allowing for uncertainty in Arrhenius and equilibrium parameters.
