Organization: **Lawrence Livermore National Laboratory**

Title: Lattice Boltzmann Simulation of Particle Laden Flows in Microfluidic

Start Date: August 2000 **End Date:** September 2002

MTO **Simbiosys**

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Project Goals

The objective of the work proposed here is to develop predictive simulation tools to study the dynamic behavior of particles and macromolecules in microfluidic subsystems. Here the focus is on the particulate phase in a suspending fluid. The targeted micro-systems include Dielectrophoretic separators with frequency dependent particle properties and suspension behavior in microflows with sudden contractions and expansions. The simulation capability is also set-up to handle species bouyancy forces. It is the goal of this effort to enable the study of suspensions and suspension properties when subject to pressure driven flow with intermolecular and surface forces and external field effects in microflows.

Technical Approach

- Develop relevant theory for Physics Modules,
- Develop interface to incoporate Physics Modules into the LB capability,
- Validate the capability with theoretical and experimental results (when available) ,
- Target development effort to solve real world problems through BioFlips program collaborations.
- Develop understanding into observed phenomena through simulation results, experimental results, and new & existing theory.
- Developed phenomenological models (and order of magnitude estimates) on phenomena studied to augment and guide mirodevice designs.

Recent Accomplishments

- Incorporated Clausius-Mossotti factor for multi-layered, complex species.
- Developed Double Layer model for Dielectrophoretic manipulation.
- Set-up multi-particle simulation capability to study the Dielectrophoretic manipulation of polystyrene beads, functionalized nano-particles and pathogen simulants.
- Developed new initialization approaches necessary to simulate concentrated suspensions in microflows.
- Instituted new pressure boundary conditions to enable the study of fluid/suspension behavior in sudden contractions.
- Developed representations for microneedle geometries with sudden contraction.
- Set-up LB code to produce HDF output files for data analysis and flow visualization.

Six-Month Milestones

- Develop traveling wave DEP capability and integrate into the LB capability.
- Use new standing and traveling wave DEP capability to assist in the design of UCD species detection system. This includes optimization of DEP operating conditions for target species, "tags" and species complexes.
- Use double layer model and DEP capability to teams with characterization of mobility of polystyrene during manipulation.
- Incorporate near-field interaction module with colloidal interactions to characterize suspension transport through microneedle geometries. Provide analysis via simulation for UCB.
- Publish traveling wave DEP capability, double layer model and suspension results from suspension capability.

Team Member Organizations

Dr. E. Wheeler, LLNL
Dr. T. Weisgraber, LLNL
Gary Hon UCB/LLNL

Design tools to optimize Dielectrophoretic separations

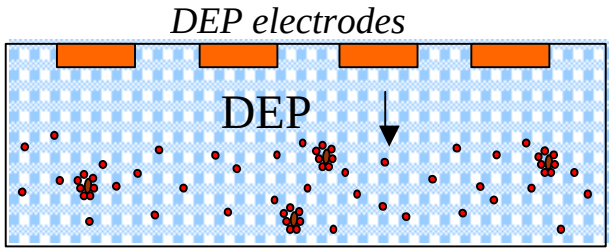

Figure 1a. Standing wave Dielectrophoretic manipulation of target species, tags and species complex for sample preparation for detection.

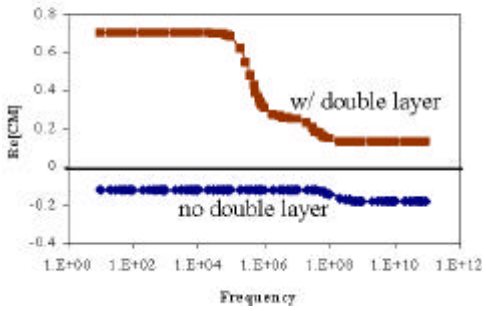

Figure 1b. Frequency dependence of the real part of the Clausius-Mossotti factor for the species complex in Figure 1 a with and without double layer effects.

Design tools to characterize and optimize suspension flows in microchannels and microneedles

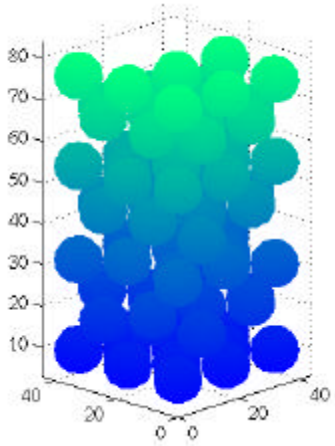

Figure 2a. New optimized, initialization for the study of concentrated suspensions. The volume fraction, ϕ, shown here is 0.4

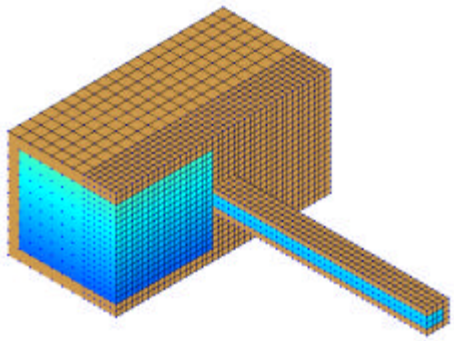

Figure 2b. Lattice Boltzmann representation a microneedle with a sudden contraction. Flow for this configuration is achieved using inlet and outlet pressure boundary conditions.