



Particle Separation by Capillary Electrophoresis in Nanochannels

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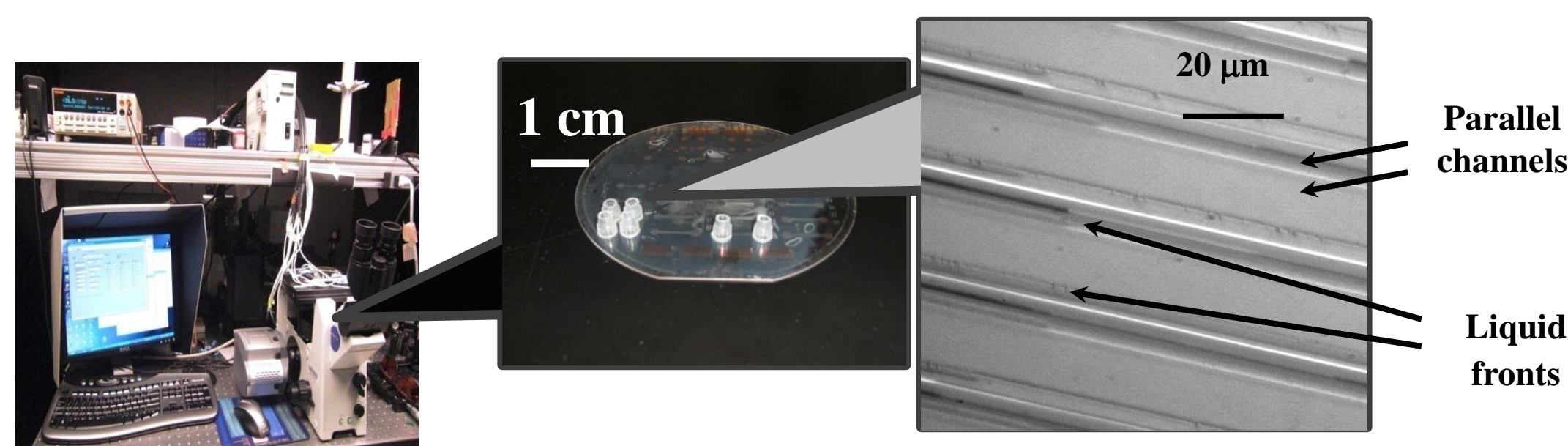
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Abstract

Our experimental / theoretical collaboration investigates recent results from Dr. Pennathur's lab (UCSB, Dept. ME). It is found that short double-strands of DNA exhibit enhanced electrophoretic separation in nanochannels when compared to separation in microchannels. We develop models to investigate for nanochannels the potential role of the large surface area to volume ratio, comparable width of the channel to electric double layer thickness, steric particle-wall and particle-particle interactions, and the van der Waals interactions. To explore the relative importance of these effects a three dimensional mathematical model is developed along with computational methods to solve the non-linear PDEs using spatially adaptive discretizations. This work is in an early stage and this poster primarily presents our specific model and overall approach for feedback.

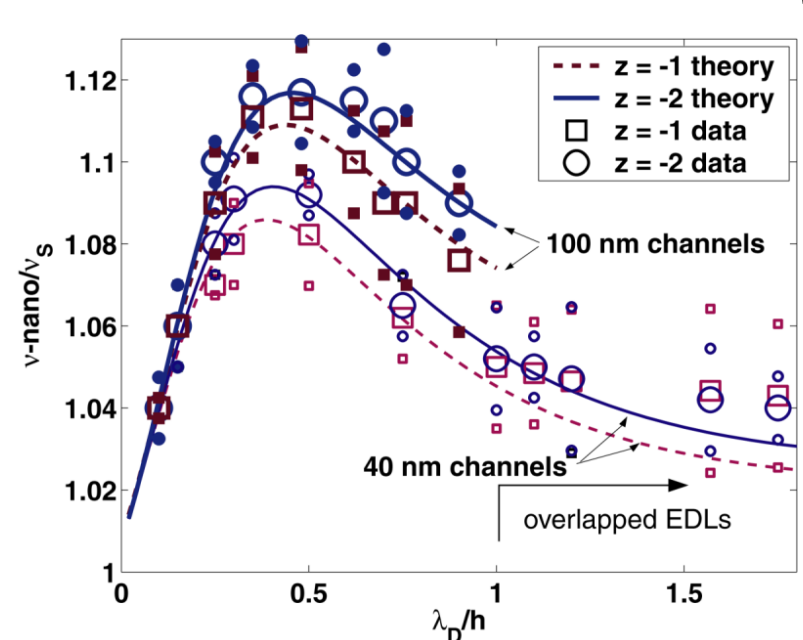
Nanochannels



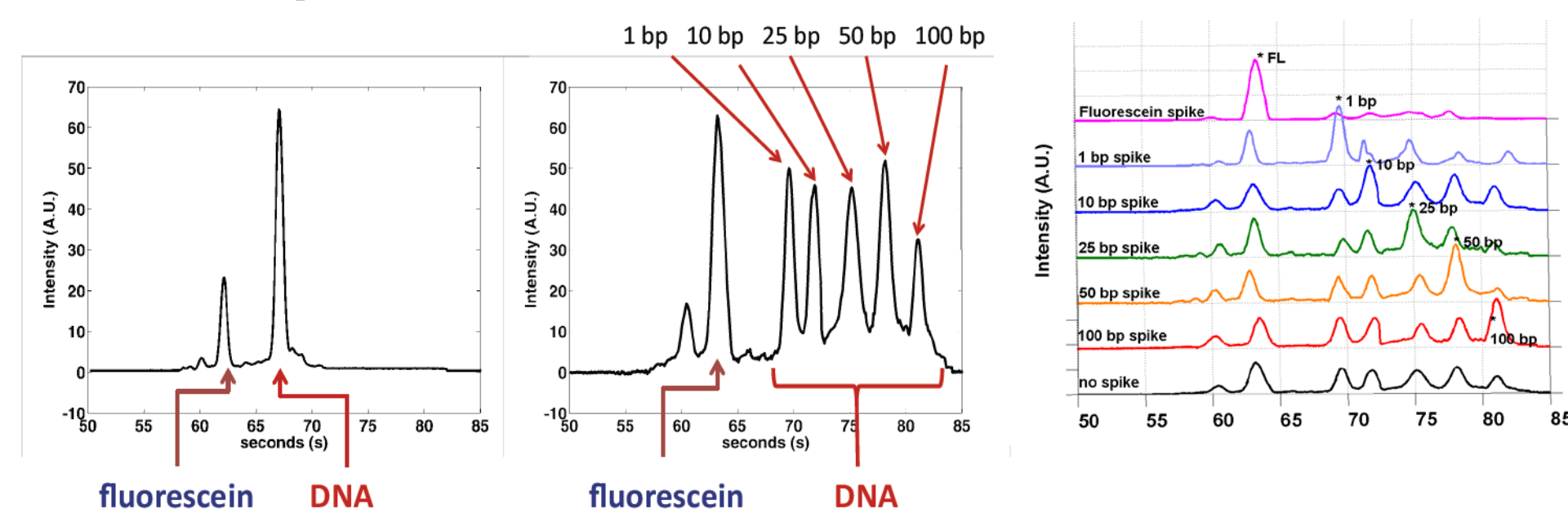
- Channels fabricated in silicon with depths ranging from 40 – 100nm.
- Custom mounting developed for wafer and fluidic inlets.
- Lithography approach allows for many channels to be fabricated on a single wafer (parallel processing for fluidics).

Experimental Results

Small Ions and Theory

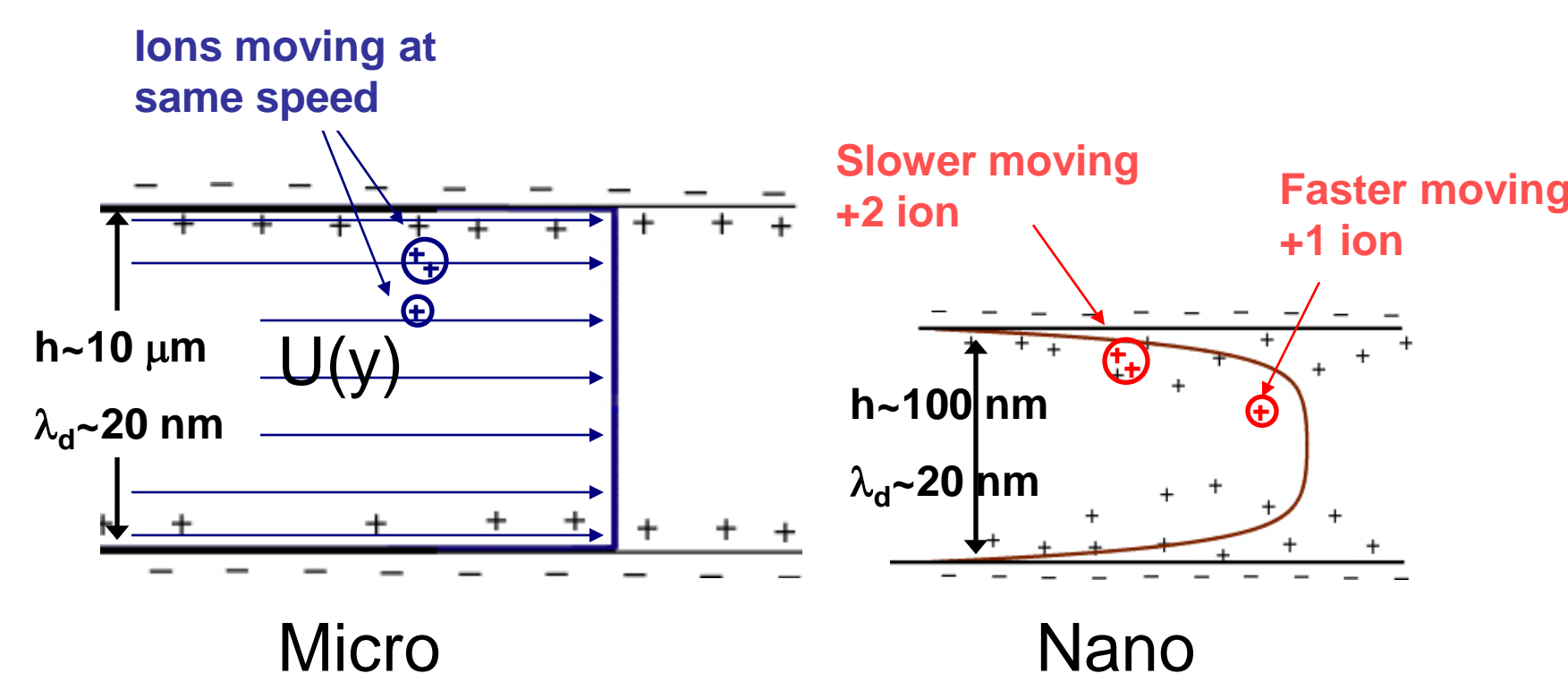


DNA Separation: Microchannel / Nanochannel



- Separation of ds-DNA in microchannel is not as pronounced as in nanochannel.
- Theory developed for small ions in nanochannels.
- Experimental measurements show good agreement with the theory, but not for larger particles.
- Larger particles are expected to exhibit more complex behaviors than small ions.
- Excluded volume (role of shape), and interactions through double-layers, wall interactions, hydrodynamics.

Motivation



- Many effects become stronger in nanochannels.
- Electro-osmotic flow deviates from plug-flow (double-layer thickness ~ channel width).
- Solute particles experience significant steric restriction by channel walls.
- Proximity of solutes relative to the walls plays an important role in hydrodynamic coupling.
- High surface area to volume ratio.
- Hydrophobic surfaces / slip boundary for flow.
- Van der Waals attraction of solute particles to the walls.

Mathematical Model

- (\mathbf{X}, θ) : Particle Rigid Body Configuration
- c_k : Ionic Species Concentration
- $\mathbf{u}(\mathbf{x}, t)$: Solvent Fluid Velocity
- $\Phi[c, \mathbf{X}, \theta]$: Total Energy

Electrostatics

$$-\nabla \cdot \epsilon \nabla \phi = q(\mathbf{x}, t)$$

$$q(\mathbf{x}, t) = q_{\text{ion}}(\mathbf{x}, t) + q_{\text{wall}}(\mathbf{x}, t) + q_{\text{prt}}(\mathbf{x}, t)$$

$$q_{\text{ion}}(\mathbf{x}, t) = \sum_k q_k c_k, \quad q_{\text{wall}}(\mathbf{x}, t), \quad q_{\text{prt}}(\mathbf{x}, t)$$

$$\frac{\partial c_k}{\partial t} = -\nabla \cdot \mathbf{J}_k$$

$$\mathbf{J}_k = -D_k \nabla c_k - \alpha_k \nabla \Phi c_k + u c_k$$

$$\Phi = \phi + \psi + E_{\text{electrodes}}$$

Steric Interactions

$$\psi = \psi_{\text{steric-ion}} + \psi_{\text{particle-wall}} + \psi_{\text{particle-particle}}$$

$$\psi_{\text{steric-ion}} = C \frac{c^2(\mathbf{x})}{c_0 - c(\mathbf{x})}$$

$$\psi_{\text{particle-(-)}} = \int \int C_1 (|\mathbf{x} - \mathbf{y}| + \delta)^{-12} dx dy - \int \int C_2 (|\mathbf{x} - \mathbf{y}| + \delta)^{-6} dx dy$$

Hydrodynamic Coupling

$$\mu \Delta \mathbf{u} = -\nabla p + \mathbf{f}$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\mathbf{u} = 0, \quad \mathbf{x} \in \partial \Omega_{\text{wall}}$$

$$\mathbf{u} = V_{\ell}, \quad \mathbf{x} \in \partial \Omega_{\text{particle } \ell}$$

$$\mathbf{f} = \sum_k \alpha_k \nabla \Phi c_k$$

Translational and Rotational Diffusion

$$\frac{d\mathbf{X}}{dt} = -\Gamma_{\text{hyd}}^{-1} \mathbf{F} + \mathbf{g}_{\text{thm}}$$

$$\frac{d\theta}{dt} = -\Lambda_{\text{hyd}}^{-1} \tau + \mathbf{h}_{\text{thm}}$$

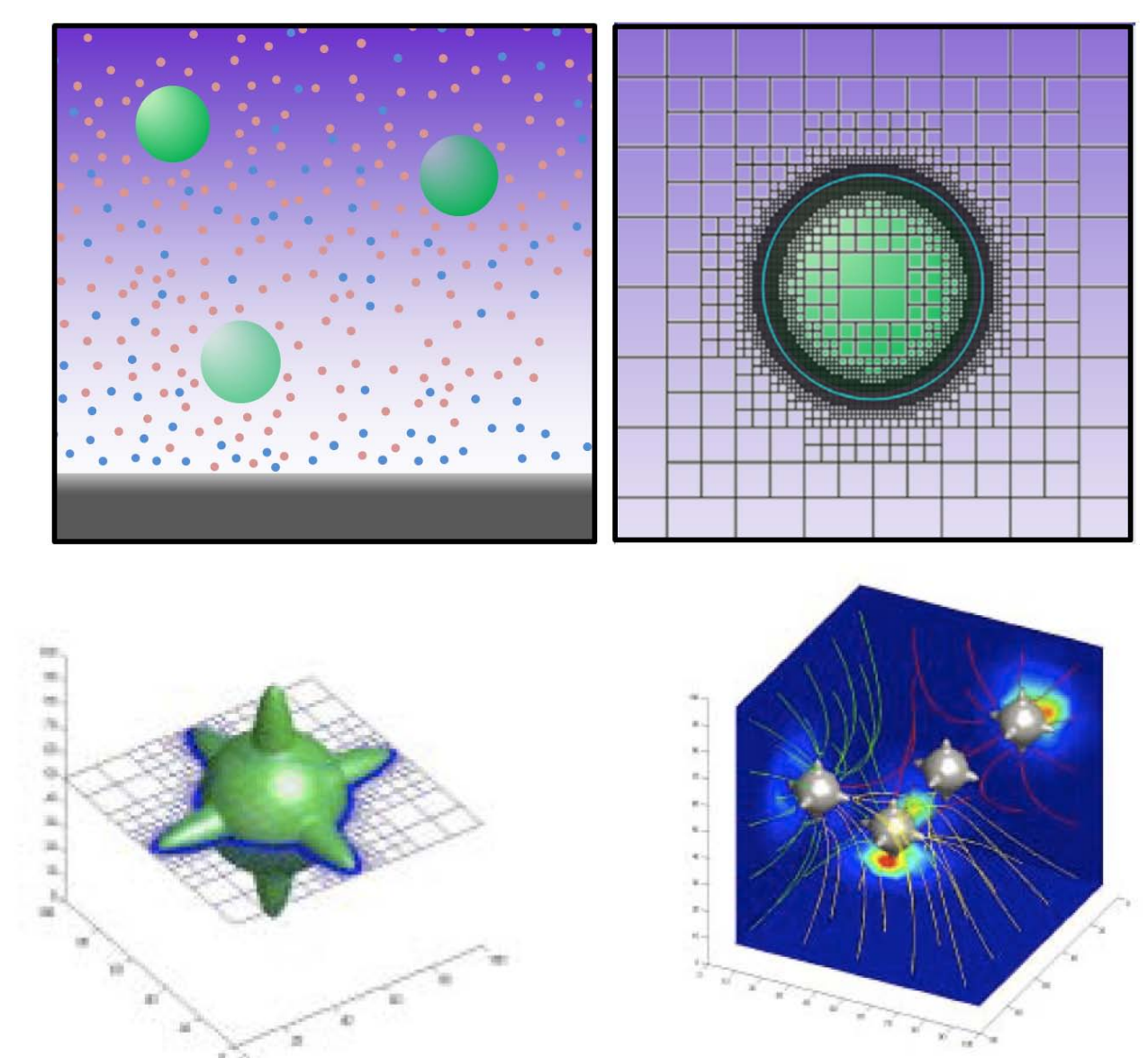
$$\mathbf{g}_{\text{thm}} = Q \frac{d\mathbf{B}_t}{dt}$$

$$\langle \mathbf{g}_{\text{thm}}(s) \mathbf{g}_{\text{thm}}^T(t) \rangle = Q Q^T \delta(t - s)$$

$$Q Q^T = 2k_B T \Gamma_{\text{hyd}}^{-1}$$

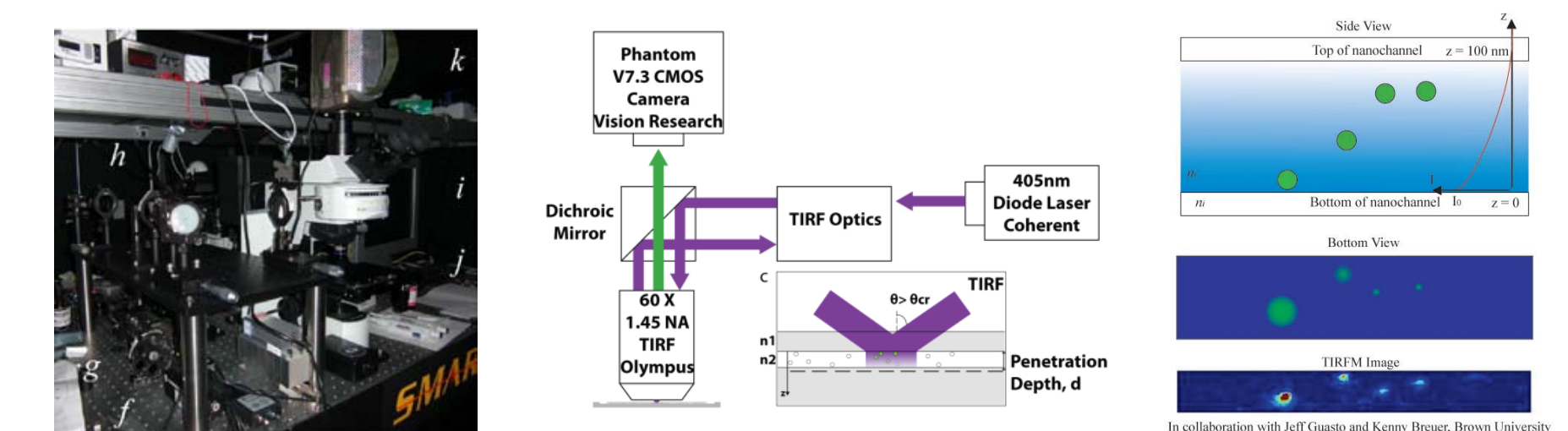
\mathbf{h}_{thm} : handled similarly

Computational Approach



- Electrostatic and hydrodynamic equations approximated by spatially adaptive discretizations.
- Electrostatic equations approximated on a domain including the channel walls and particles.
- Hydrodynamics approximated on a geometric domain defined by the channel and the exterior of the particles.
- Non-spherical particles can be handled by the approach.

Proposed TIRF Experiments



- What can be learned from TIRF measurements of quantum dots? (exp. time / blinking : potential issues).
- Three dimensional data time series will be used to obtain particle distribution functions within the channel.
- Attempt single particle tracking x-y-z for mean displacement velocity and diffusivity.

Current / Future Work

- Implementation of computational methods and development of iterative solvers for the electrostatics.
- Statistical Mechanics Theory / Monte-Carlo Simulations to develop constitutive relations for ion sterics.
- Non-dimensional analysis / time-scale analysis to develop simplified models and theory.
- Validation with respect to experimental data sets (fluorescent signals / TIRF measurements).