

# Micro and Nanoscale Transport of Biomolecules through Pores



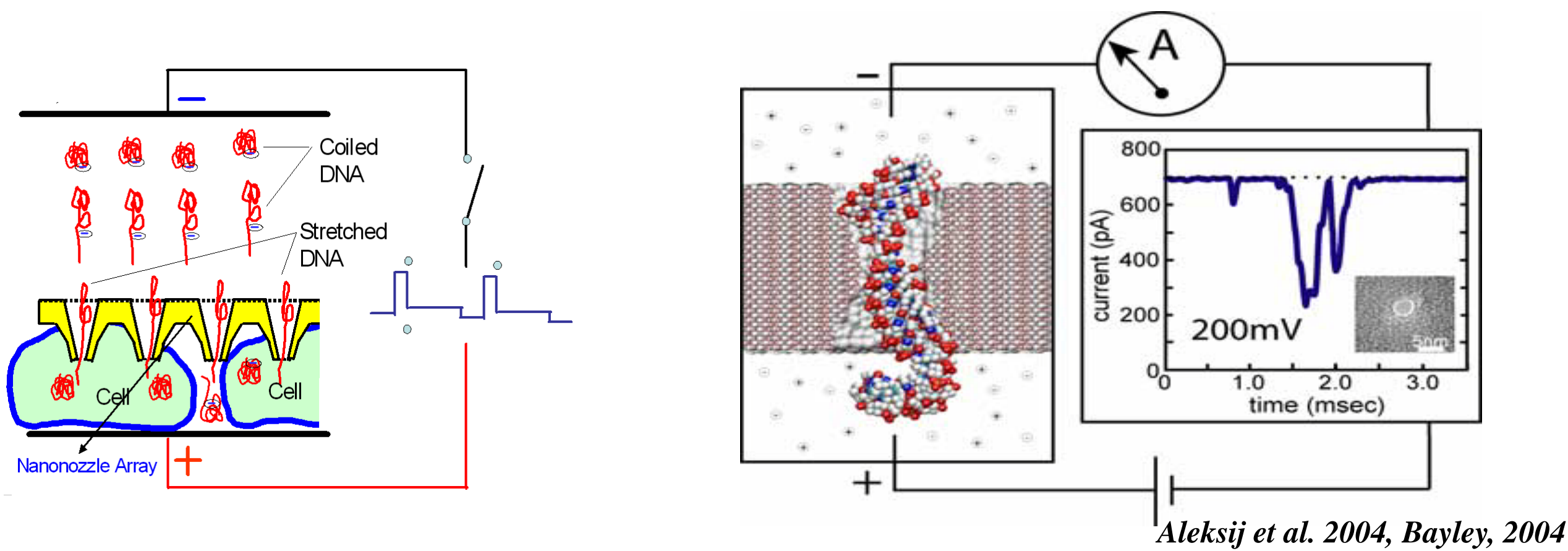
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## Motivation

- Model and analyze translocation of fluid flow and biomolecules through micro/nano channels.
- Experiments to measure velocity, mole fraction & temperature profiles at nanoscale are not possible.
- To study behaviour of electric current in channel from bio-sensing point of view.
- Impact:
  - Cut design time of nanoscale devices.
  - Reduce the number of prototype devices.

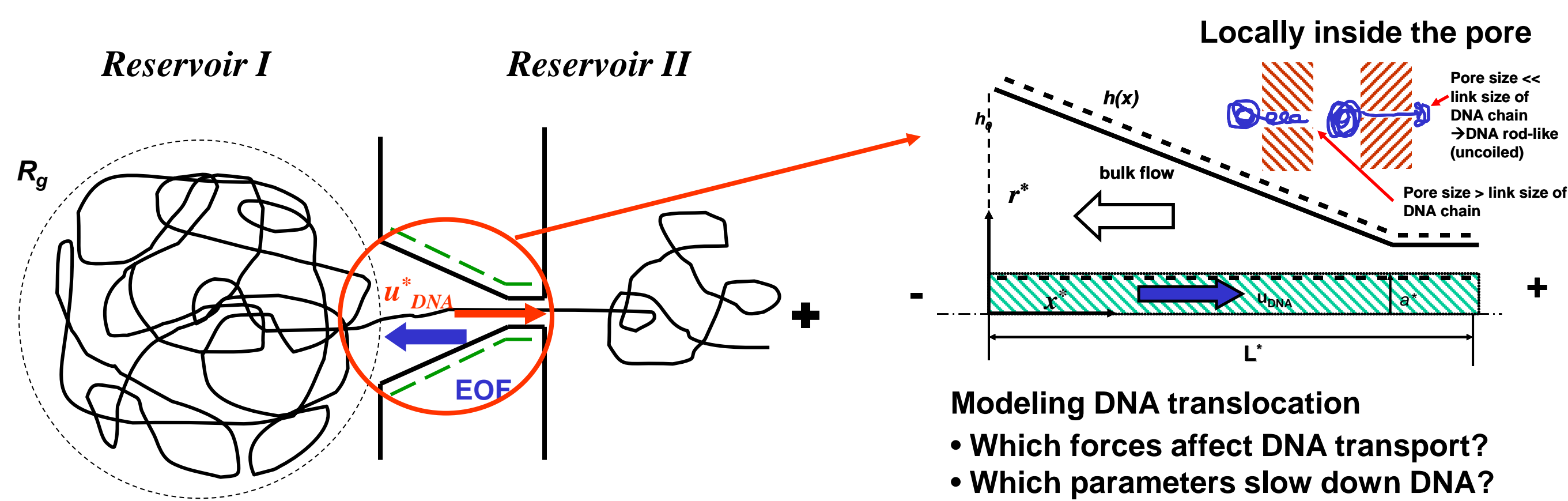
## DNA translocation through a nanopore



Gene delivery: directly transfer repaired DNA into cells

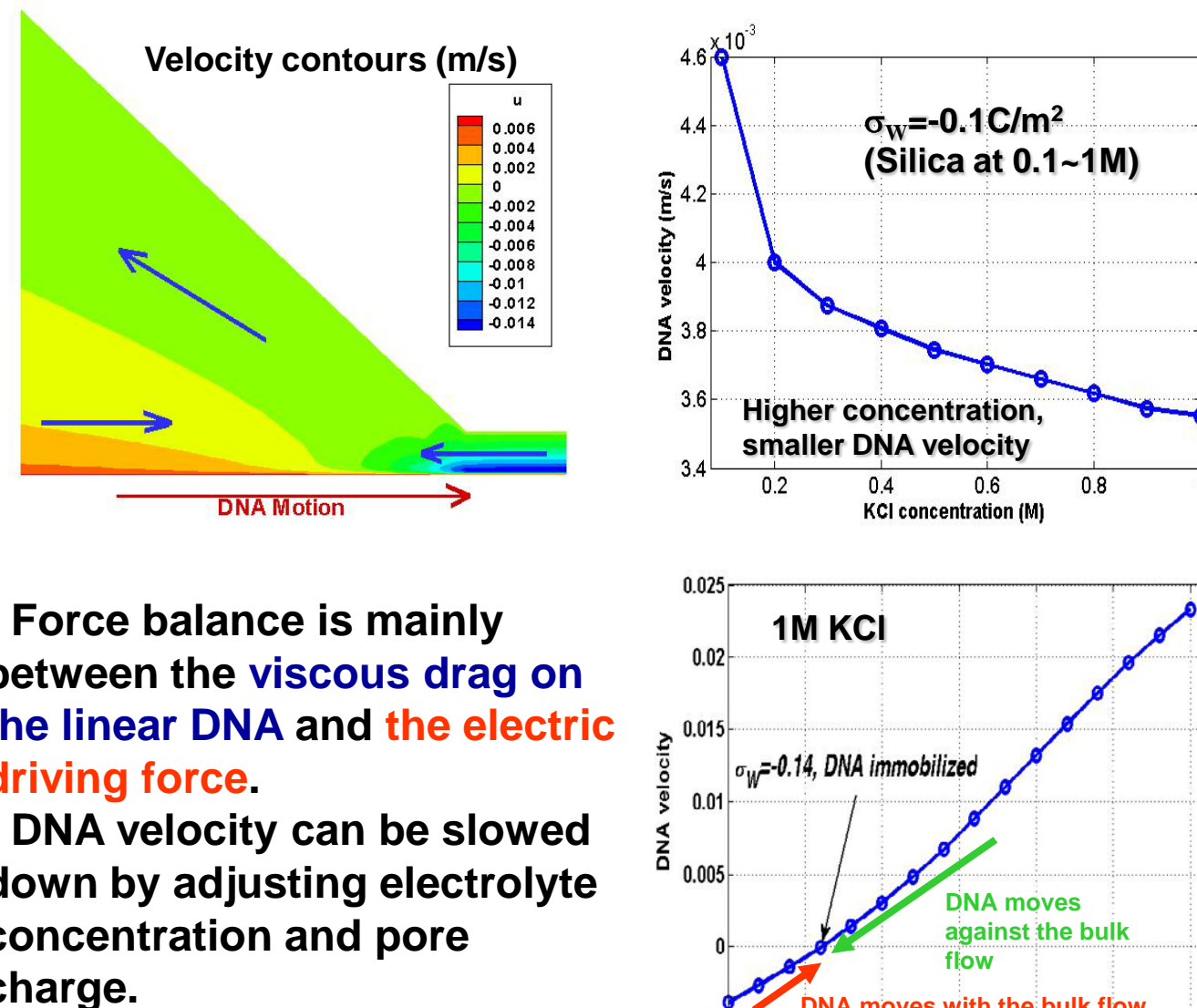
Nanopore sequencing: identity of the DNA molecule is encoded in the ionic current changes

## Model for DNA translocation



- Which forces affect DNA transport?
- Which parameters slow down DNA?

Forces	Outside/Inside the nanopore	Magnitude
Electrical driving force	Inside	O(100pN)
Viscous drag on the linear DNA	Inside	O(100pN)
Entropic uncoiling and recoiling forces	Outside	<O(1)pN
Viscous drag on the DNA blob	Outside	O(1~10pN)



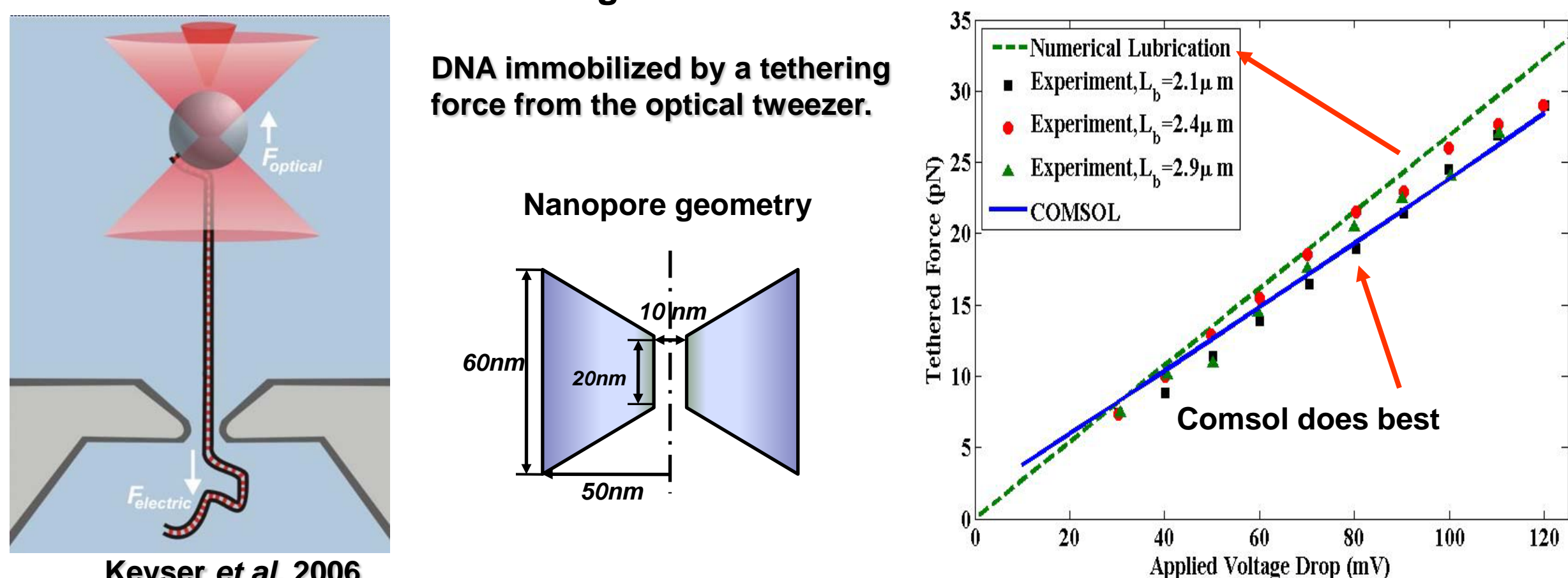
- Force balance is mainly between the viscous drag on the linear DNA and the electric driving force.
- DNA velocity can be slowed down by adjusting electrolyte concentration and pore charge.

## Experimental validation

### DNA translocation velocity validation

Source	$\sigma_w$ (C/m <sup>2</sup> )	$L_{DNA}$ ( $\mu$ m)	$c_{KCl}$ (M)	$V_{exp}$ (m/s)	$V_{num}$ (m/s)
Storm 2005	-0.2	3.91	1	0.013	0.0149
Smeets 2006	-0.14	16.5	0.5	0.012	0.0123
Li 2003	-0.14	3.4	1	0.01	0.012

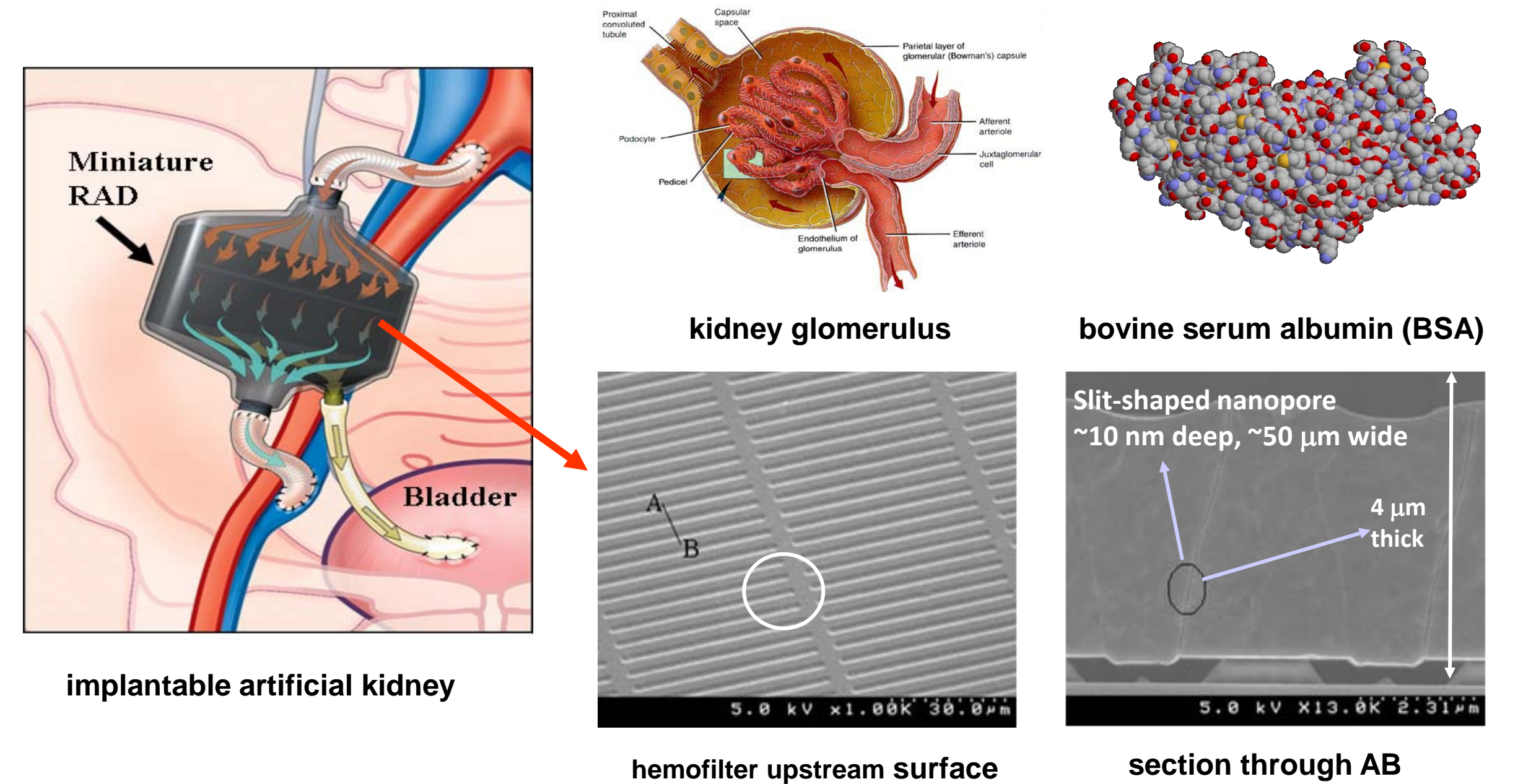
### Tethering force validation



Model validated by the good agreement between the computational results and the experimental data.

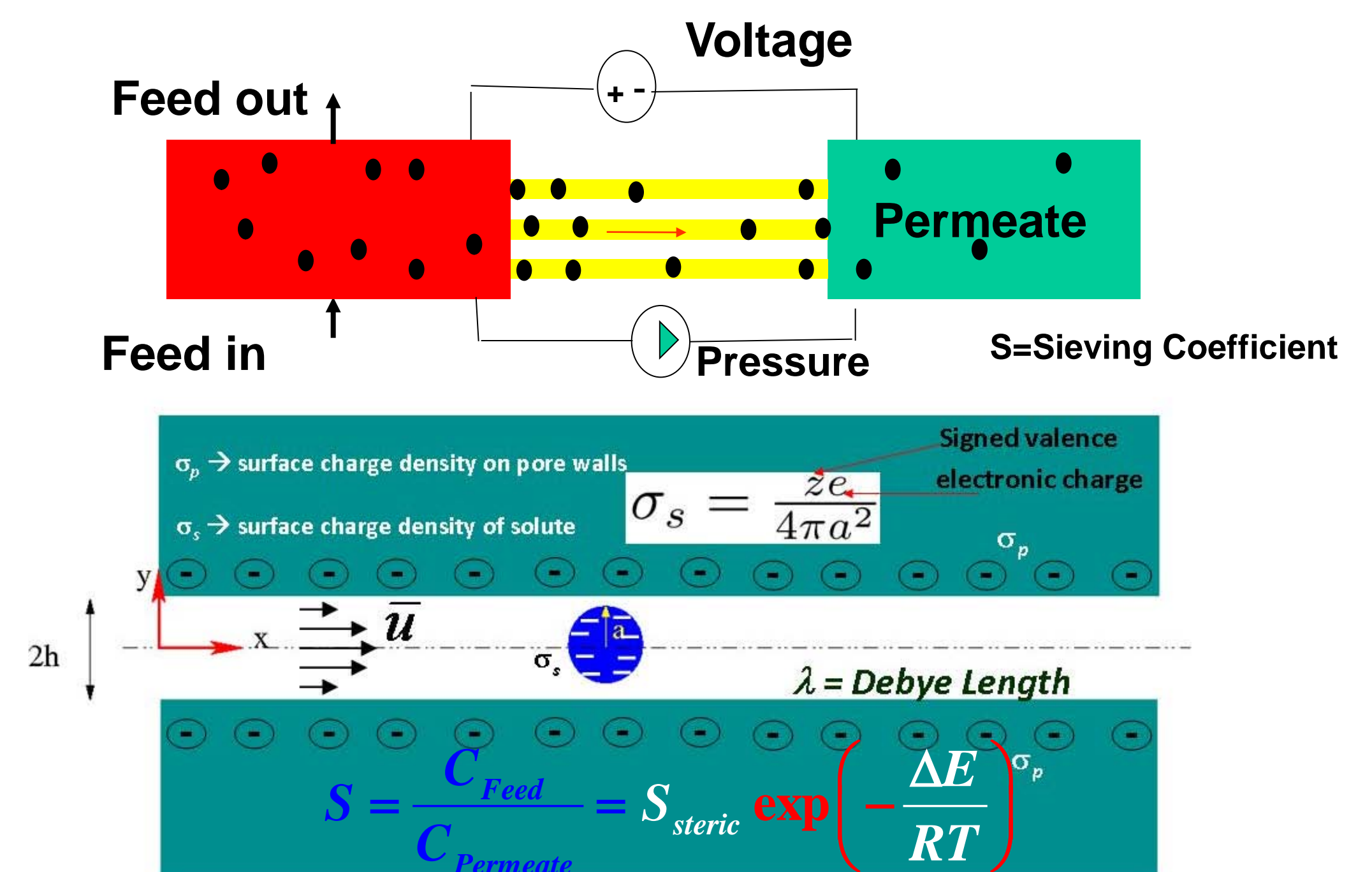
Chen, Lei, Conlisk, A. T., "DNA nanowire translocation phenomena in nanopores", *Biomedical Microdevices*, 2009, Accepted.

## Charged biomolecular transport in an implantable artificial kidney



Filtration of biomolecule (BSA) through a synthetic membrane-based implantable artificial kidney conceived to functionally substitute native kidney glomerulus in End-Stage Renal Disease Patients.

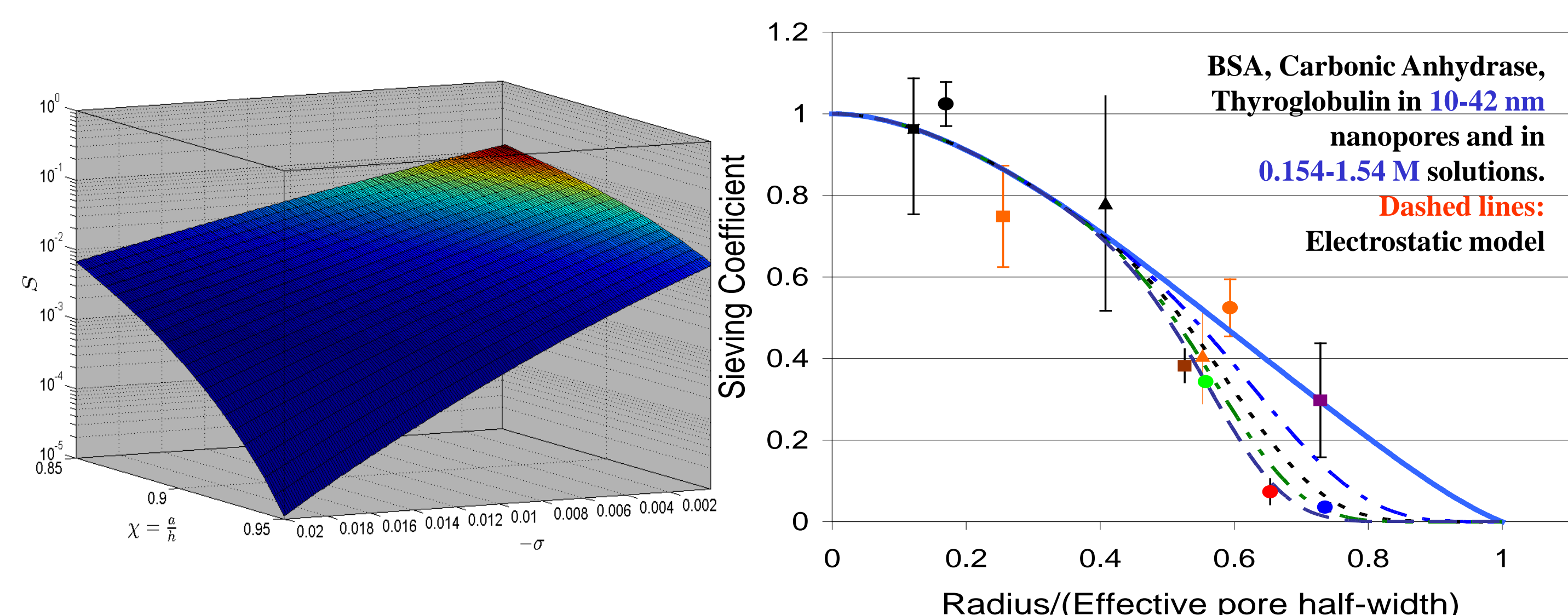
## Model for pore level transport



$$\Delta E = A\sigma_p^2 + B\sigma_p\sigma_s + C\sigma_s^2$$

- $S_{steric}$  from size-hindered equilibrium partitioning, convection, diffusion and electrophoresis.
- Change in electrostatic energy  $\Delta E$  of the solute pore electrolyte system between isolated and confined states.
- Interacting solute surfaces modeled as two paraboloids separately interacting with nearest pore wall (Deriaguin approximation).

## Porescale electrostatics in an implantable artificial kidney



- Membranes with narrow and charged pores containing dilute electrolytes are more selective.
- Satisfactory agreement with experimental data
- Modifying pore width and surface charge can improve filtration through nanopores in a membrane.

Conlisk, A. T., Datta, S., Fissell, W. H. and Roy, S. "Biomolecular transport through hemofiltration membranes", *Annals of Biomedical Engineering*, 37(4):722-736, 2009.

## Acknowledgements

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