

OPTIMAL ELECTRO-OSMOTIC FLOW THROUGH NANOCHANNELS

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NAVIER-STOKES EQUATION

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$$\begin{aligned}\nabla \cdot \mathbf{u} &= 0 \\ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) &= -\nabla P + \eta_0 \nabla^2 \mathbf{u} + \rho \mathbf{F},\end{aligned}$$

- ▶ $\rho \implies$ Density of fluid
- ▶ $\eta_0 \implies$ Shear viscosity of fluid
- ▶ $P \implies$ Pressure of the fluid
- ▶ $\mathbf{u} \implies$ Streaming velocity field of the fluid flow
- ▶ $\mathbf{F} \implies$ External body force applied to generate the flow

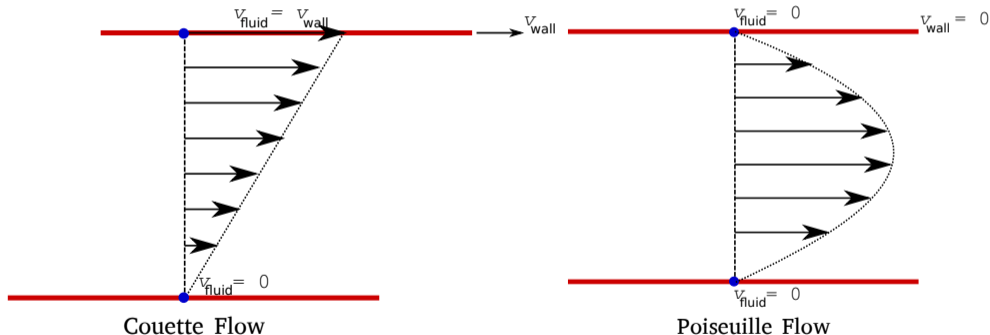
NO-SLIP BOUNDARY CONDITION

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Nanoscale hydrodynamics

Enhanced flow in carbon nanotubes

[Mainak Majumder](#), [Nitin Chopra](#), [Rodney Andrews](#) & [Bruce J. Hinds](#) 

Table 1 | Pressure-driven flow through aligned MWCNT membrane

Liquid	Initial permeability*	Observed flow velocity†	Expected flow velocity†	Slip length (mm)
Water	0.58	25	0.00057	54
	1.01	43.9	0.00057	68
	0.72	9.5	0.00015	39
Ethanol	0.35	4.5	0.00014	28
iso-Propanol	0.088	1.12	0.00077	13
Hexane	0.44	5.6	0.00052	9.5
Decane	0.053	0.67	0.00017	3.4

MWCNT, multiwalled carbon nanotube. For details of methods, see supplementary information. *Units, cm^3 per cm^2 min bar. †Flow velocities in cm s^{-1} at 1 bar. Expected flow velocity is that predicted from conventional flow.

FLUID FRICTION

- ▶ According Navier,

$$\sigma_{xy} = -\xi_0 u_x(z)$$

- ▶ $\sigma_{xy} \implies$ tangential stress exerted by the wall on the fluid,
- ▶ $u_x \implies$ velocity x -component
- ▶ $\xi_0 \implies$ interfacial friction coefficient.



Figure: Bust of Claude Louis Marie Henri Navier at the École Nationale des Ponts et Chaussées (Image courtesy: *Wikipedia*)

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- ▶ NS equation with slip boundary conditions valid up to channel widths ≈ 1 nm !

ELECTRO-OSMOTIC FLOW

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- ▶ The Navier-Stokes equation for analyzing EOF

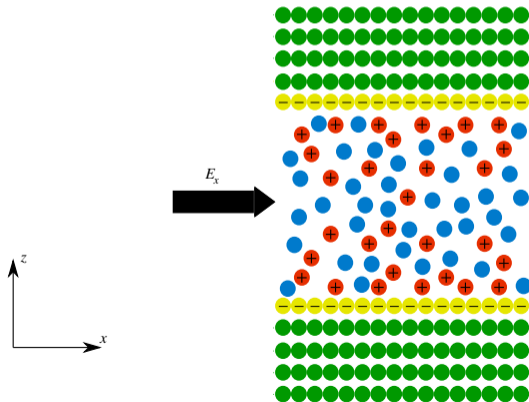
$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla P + \eta_0 \nabla^2 \mathbf{u} + \rho_f \mathbf{E},$$

- ▶ $\rho_f \implies$ Free charge density
- ▶ $\mathbf{E} \implies$ External electric field applied to generate the flow

ELECTRO-OSMOTIC FLOW

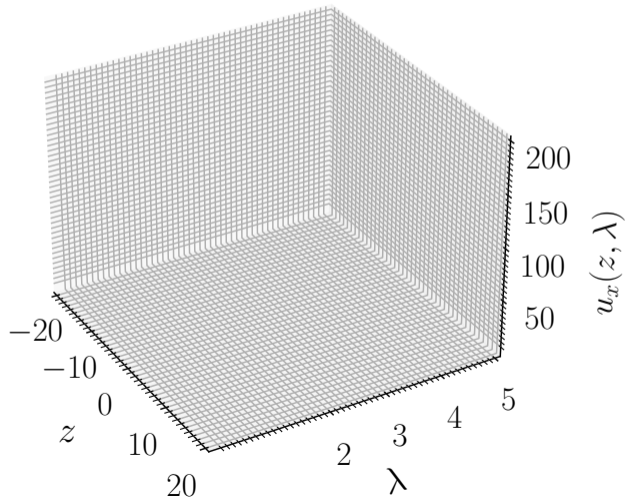
- ▶ The governing equation for a fully developed 1-D steady-state EOF, with negligible inertial effects compared to viscous forces

$$\Rightarrow \eta_0 \frac{d^2 u_x(z)}{dz^2} = -\rho_f(z) E_x$$

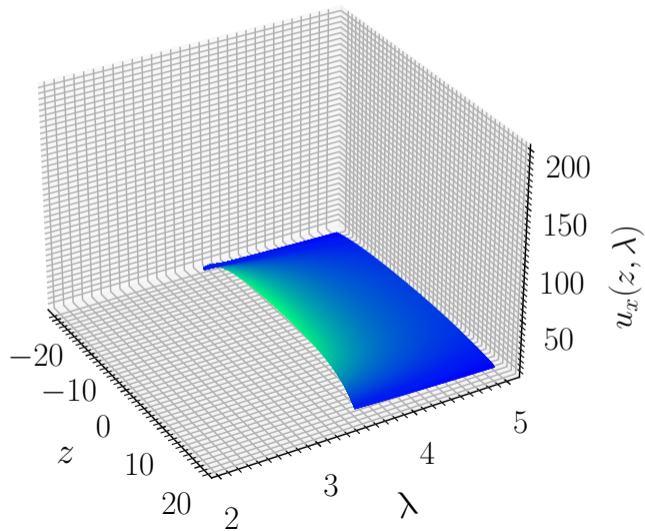


WETTING (HYDROPHILIC) NANOCHANNEL

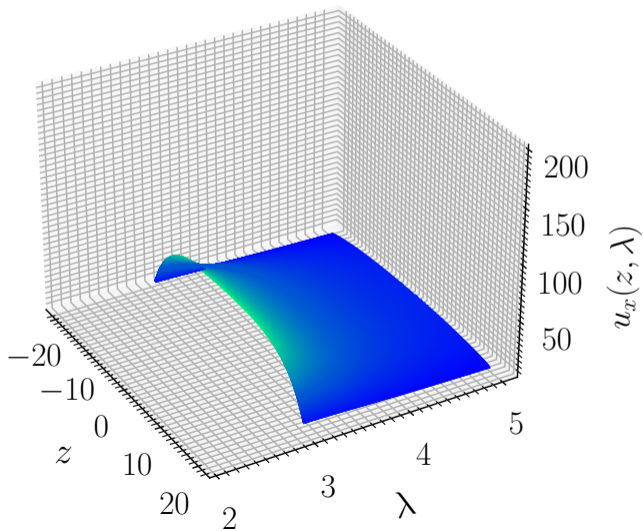
$$\lambda \propto \frac{1}{\text{ionic conc.}}$$



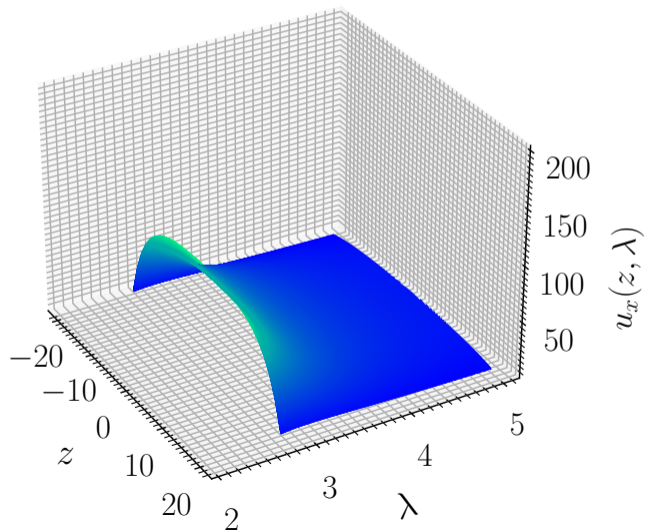
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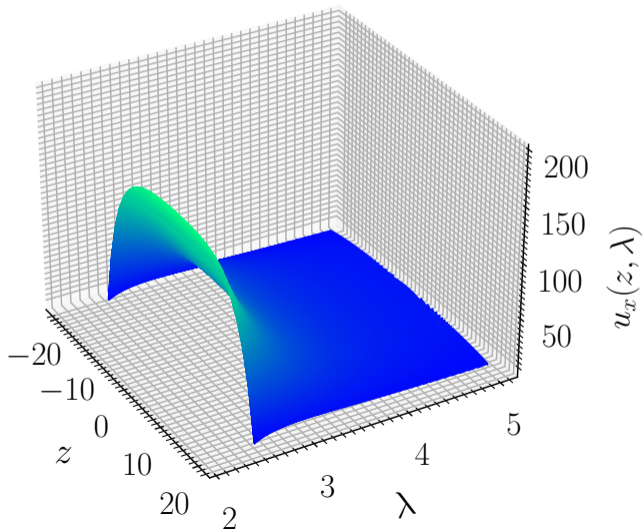
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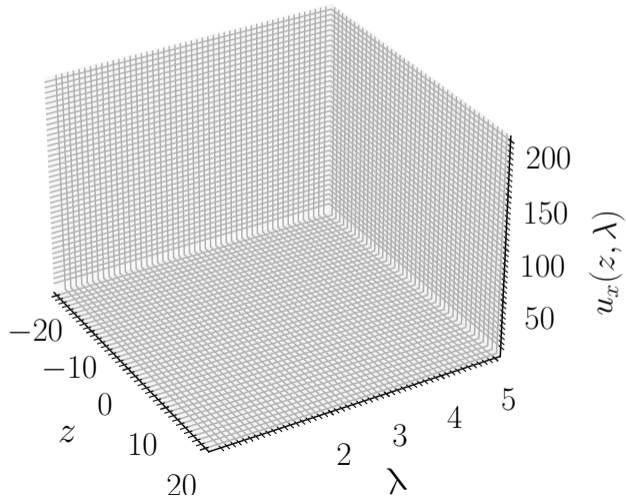


WETTING (HYDROPHILIC) NANOCCHANNEL

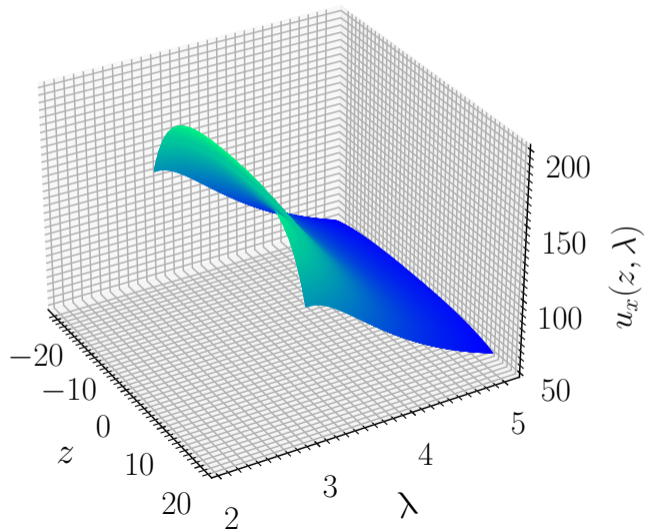


NON-WETTING (HYDROPHOBIC) NANOCHANNEL

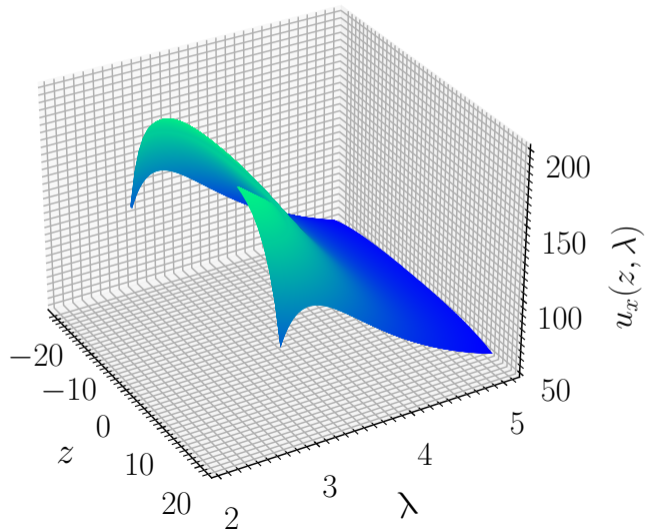
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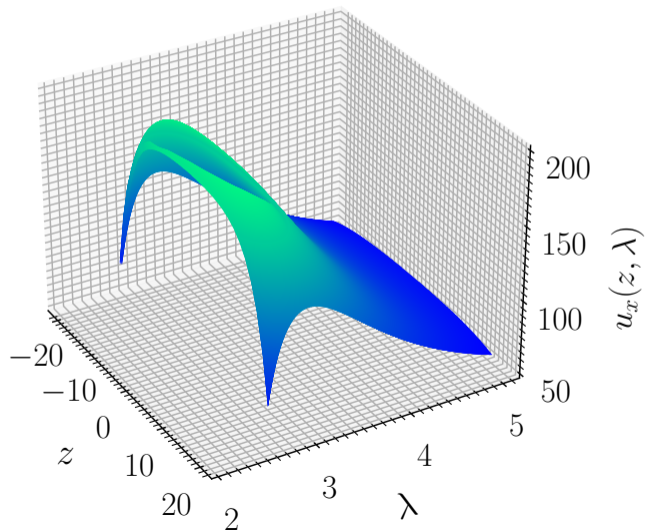
NON-WETTING (HYDROPHOBIC) NANOCHANNEL



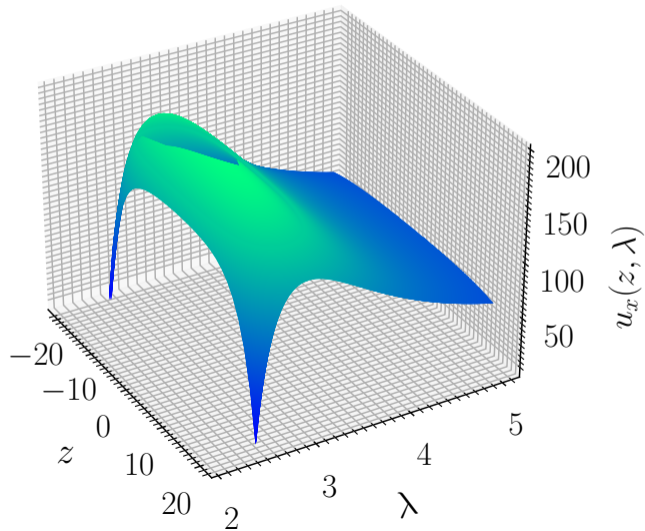
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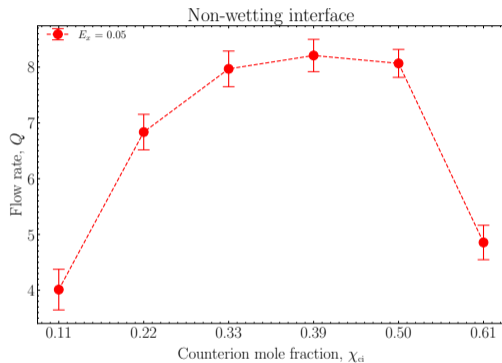
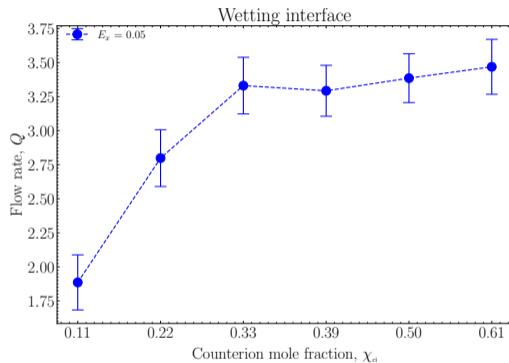
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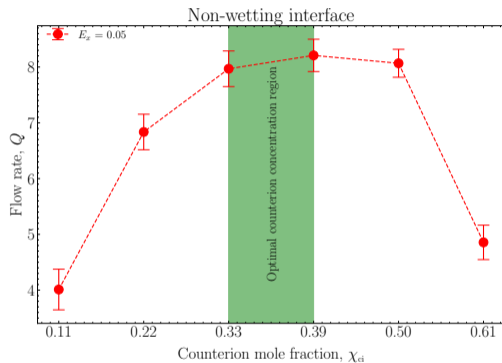
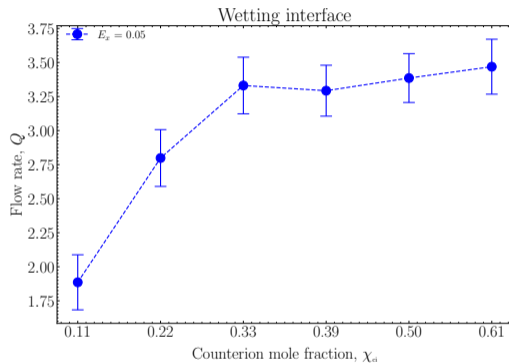
NON-WETTING (HYDROPHOBIC) NANOCHANNEL



MOLECULAR DYNAMICS SIMULATIONS



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APPLICATIONS

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- ▶ Energy storage

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- ▶ Optimizing electro-osmotic transport through nanochannels.
 - ▶ Electro-osmotic pumping does not require any mechanical moving parts such as pumps or valves to transport the fluid.
- ▶ Desalination
- ▶ Energy storage
- ▶ Understanding flow through biological nanochannels

ACKNOWLEDGEMENTS

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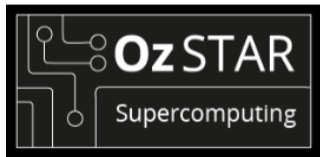
Prof. Jesper Schmidt Hansen
Roskilde University
Denmark

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Thank you!

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