



# Coupled transport in nanoscale confined fluids

## Beyond coefficient-based transport laws

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Conference Courses 18 May

A large, detailed sculpture of an elephant, possibly a water buffalo, with a person riding on its back. The sculpture is set against a blue sky and a cityscape.

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Logos: Nantes Université, oniris, Université Gustave Eiffel, enrs.

# Transport laws: a recurring structure

Ohm 1827



$$I = R^{-1}U$$

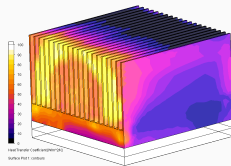
# Transport laws: a recurring structure

Ohm 1827



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Fourier 1822



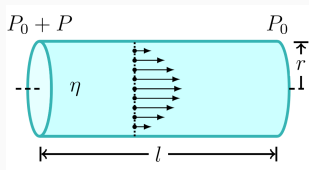
$$q = -k \nabla T$$

Fick 1855



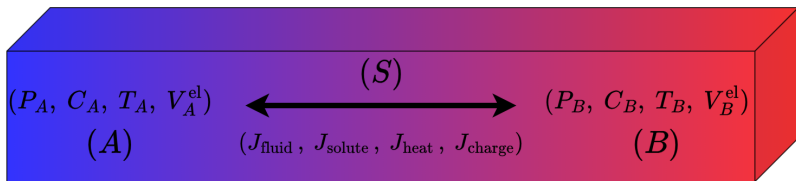
$$j = -D \nabla c$$

Newton 1687



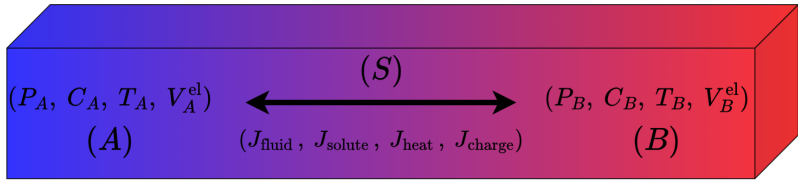
$$\sigma = \eta \nabla v$$

# Onsager (1931): Thermodynamics of irreversible processes



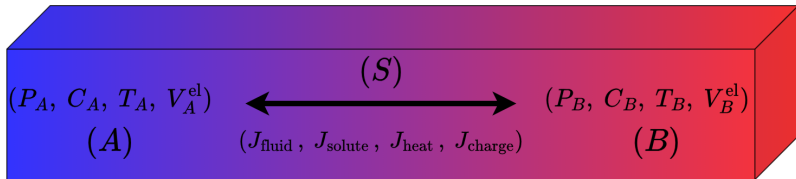
$$\begin{bmatrix} J_{\text{fluid}} \\ J_{\text{solute}} \\ J_{\text{heat}} \\ J_{\text{charge}} \end{bmatrix} = \begin{bmatrix} L_{\text{fluid}} \times \Delta P \\ L_{\text{solute}} \times \Delta C \\ L_{\text{heat}} \times \Delta T \\ L_{\text{charge}} \times \Delta V^{\text{el}} \end{bmatrix}$$

# Onsager (1931): Thermodynamics of irreversible processes



$$\begin{bmatrix} J_{\text{fluid}} \\ J_{\text{solute}} \\ J_{\text{heat}} \\ J_{\text{charge}} \end{bmatrix} = \begin{bmatrix} L_{\text{fluid}}^P \Delta P & +L_{\text{fluid}}^C \Delta C & +L_{\text{fluid}}^T \Delta T & +L_{\text{fluid}}^{\text{el}} \Delta V^{\text{el}} \\ L_{\text{solute}}^P \Delta P & +L_{\text{solute}}^C \Delta C & +L_{\text{solute}}^T \Delta T & +L_{\text{solute}}^{\text{el}} \Delta V^{\text{el}} \\ L_{\text{heat}}^P \Delta P & +L_{\text{heat}}^C \Delta C & +L_{\text{heat}}^T \Delta T & +L_{\text{heat}}^{\text{el}} \Delta V^{\text{el}} \\ L_{\text{charge}}^P \Delta P & +L_{\text{charge}}^C \Delta C & +L_{\text{charge}}^T \Delta T & +L_{\text{charge}}^{\text{el}} \Delta V^{\text{el}} \end{bmatrix}$$

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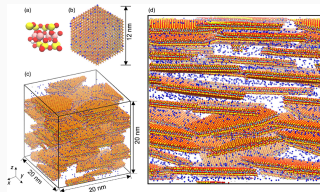
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Onsager Matrix :  $L \equiv$  transport properties of (S)

1968 Nobel Prize in Chemistry

# A different picture emerges at the nanoscale

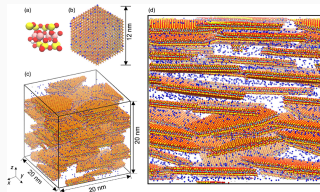
## Soils



Zheng *et al.* 2023

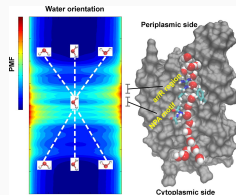
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## Soils



Zheng *et al.* 2023

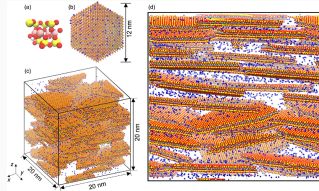
## Cells



Padhi *et al.* 2017

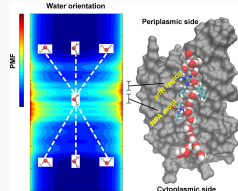
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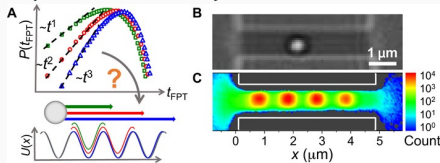
Zheng *et al.* 2023

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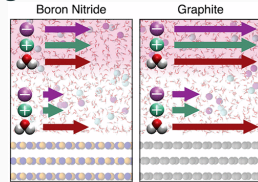
Padhi *et al.* 2017

## Experimental reality



Thornework *et al.* 2020

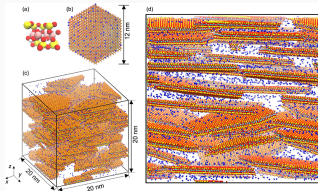
## New grounds



Helms *et al.* 2023

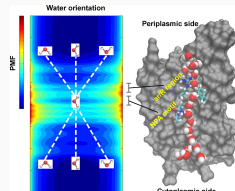
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## Soils



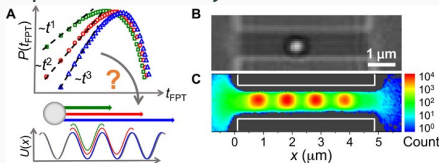
Zheng *et al.* 2023

## Cells



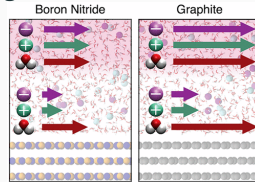
Padhi *et al.* 2017

## Experimental reality



Thorneywork *et al.* 2020

## New grounds



Helms *et al.* 2023

- There is no such thing as a bulk stationary fluid at the nanoscale.
- This is the regime where emerging technologies operate.

Coefficients might not be enough, can we do better?

## Classical coefficients framework

$$J_a = \sum_b L_{ab} F_b, \quad a, b = \text{fluid, solute, heat, charge...}$$

# Promoting coefficients to fields

## Classical coefficients framework

$$J_a = \sum_b L_{ab} F_b, \quad a, b = \text{fluid, solute, heat, charge...}$$

## Field-based framework

$$j_a(\mathbf{r}, t) = - \sum_b \int_V \int_{-\infty}^t \mathbf{R}_{ab}(\mathbf{r}, \mathbf{r}', t - t') \cdot \nabla \phi_b(\mathbf{r}', t') dt' d\mathbf{r}'$$

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$J_a \Rightarrow j_a(\mathbf{r}, t)$ : current density ( $a$ ) at position  $\mathbf{r}$  and time  $t$

$F_b \Rightarrow -\nabla \phi_b(\mathbf{r}', t')$ : local thermodynamic force ( $b$ ) at  $\mathbf{r}'$  and time  $t'$

$L_{ab} \Rightarrow \mathbf{R}_{ab}(\mathbf{r}, \mathbf{r}', t - t')$ : **generalized transport coefficient**

$\int$  Coupled responses through space-time convolution

# Averaging microscopic transport

Integrating  $R_{ab}(\mathbf{r}, \mathbf{r}', t)$  over space and/or time  
 $\equiv$  Averaging assuming homogeneous and/or constant forcing

Recovering the traditional coefficients

$$L_{ab} = \lim_{t \rightarrow \infty} \int_0^t \int_V \int_V R_{ab}(\mathbf{r}, \mathbf{r}', t) d\mathbf{r} d\mathbf{r}' dt ,$$

and many other *intermediate projections!*

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















What does  $R_{ab}(\mathbf{r}, \mathbf{r}', t)$  look like?

# $R_{ab}(r, r', t)$ : a high-dimensional object

	pressure $-\nabla P$	chemical pot. $-\nabla \mu_s$	temperature $-\nabla T$	electrical pot. $-\nabla V^{\text{el}}$
$\dot{j}_n$ fluid	$R_{nn}^{ij}(\vec{r}, \vec{r}', t)$	$R_{ns}^{ij}(\vec{r}, \vec{r}', t)$	$R_{nh}^{ij}(\vec{r}, \vec{r}', t)$	$R_{nc}^{ij}(\vec{r}, \vec{r}', t)$
$\dot{j}_s$ solute	$R_{sn}^{ij}(\vec{r}, \vec{r}', t)$	$R_{ss}^{ij}(\vec{r}, \vec{r}', t)$	$R_{sh}^{ij}(\vec{r}, \vec{r}', t)$	$R_{sc}^{ij}(\vec{r}, \vec{r}', t)$
$\dot{j}_h$ heat	$R_{hn}^{ij}(\vec{r}, \vec{r}', t)$	$R_{hs}^{ij}(\vec{r}, \vec{r}', t)$	$R_{hh}^{ij}(\vec{r}, \vec{r}', t)$	$R_{hc}^{ij}(\vec{r}, \vec{r}', t)$
$\dot{j}_c$ charge	$R_{cn}^{ij}(\vec{r}, \vec{r}', t)$	$R_{cs}^{ij}(\vec{r}, \vec{r}', t)$	$R_{ch}^{ij}(\vec{r}, \vec{r}', t)$	$R_{cc}^{ij}(\vec{r}, \vec{r}', t)$

$R_{ab}(r, r', t) \equiv \text{size ?}$

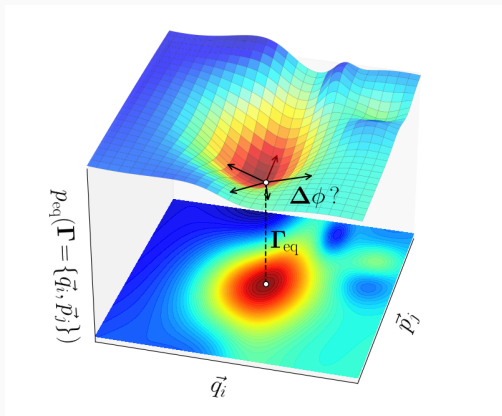
# $R_{ab}(r, r', t)$ : a high-dimensional object

	pressure $-\nabla P$	chemical pot. $-\nabla \mu_s$	temperature $-\nabla T$	electrical pot. $-\nabla V^{\text{el}}$
$j_n$ fluid				
$j_s$ solute				
$j_h$ heat				
$j_c$ charge				

$R_{ab}(r, r', t) \equiv 16 \times \mathcal{C}(\mathbb{R}^{3+3+1}, \mathbb{R}^{3 \times 3}) \equiv 16 \text{ tensor fields on } \mathbb{R}^7$

→ **MASSIVE!** How can we sample it?

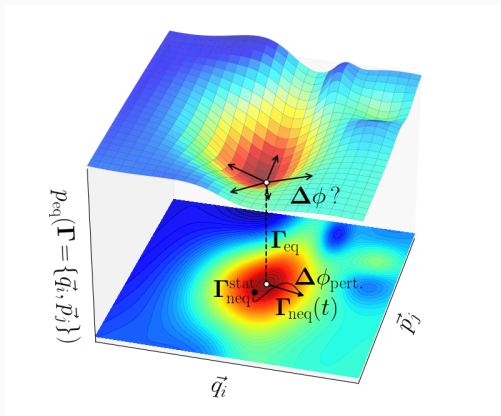
# Accessing local transport in high dimensions



# Accessing local transport in high dimensions

## Nonequilibrium MD

You apply and you measure



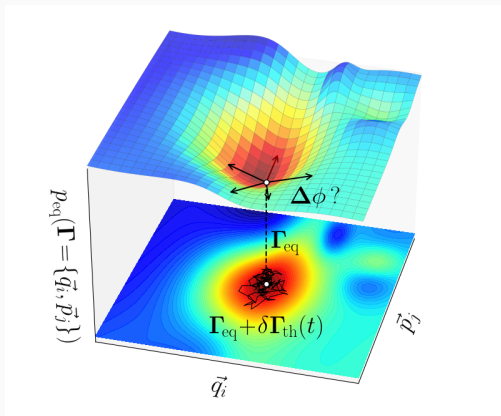
# Accessing local transport in high dimensions

## Nonequilibrium MD

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## Equilibrium MD

You let the system explore itself



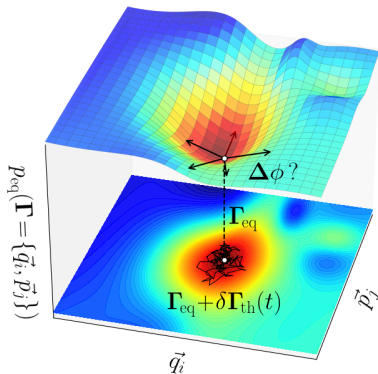
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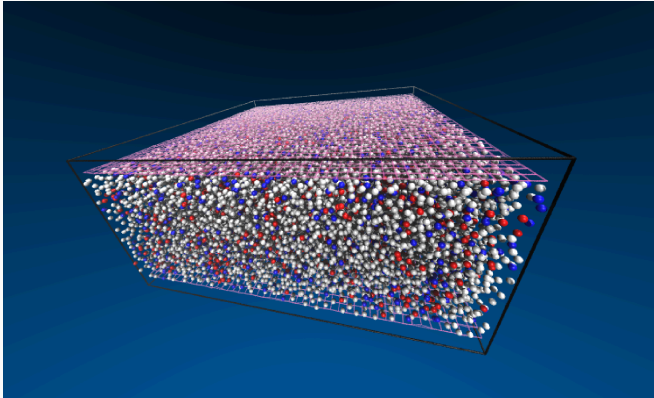


The average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process.

L. Onsager, 1931

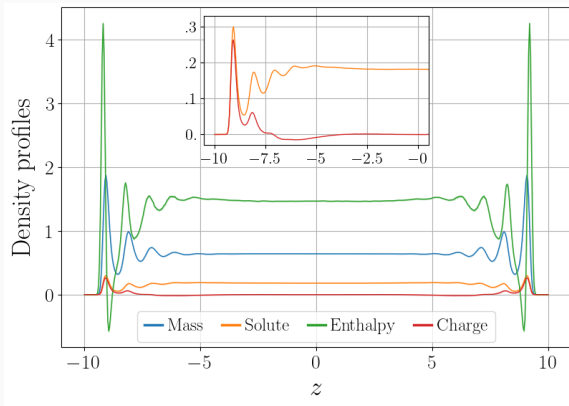
$$R_{ab}(r, r', t) = \frac{\langle j_a(r, t) \otimes j_b(r', 0) \rangle_{\text{eq}}}{k_B T}$$

# Molecular Dynamics simulations of confined fluid



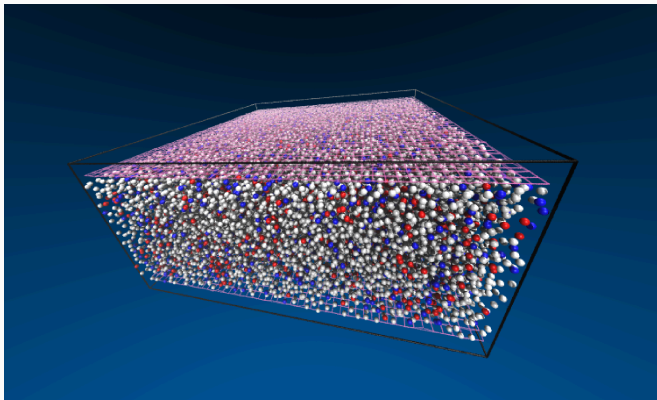
- Charged tertiary LJ fluid ( $\sim 30000$  atoms)
- $T = 1.4$ ,  $\rho_{\text{tot}} \sim 0.7$ ,  $V \sim 50 \times 50 \times 20$
- $\rho_s/\rho_{\text{tot}} \sim 0.25$ ,  $q_{\pm} = \pm 1$ ,  $\epsilon_r \epsilon_0 = 1$
- Thermalized solid with surface charge  $\Sigma = -0.1$

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# Molecular Dynamics simulations of confined fluid



Exploiting the effective 1D geometry:

$$\mathbf{j}(\mathbf{r}, t) \rightarrow j(z, t) = \frac{1}{S} \int_S \mathbf{j}(\mathbf{r}, t) \cdot \hat{\mathbf{e}}_{\parallel} d^2s$$

$$\begin{aligned} R_{ab}(\mathbf{r}, \mathbf{r}', t) \rightarrow R_{ab}(z, z', t) &= \frac{1}{S^2} \int_S \int_S [\hat{\mathbf{e}}_{\parallel} \cdot \mathbf{R}_{ab}(\mathbf{r}, \mathbf{r}', t) \cdot \hat{\mathbf{e}}_{\parallel}] d^2s d^2s' \\ &\equiv 16 \times \mathcal{C}(\mathbb{R}^3, \mathbb{R}) \equiv 16 \text{ scalar fields on } \mathbb{R}^3 \end{aligned}$$

# Beyond Poiseuille $R_{nn}(z, z', t)$

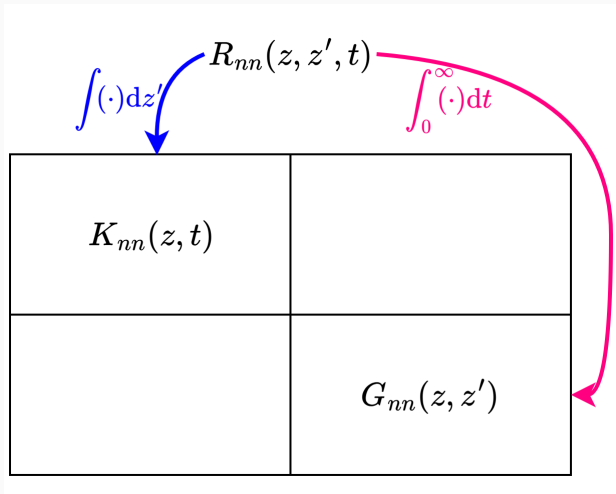
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$j_n$ fluid	$R_{nn}(z, z', t)$	$R_{ns}(z, z', t)$	$R_{nh}(z, z', t)$	$R_{nc}(z, z', t)$
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$j_h$ heat	$R_{hn}(z, z', t)$	$R_{hs}(z, z', t)$	$R_{hh}(z, z', t)$	$R_{hc}(z, z', t)$
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# Beyond Poiseuille $R_{nn}(z, z', t)$

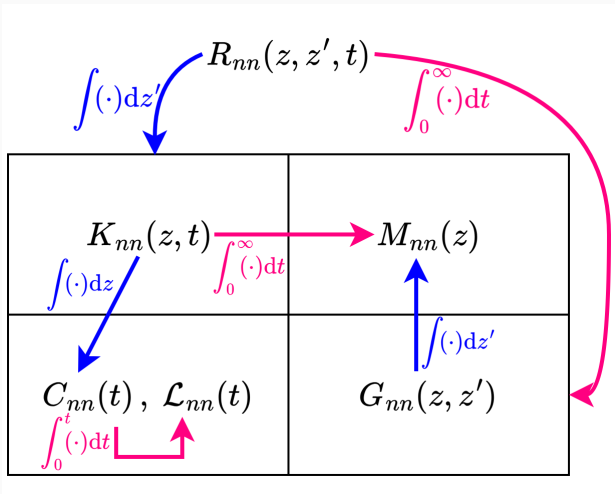
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$$R_{nn}(z, z', t)$$

# Beyond Poiseuille $R_{nn}(z, z', t)$

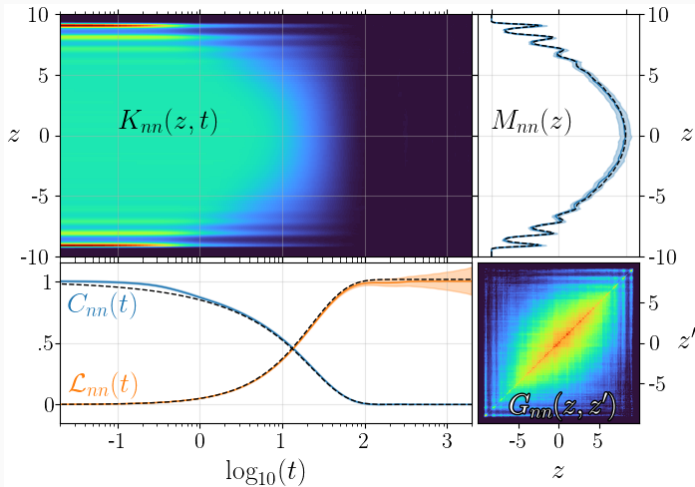


# Beyond Poiseuille $R_{nn}(z, z', t)$



$K_{nn}(z, t)$	$M_{nn}(z)$
$C_{nn}(t), \mathcal{L}_{nn}(t)$	$G_{nn}(z, z')$

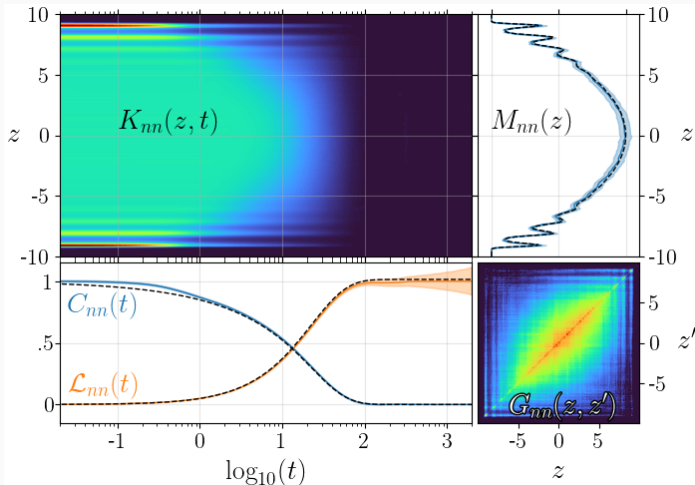
# Beyond Poiseuille $R_{nn}(z, z', t)$



• Space-time resolution of transport

• Layered structure close to interface

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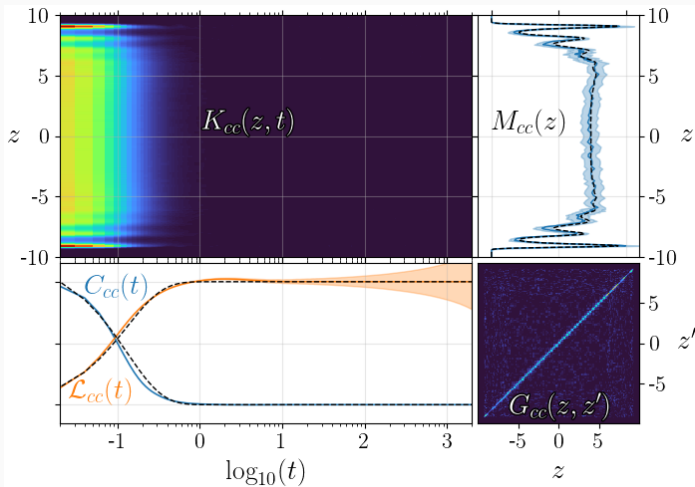


- Space-time resolution of transport
- Layered structure close to interface
- Position-dependent relaxation due to inhomogeneous density
- Slow viscous effects and large correlation time and length

# Beyond Nernst-Einstein $R_{cc}(z, z', t)$

	pressure $-\nabla P$	chemical pot. $-\nabla \mu_s$	temperature $-\nabla T$	electrical pot. $-\nabla V^{\text{el}}$
$j_n$ fluid	$R_{nn}(z, z', t)$	$R_{ns}(z, z', t)$	$R_{nh}(z, z', t)$	$R_{nc}(z, z', t)$
$j_s$ solute	$R_{sn}(z, z', t)$	$R_{ss}(z, z', t)$	$R_{sh}(z, z', t)$	$R_{sc}(z, z', t)$
$j_h$ heat	$R_{hn}(z, z', t)$	$R_{hs}(z, z', t)$	$R_{hh}(z, z', t)$	$R_{hc}(z, z', t)$
$j_c$ charge	$R_{cn}(z, z', t)$	$R_{cs}(z, z', t)$	$R_{ch}(z, z', t)$	$R_{cc}(z, z', t)$

# Beyond Nernst-Einstein $R_{cc}(z, z', t)$



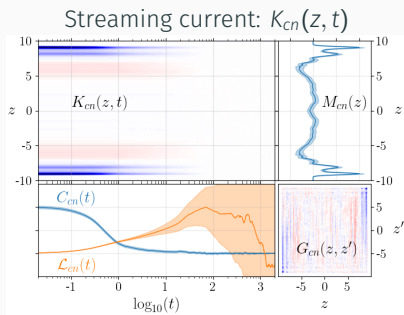
• Ionic friction and relaxation

• Fast dynamics and short correlation

# Streaming current $R_{cn}(z, z', t)$ and Electroosmotic flow $R_{nc}(z, z', t)$

	pressure $-\nabla P$	chemical pot. $-\nabla \mu_s$	temperature $-\nabla T$	electrical pot. $-\nabla V^{\text{el}}$
$j_n$ fluid	$R_{nn}(z, z', t)$	$R_{ns}(z, z', t)$	$R_{nh}(z, z', t)$	$R_{nc}(z, z', t)$
$j_s$ solute	$R_{sn}(z, z', t)$	$R_{ss}(z, z', t)$	$R_{sh}(z, z', t)$	$R_{sc}(z, z', t)$
$j_h$ heat	$R_{hn}(z, z', t)$	$R_{hs}(z, z', t)$	$R_{hh}(z, z', t)$	$R_{hc}(z, z', t)$
$j_c$ charge	$R_{cn}(z, z', t)$	$R_{cs}(z, z', t)$	$R_{ch}(z, z', t)$	$R_{cc}(z, z', t)$

# Streaming current $R_{cn}(z, z', t)$ and Electroosmotic flow $R_{nc}(z, z', t)$



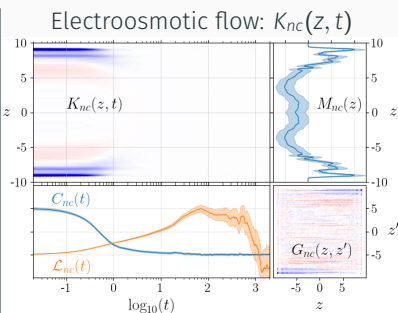
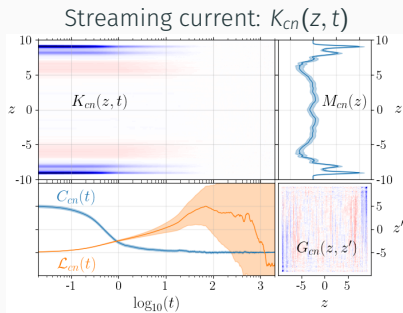
$$\nabla P \longrightarrow j_{\text{charge}}(z, t)$$

$$\downarrow \qquad \uparrow$$

$$\text{flow} \longrightarrow \text{charge drift}$$

Uniform drift of charge carriers

# Streaming current $R_{cn}(z, z', t)$ and Electroosmotic flow $R_{nc}(z, z', t)$



$$\nabla P \longrightarrow j_{\text{charge}}(z, t)$$

$$\downarrow \qquad \uparrow$$

$$\text{flow} \longrightarrow \text{charge drift}$$

Uniform drift of charge carriers

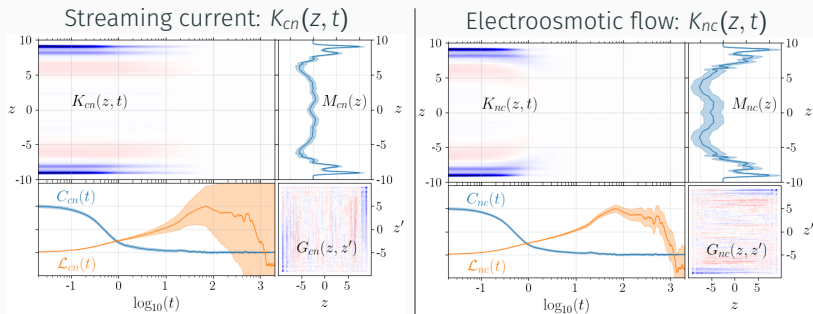
$$\nabla V^{\text{el}} \longrightarrow j_{\text{fluid}}(z, t)$$

$$\downarrow \qquad \uparrow$$

$$\text{charge sep.} \longrightarrow \text{stress}$$

Viscous diffusion

# Streaming current $R_{cn}(z, z', t)$ and Electroosmotic flow $R_{nc}(z, z', t)$



$$\nabla P \longrightarrow j_{\text{charge}}(z, t)$$

$$\downarrow \qquad \uparrow$$

$$\text{flow} \longrightarrow \text{charge drift}$$

Uniform drift of charge carriers

$$\nabla V^{\text{el}} \longrightarrow j_{\text{fluid}}(z, t)$$

$$\downarrow \qquad \uparrow$$

$$\text{charge sep.} \longrightarrow \text{stress}$$

Viscous diffusion

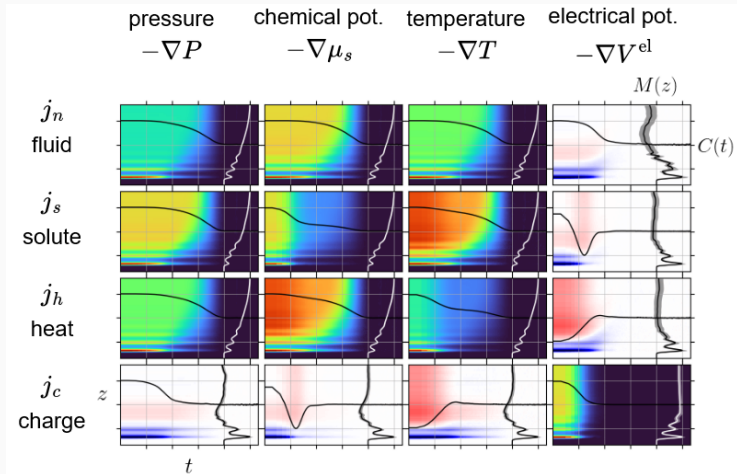
$$K_{cn}(z, t) \neq K_{nc}(z, t)$$

«Spatial breakdown» of Onsager reciprocal symmetry

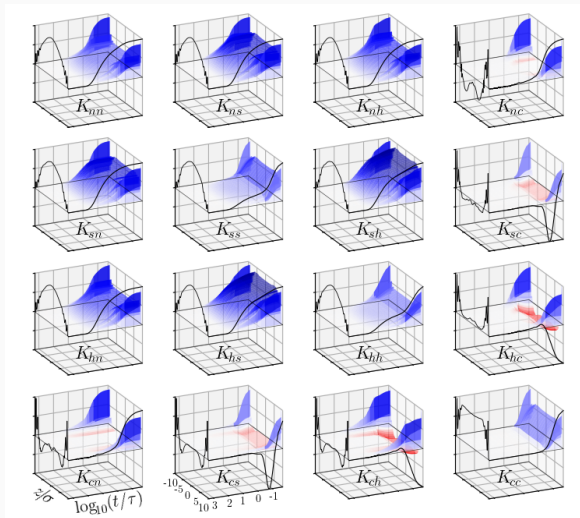
# 4 × 4 coupled kernel

	pressure $-\nabla P$	chemical pot. $-\nabla \mu_s$	temperature $-\nabla T$	electrical pot. $-\nabla V^{\text{el}}$
$j_n$ fluid	$K_{nn}(z, t)$	$K_{ns}(z, t)$	$K_{nh}(z, t)$	$K_{nc}(z, t)$
$j_s$ solute	$K_{sn}(z, t)$	$K_{ss}(z, t)$	$K_{sh}(z, t)$	$K_{sc}(z, t)$
$j_h$ heat	$K_{hn}(z, t)$	$K_{hs}(z, t)$	$K_{hh}(z, t)$	$K_{hc}(z, t)$
$j_c$ charge	$K_{cn}(z, t)$	$K_{cs}(z, t)$	$K_{ch}(z, t)$	$K_{cc}(z, t)$

# $4 \times 4$ coupled kernel

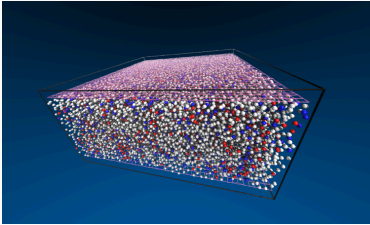


# Reconstructing time-dependent profiles

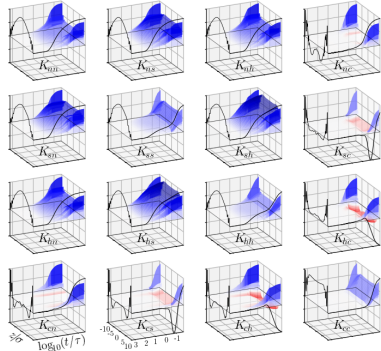


Step-response to uniform forcings

# Take-home message(s)

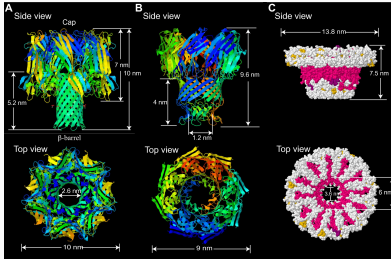


$$R_{ab}(r, r', t) = \frac{\langle j_a(r, t) \otimes j_b(r', 0) \rangle_{\text{eq}}}{k_B T}$$



- 1 Nanoscale transport is spatially and temporally structured.
- 2 Transport coefficients can be promoted to space-time fields.
- 3 Fluctuations provide efficient access to these properties.

Can  $R_{ab}(r, r', t)$  be engineered?

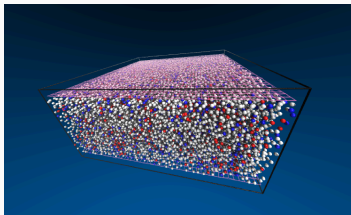
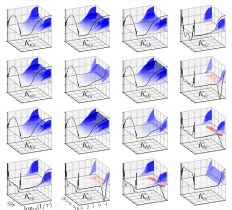


Feng et al. 2015

Tailored energy storage and recovery  
Selective water transport & desalination  
Tunable electrohydrodynamics  
Iontronics & Neuromorphic computing



# Take-home message and outlook



Confinement reveals structure

Coefficients are projections

Music is hidden in the noise

Room for structure-aware inference

Towards exciting technologies



Thank you for your attention

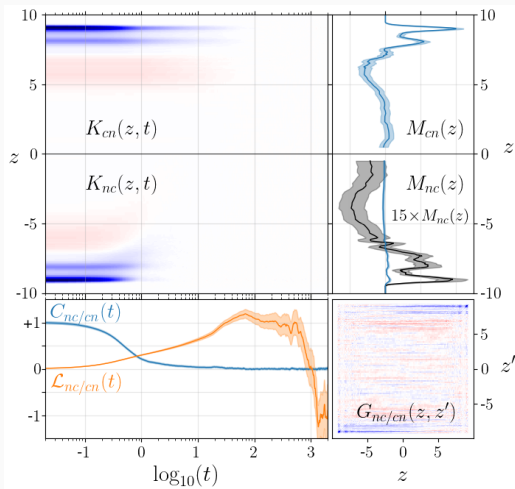
*mh7003@princeton.edu*



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# Did we really violate Onsager reciprocity?



$$R_{ab}(z, z', t) = R_{ba}(z', z, t)$$

$$\implies L_{ab} = L_{ba}$$

$$\not\Rightarrow K_{ab}(z, t) = K_{ba}(z, t)$$

$$\not\Rightarrow M_{ab}(z) = M_{ba}(z)$$

$$\implies \text{Onsager is safe}$$

$$R_{ab}(z, z', t) = \beta \langle j_a(z, t) j_b(z', 0) \rangle_{\text{eq}}, \quad L_{ab} = \int_0^\infty \iint R_{ab}(z, z', t) dz dz' dt$$

$$R_{ab}(z, z', t) = R_{ba}(z', z, -t) = R_{ba}(z', z, +t)$$

# The Real Onsager matrix

