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From pore- to membrane-scale filtration: a homogenization perspective

EPFL

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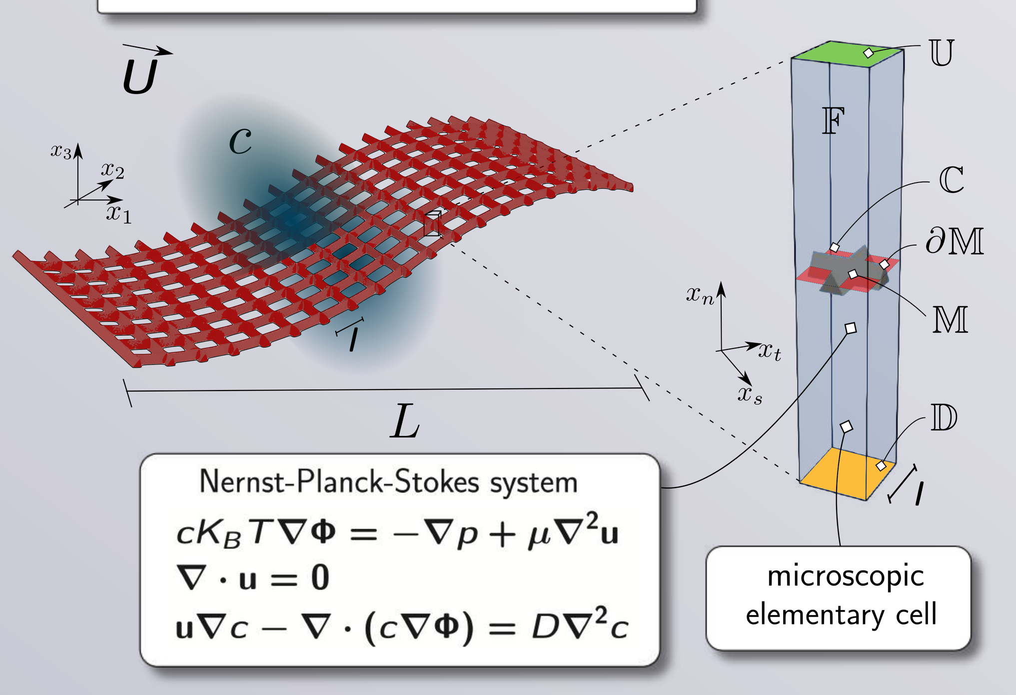
EPFL-STI-IGM-LFMI

A powerful tool for membrane flows modelling: multiscale homogenization

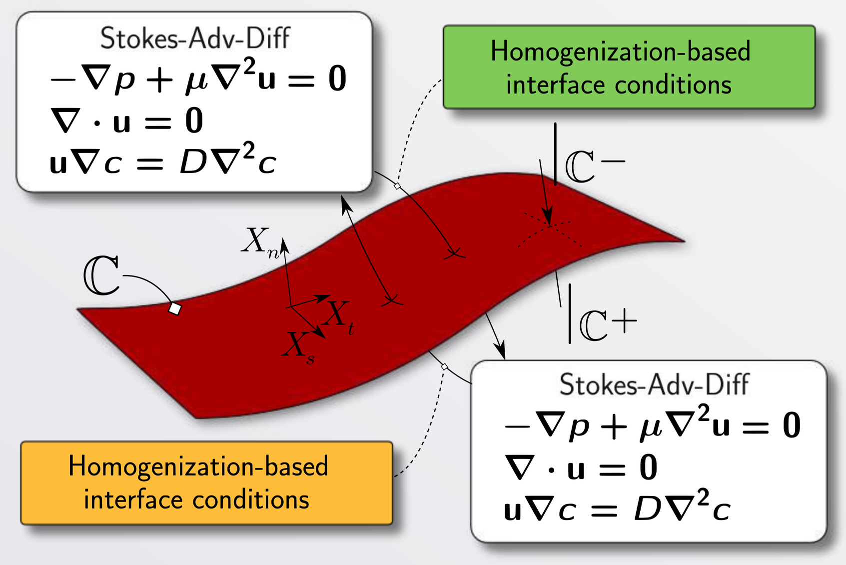
PORE-SCALE DESCRIPTION

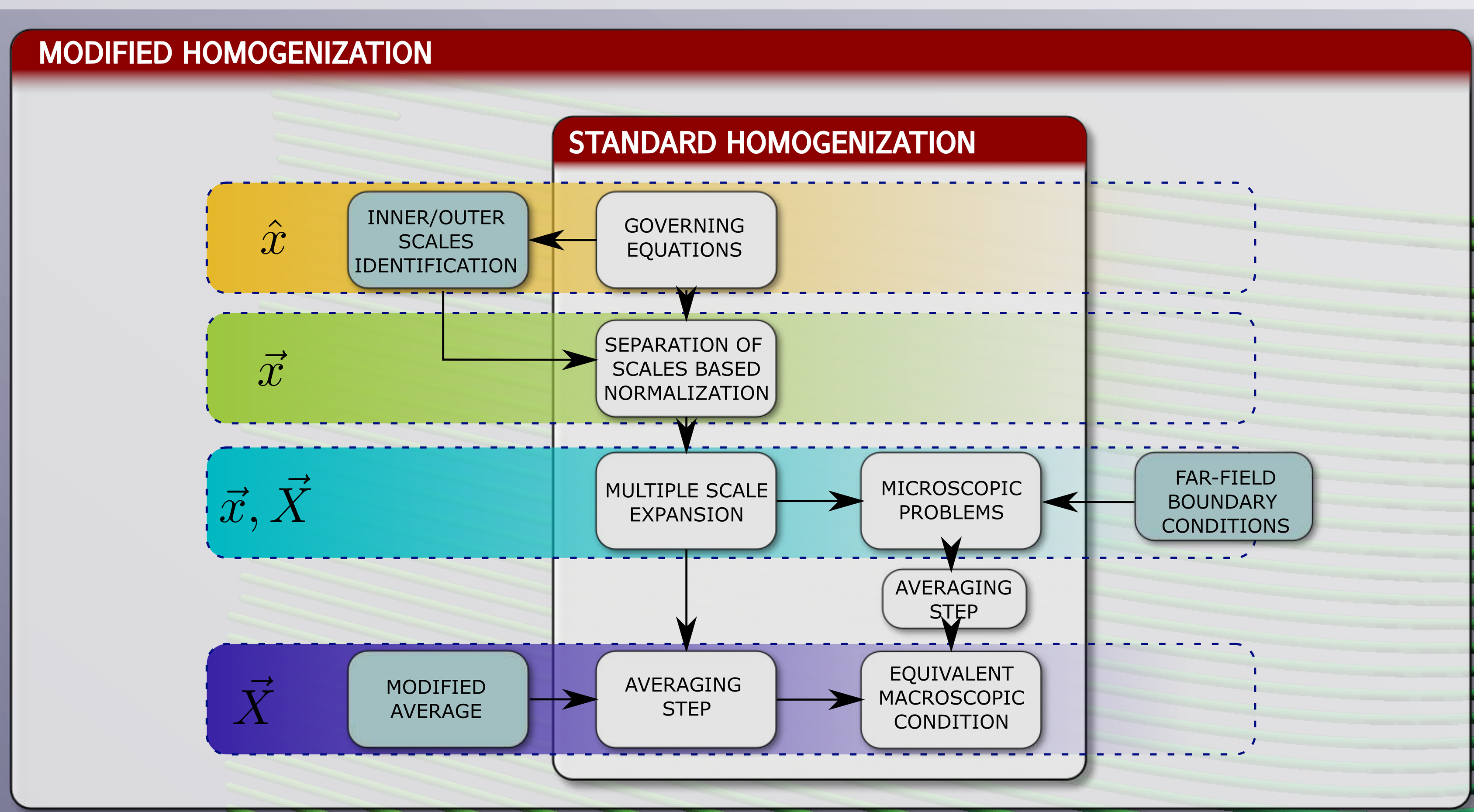


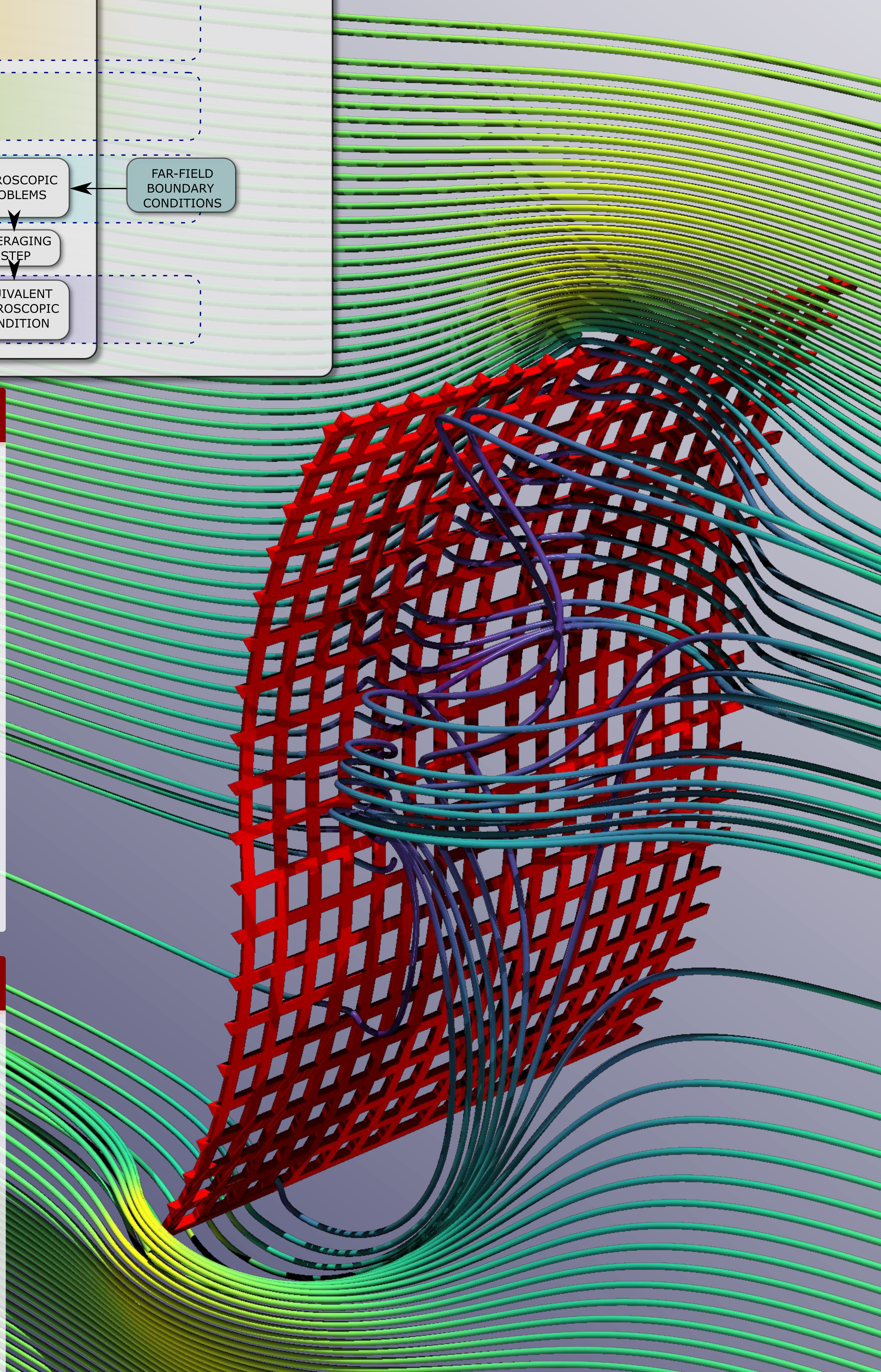
Osmotic flow of a solvent of density ρ and viscosity μ and a solute of diffusivity D through a thin porous structure of chemical potential $K_BT\Phi$ via the Nernst-Planck-Stokes system. Homogenization works like a selective magnification lens and provides interface conditions valid on a fictitious macroscopic membrane $\mathbb{C}$.

HOMOGENIZATION

MEMBRANE-SCALE DESCRIPTION







Effective stress and flux jump conditions

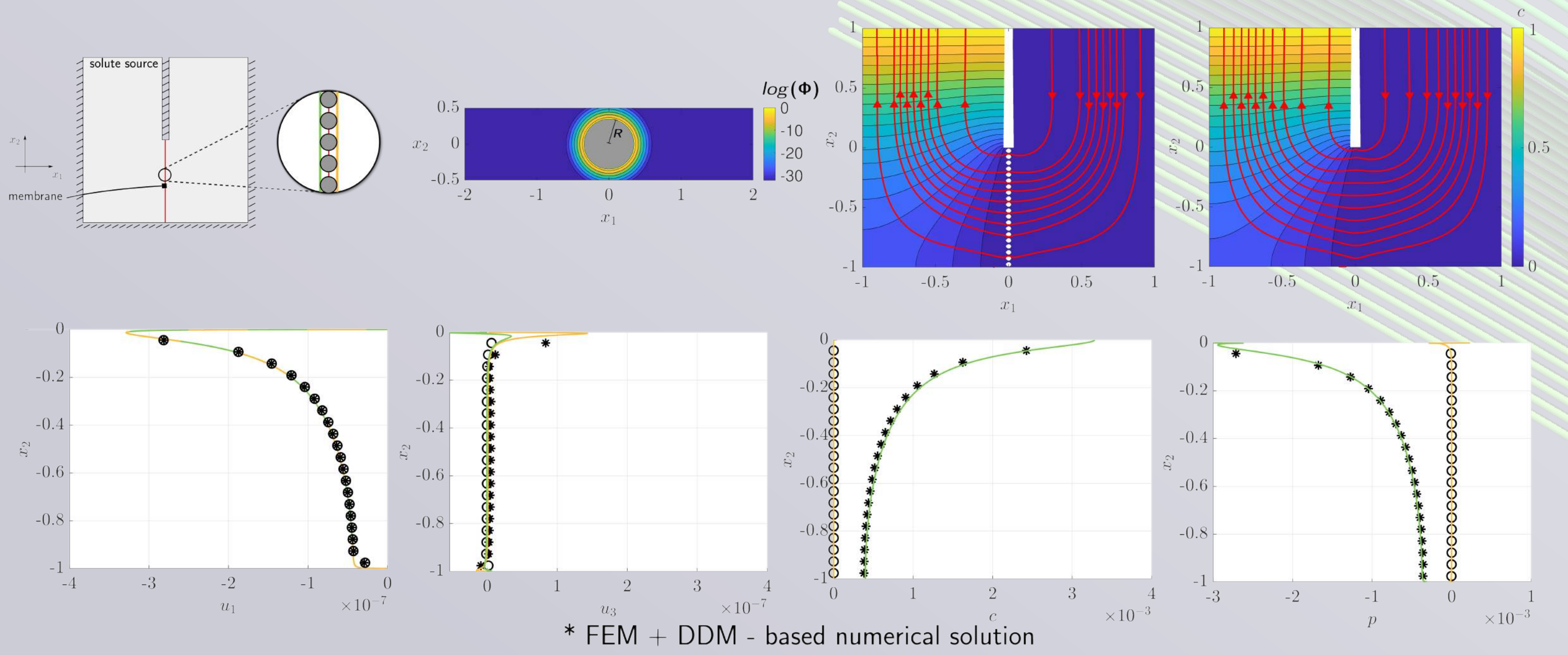
The solvent velocity and pressure, and solute concentration fields, $\mathbf{u}$, p and c, satisfy

$$\begin{cases} \mathbf{u}|_{\mathbb{C}^-} = \mathcal{M}^- : \boldsymbol{\Sigma}|_{\mathbb{C}^-} + \mathcal{N}^- : \boldsymbol{\Sigma}|_{\mathbb{C}^+} + \alpha^- \mathbf{F}|_{\mathbb{C}^-} + \beta^- \mathbf{F}|_{\mathbb{C}^+} \\ c|_{\mathbb{C}^-} = \mathcal{T}^- \cdot \mathbf{F}|_{\mathbb{C}^-} + \mathcal{Y}^- \cdot \mathbf{F}|_{\mathbb{C}^+} \\ \mathbf{u}|_{\mathbb{C}^+} = \mathcal{M}^+ : \boldsymbol{\Sigma}|_{\mathbb{C}^-} + \mathcal{N}^+ : \boldsymbol{\Sigma}|_{\mathbb{C}^+} + \alpha^+ \mathbf{F}|_{\mathbb{C}^-} + \beta^+ \mathbf{F}|_{\mathbb{C}^+} \\ c|_{\mathbb{C}^+} = \mathcal{T}^+ \cdot \mathbf{F}|_{\mathbb{C}^-} + \mathcal{Y}^+ \cdot \mathbf{F}|_{\mathbb{C}^+} \end{cases}$$

where $\boldsymbol{\Sigma}|_{\mathbb{C}^\pm} = -\mathbf{I}p|_{\mathbb{C}^\pm} + \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)|_{\mathbb{C}^\pm}$ and $\mathbf{F}|_{\mathbb{C}^\pm} = \mathbf{u}c - D\nabla c$ are the solvent stresses and solute fluxes and $\mathcal{M}^\pm$, $\mathcal{N}^\pm$, $\alpha^\pm$, $\beta^\pm$, $\mathcal{T}^\pm$ and $\mathcal{Y}^\pm$ are upward $(\cdot^-)$ and downward $(\cdot^+)$ spatial averages of microscopic quantities, representing effective properties of the membrane. These quantities, computed once and for all for a given membrane within the microscopic elementary cell, allow a *predictive* determination of the *mobility* matrix. The macroscopic conditions, valid on $\mathbb{C}^\pm$, quantify jumps in the solvent velocity, pressure, and stresses and in the solute concentration and fluxes.

Predictive macroscopic modelling of osmotic flows*

- Test case: U-shaped container split by a membrane at $Re = \frac{\rho U l}{\mu} = 0 = Pe = \frac{Ul}{D}$ and $\Phi = A(1 - tanh\frac{\sqrt{x_t^2+x_n^2}-R}{\delta})$, $A = 10, \delta = 10^{-3}$.



* FEM + DDM - based numerical solution

References

[1] Zampogna, Gallaire 2020 *JFM*, 892, A9.
[2] Ledda, Boujo, Camarri, Gallaire, Zampogna 2021 *JFM*, 927 A31.
[3] Zampogna, Ledda, Gallaire 2022 *PoF*, 34, 083113.
[4] Zampogna, Ledda, Wittkowski, Gallaire 2023 *JFM*, 970, A39.

Conclusion & Perspectives

- We developed and validated an effective macroscopic model describing osmotic flows across thin microstructured porous membranes
- We know the link between the mobility matrix and the microscopic membrane properties, i.e. we can implement objective-based optimization strategies (done for the hydrodynamics problem in **[2]**)
- Extension to electro-osmosis and to membranes with (sub-)nanoscopic pores are foreseen
- Establish a link between our model and the Spiegler-Kedem-Kaltchalsky equations

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