# Dynamics of charged fluids in nanodevices. Grant 3720

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## Purpose of the visit . March 5th- April 7th

The main purpose of the visit at the University of Barcelona was to establish a collaboration between Umberto Marini Bettolo Marconi and Ignacio Pagonabarraga on subjects related to charge transport in electrolytes through membranes and nanochannels, a field in rapid evolution, nowadays.

## Description of the work carried during the visit

We investigated a theoretical and numerical framework to study transport in non-uniform charged systems and the interplay between structural and dynamical properties varying on the atomic scale. The method bridges different areas of liquid state theory, namely kinetic and density functional theory and is implemented numerically based on the evolution of the singlet phase space distribution function. The resulting transport equation is a self-consistent dynamical equation applicable to generic fluids and mixtures, and it is

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particularly useful when studying systems under extreme confinement, where standard hydrodynamics becomes questionable. In a mixture representative of electro-osmotic and electro-phoretic flows, we study the competition between density layering, the role of electrostatic forces and the organization of the velocity field.

## Main results obtained

Simulations show how excluded volume affects flow rates at different Debye lengths, surface charge and degree of confinement, together with discriminating electro-osmotic from electro-phoretic mobility at varying packing fractions. A clear-cut distinction between micro and nanoscopic behavior emerges when the geometry and/or the surface charge is modulated, where non-trivial characteristic curves are observed and interpreted.

## Future work and collaboration

The visit has been extremely useful and we are planning to continue the collaboration.

With Prof. Ignacio Pagonabarraga and Dr. Simone Melchionna we shall conduct further studies about the behavior of electrolytes in membrane channels by means of the so called Planck-Nernst-Poisson theory in the case where the channels have non uniform shapes. The techniques we are using are similar to those employed to derive the so called Fick-Jacobs equation, where starting from a three dimensional model one derives an effective one-dimensional equation for the concentration field. We have already some result which show the importance of the geometry and interpret these by means of entropic forces.

## Future publications

The results of these investigations will be concluded soon and form the subject of a forthcoming publications.