Outline

3-D Quantum Mechanical Simulation of Nano-MOSFETs vs. Electro-Magnetic simulation

The transverse mode representation

Applications to

- **nMOS/pMOS I-V characteristics**
- **Analysis of a super-steep subthreshold slope MOSFET**

Analogies to RCWA EM simulation

- **Application to solar-cell analysis**

From Monte Carlo Device Simulation to Ionic Transport through Biological and Synthetic Nano-Scale Channels

NUMERICAL SIMULATION OF ION TRANSPORT THROUGH ION CHANNELS AND SOLID-STATE NANOPORES

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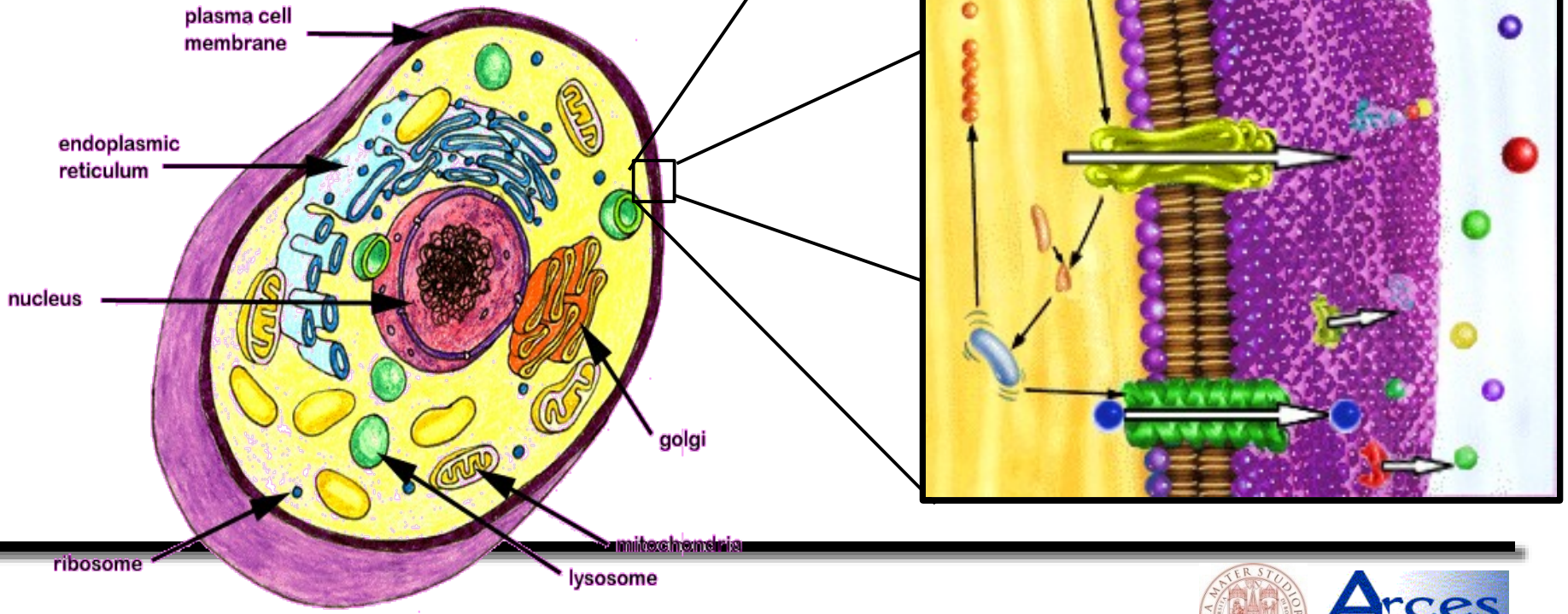
Particle based simulation

- Particle based simulation has been largely applied to the analysis of MOSFETs since mid 80's
  - Hot Carriers
  - Quasi-Ballistic Effects
  - 2-D transport in ultra-thin SOI MOSFETs
- Competences acquired in the field of MOSFET simulation can be transferred to other fields
- The case for ion transport in cellular ion channels and nanopores

ION CHANNELS

- Ion channels are pore-forming proteins across the cell membrane that allow the cell to exchange ions with the extracellular environment
  - Not simple pores but switches
  - Several gating mechanisms
  - High selectivity
  - High throughput
  - ...

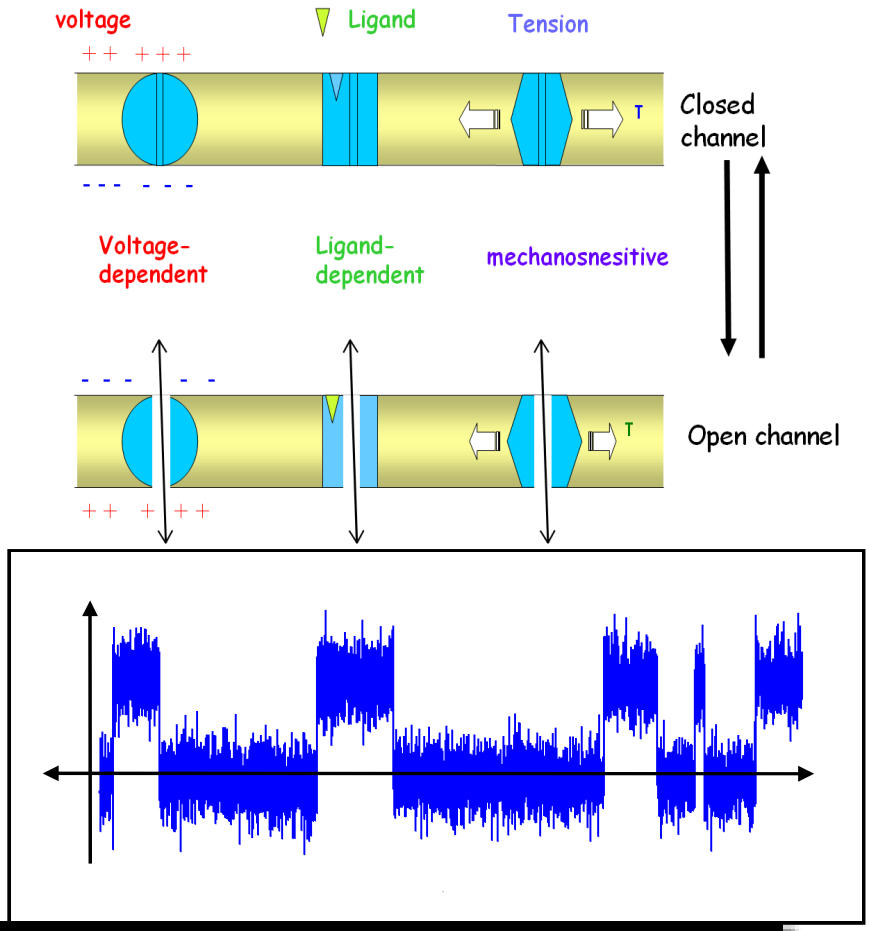


ION CHANNELS

- Ion channels are classified by the gating mechanism that determines their permeability

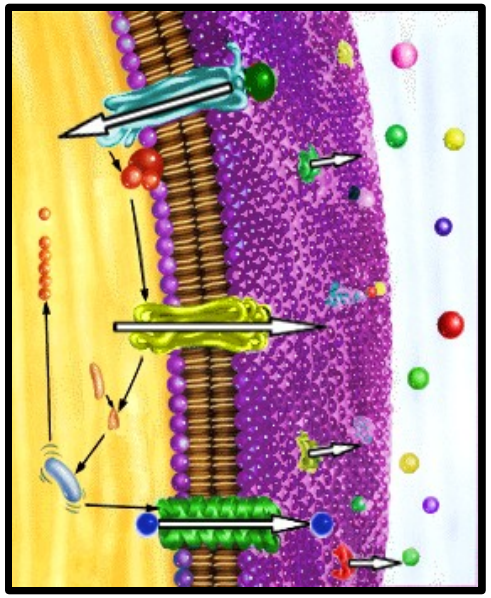
- Voltage-dependent
- Ligand-dependent
- Mechanosensitive channels

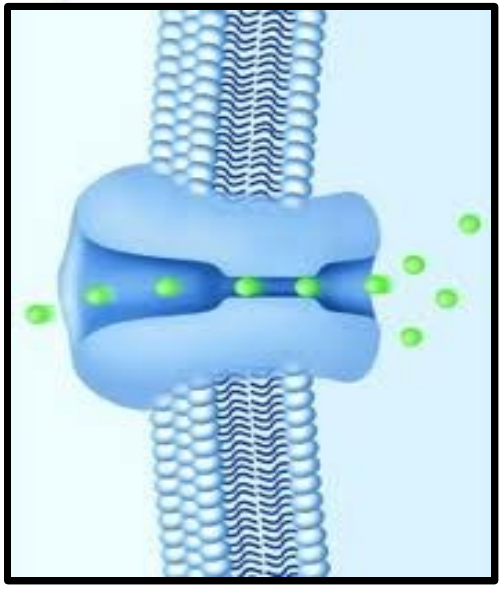
- Open and closed states are stochastic events determined by the gate mechanism
- Usually for a single channel:
- Conductance of open state has a typical mean value
- When a constant transmembrane potential is applied the current becomes a two-level random signal (RTS)

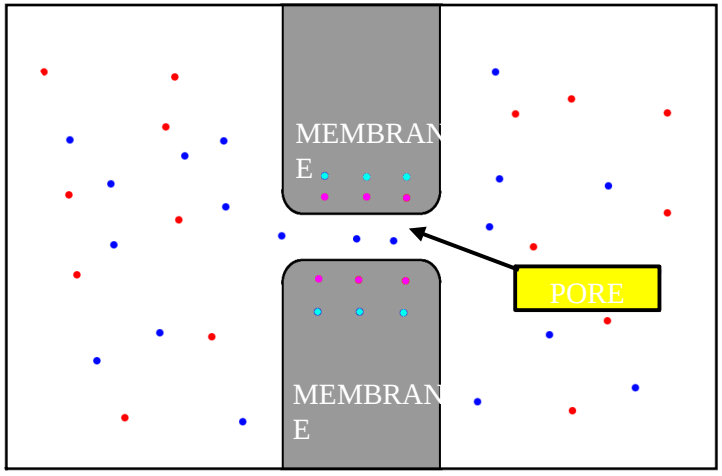


SIMULATION DOMAIN

- A membrane separates two ionic baths
- Ions can cross the membrane only through the pore
- Rotational symmetry

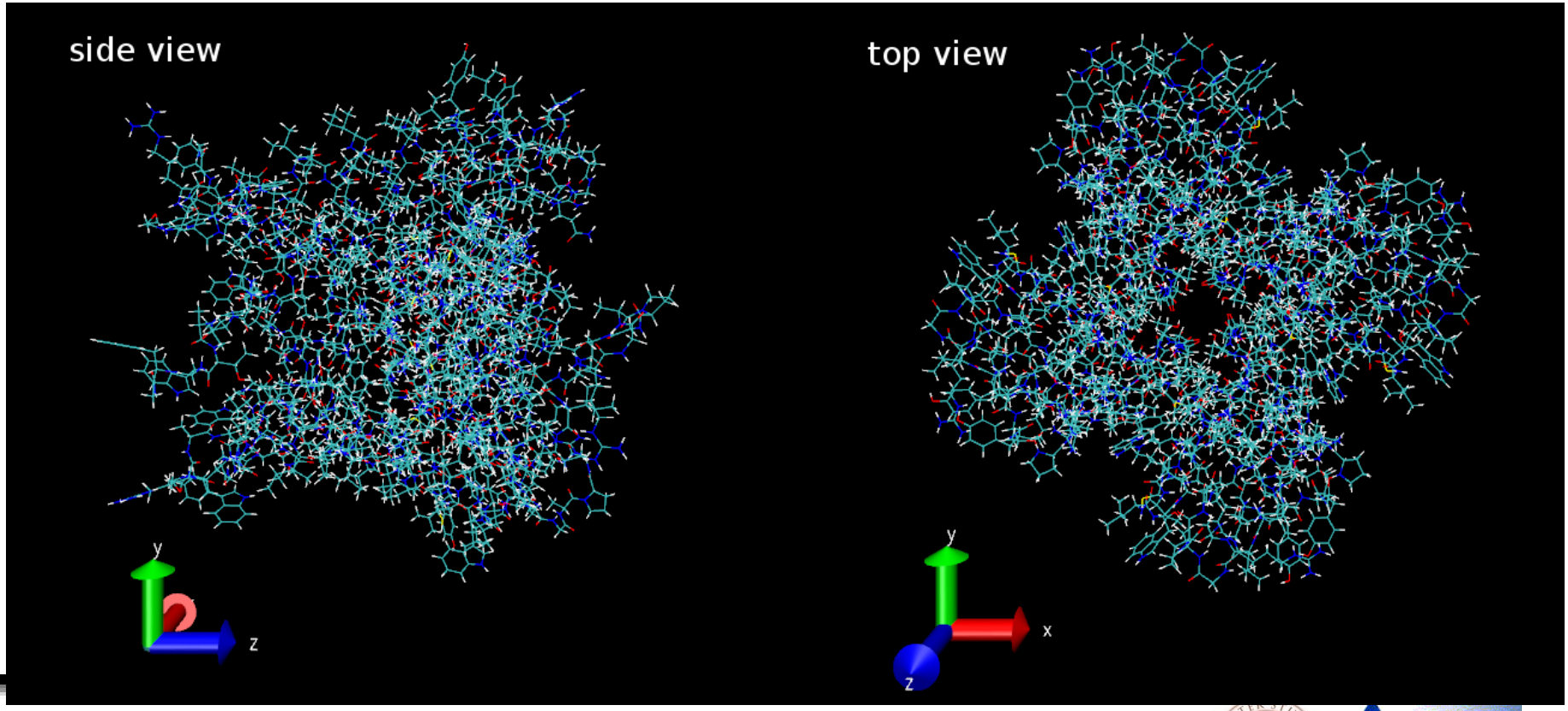






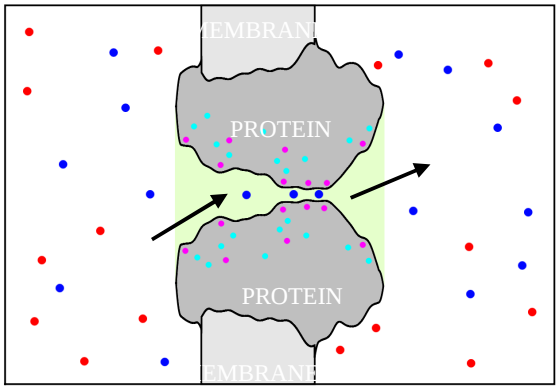
SIMULATION DOMAIN GENERATION

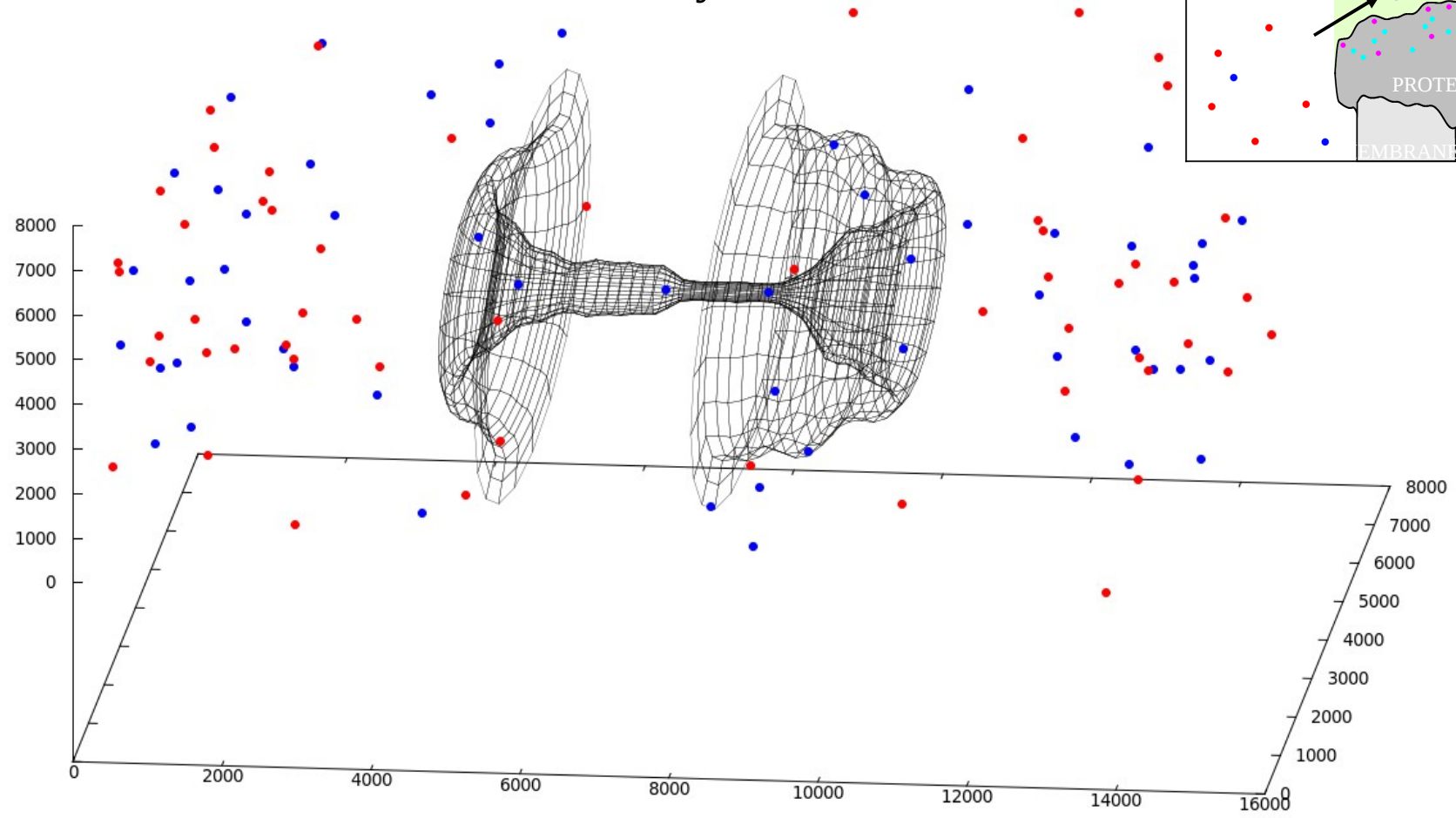
- For a synthetic nanopore the simulation domain is built imposing geometrical constraints
- An ion channel is defined by the charge distribution of the protein and the characteristics of the membrane



SIMULATION DOMAIN

- Phase boundary is determined by the charge distribution of the channel and the membrane
- Ions cannot cross the boundary





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SIMULATION APPROACHES

- Molecular Dynamics (MD)
  - Interactions between every couples of atoms in the system are taken into account
  - Highly accurate
  - Computationally too expensive

- Poisson-Nernst-Planck Approach (PNP)
  - Based on continuum charge distribution
  - Became more and more critical when dimensions of the channel decrease
  - Loss of characteristic effects (gating and selectivity)

- Brownian Dynamics (BD)
  - Something in between..

BROWNIAN DYNAMICS

- Something in between MD and PNP
- Only the trajectories of the ions are modeled
- Water molecules trajectories are neglected
- Interactions between ions and waters are included trough a friction force and random forces (collisions) acting on the ions
- Ions trajectories are generated according to the Langevin's equation:

$$m_i \frac{d\vec{v}_i}{dt} = -q_i \frac{dV_i}{d\vec{r}_i} - \gamma_i \frac{d\vec{r}_i}{dt} + \vec{F}_R(t)$$

Force acting on ion i

Force due to the electric field

Force due to friction with surrounding water

collisions with surrounding water

BROWNIAN DYNAMICS

- Only the trajectories of the ions are modeled
- Water molecules trajectories are neglected
- The dynamics of ions is described by Langevin's equation:

$$m_i \dot{v}_i(t) = -m_i \gamma_i v_i(t) + F_i(r(t)) + R_i(t)$$

- Ion trajectories are computed according according Verlet algorithm [1]:

$$x(t_n + \Delta t) = x(t_n)\left[1 + e^{-\gamma \Delta t}\right] - x(t_n - \Delta t)\, e^{-\gamma \Delta t}$$
$$+ m^{-1} F(t_n)(\Delta t)^2 (\gamma \Delta t)^{-1}\left[1 - e^{-\gamma \Delta t}\right]$$
$$+ m^{-1} \dot{F}(t_n)(\Delta t)^3 (\gamma \Delta t)^{-2}\left[1/2\, \gamma \Delta t\left[1 + e^{-\gamma \Delta t}\right] - \left[1 - e^{-\gamma \Delta t}\right]\right]$$
$$+ X_n(\Delta t) + e^{-\gamma \Delta t} X_n(-\Delta t) + O\left[(\Delta t)^4\right]$$

[1] Van Gunsteren and Berendsen, Algorithms for *Brownian dynamics* (Molecular Physics Vol. 45, No. 3,1982, 637-647)

ELECTROSTATICS

POISSON EQUATION

$$\nabla^2 \varphi(r) = -\frac{\rho(r)}{\varepsilon_0 \varepsilon(r)}$$

Multiple dielectrics – inhomogeneous media

$$\varepsilon_0 \nabla \cdot [\varepsilon(r) \nabla \varphi(r)] = -\rho(r)$$

Introducing the electric field and the polarization

$$E(r) = -\nabla \varphi(r) \qquad P(r) = (\varepsilon(r) - 1)\varepsilon_0 E(r)$$

Poisson equation takes the form:

$$\varepsilon_0 \nabla \cdot E(r) = \rho(r) - \nabla \cdot P(r)$$

ELECTROSTATICS

Introducing the polarization charge density: $h(r) = -\nabla \cdot P(r)$

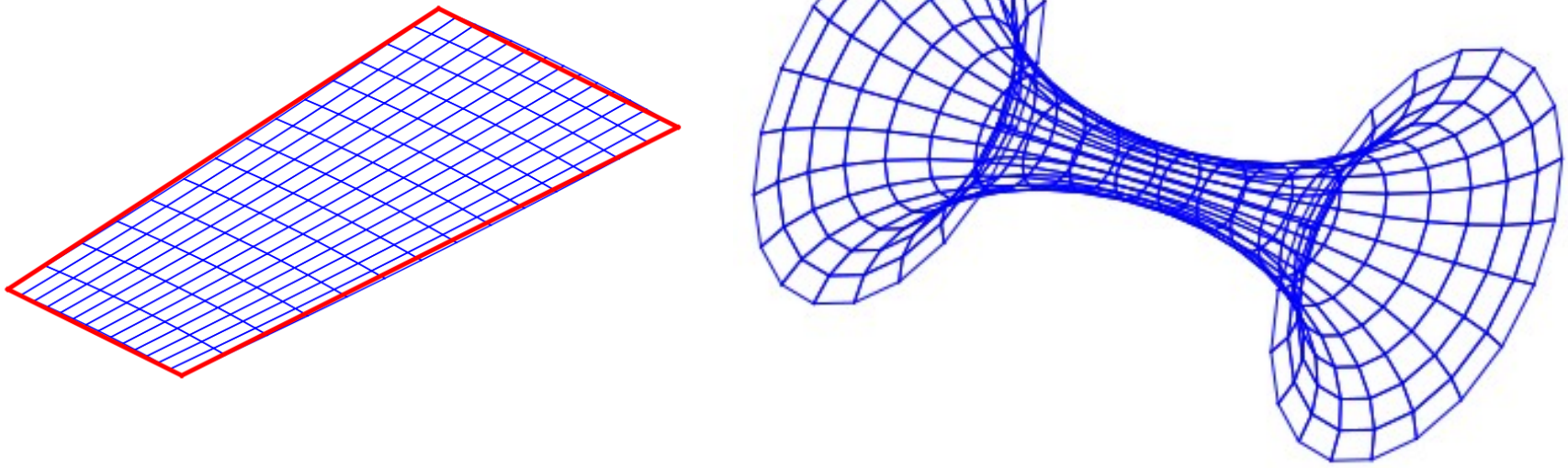
And substituting it in the Poisson equation, we obtain

$$h(r) = \frac{1-\varepsilon(r)}{\varepsilon(r)}\rho(r) - \varepsilon_0 \frac{\nabla \varepsilon(r)}{\varepsilon(r)} \cdot E(r)$$

- **Polarization induced charges are calculated according to the ICC method [D. Boda, et al., *Phys. Rev. E*, 69, 046702, 2004.]**
- **Calculation of *h(r)* is performed numerically on a discretization grid for the surface boundaries where discontinuity of permittivity occurs.**

ICC – Discretization of surface boundaries

- ICC methods work on an approximation of the phase boundary
- Surface elements are called “tiles” and can be flat or curved
- Tiles can be divided in subtiles
-



ELECTROSTATICS

• Once h(r) is calculated, we can solve the particle-particle electrostatic problem by superimposing several contributions

Total electric field

Electric field generated by fixed charges in the membrane

Electric field generated by other ions in the system (Coulombic term)

$$\vec{E}_i = \vec{E}_{S,i} + \vec{E}_{FC,i} + \vec{E}_{EXT,i} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \vec{E}_{C,i} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \vec{E}_{I,i}$$

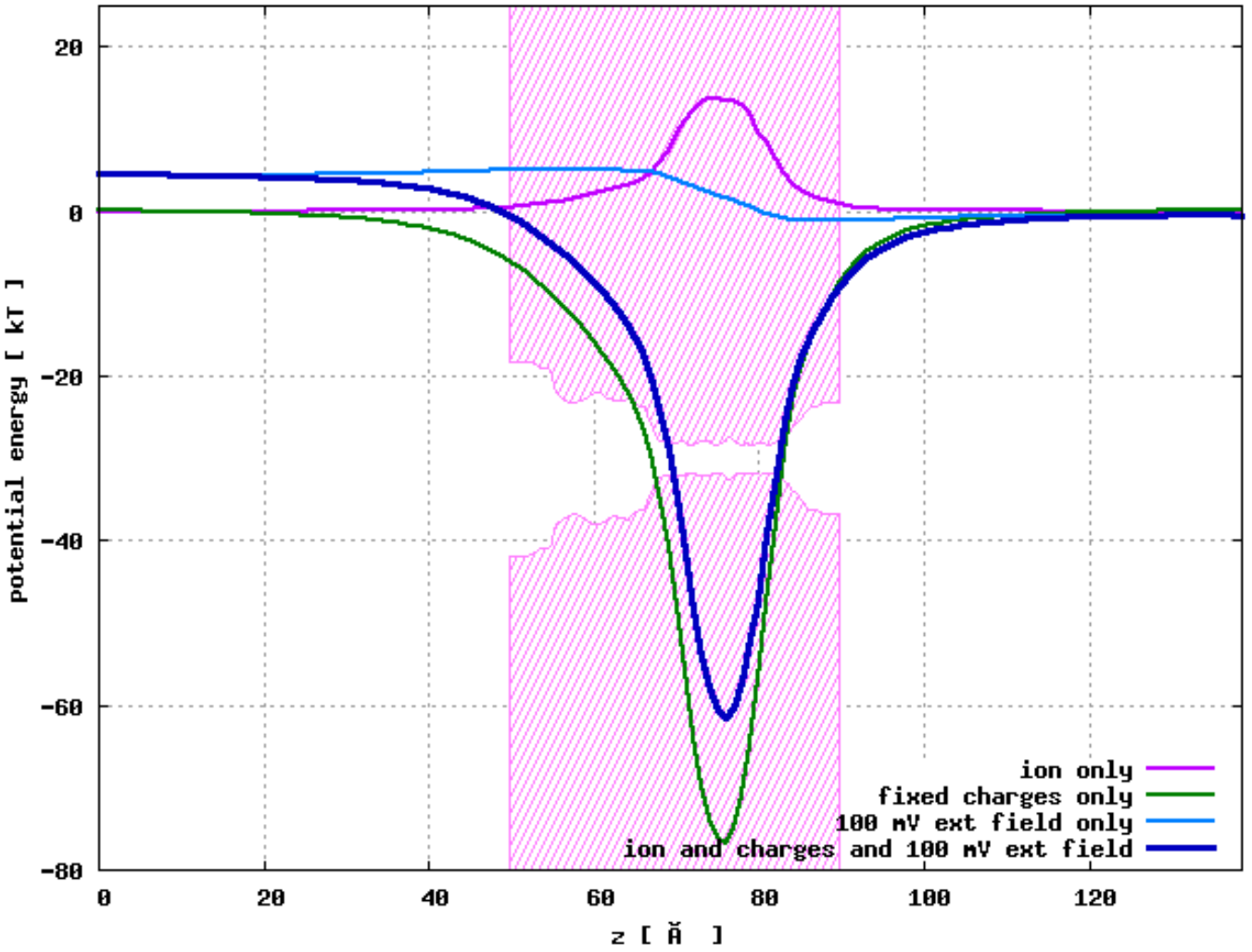
Self-induced electric field

Electric field generated by an applied transmembrane potential

Electric field generated by other ions in the system (polarization term)

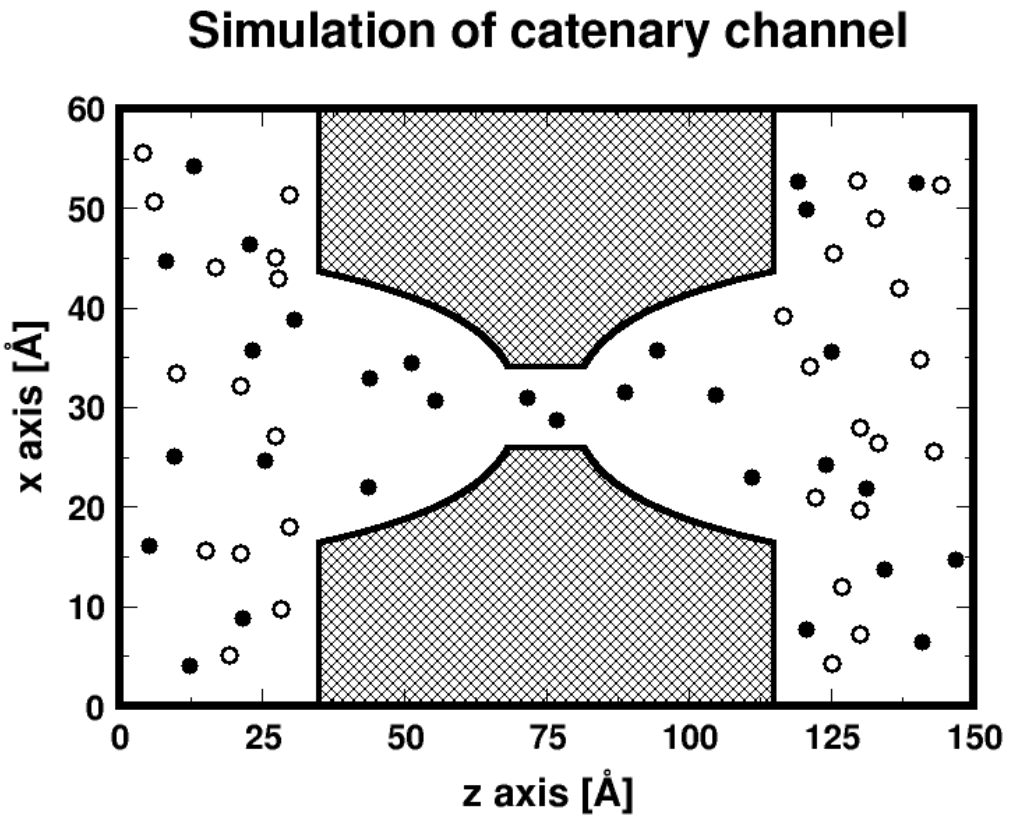
ELECTROSTATICS

- Total potential energy



TEST CHANNELS – CATENARY CHANNEL

- The simulator has been tested with catenary channel test case [3]:



[3] M. Hoyles et al., *Computer simulation of ion conductance in membrane channels* (Phys. Rev. E. 58:3654-3661, 1998)

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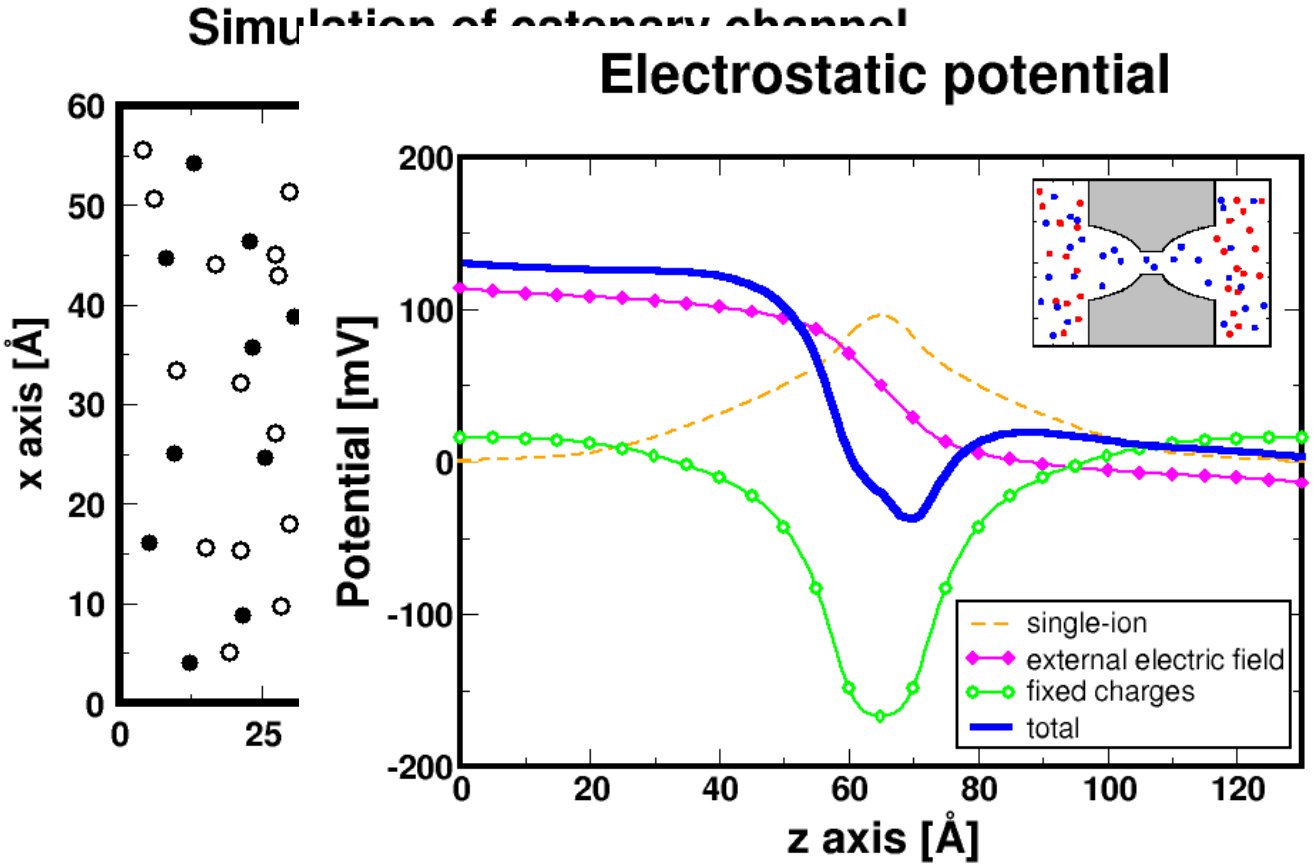

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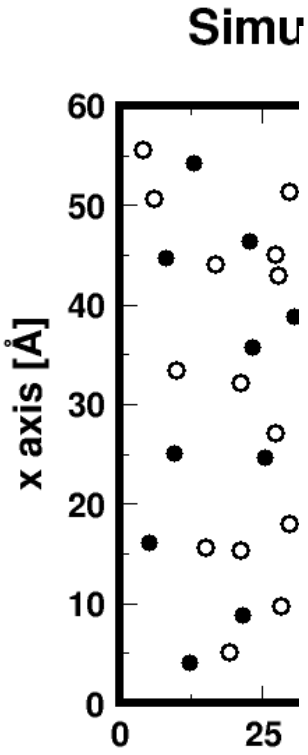

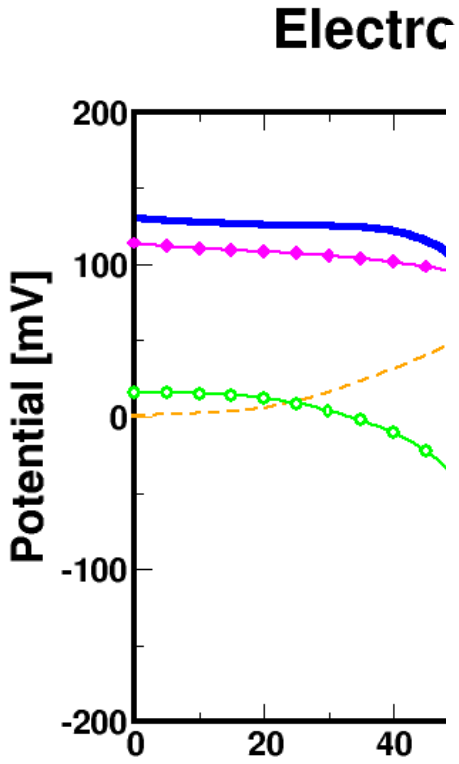

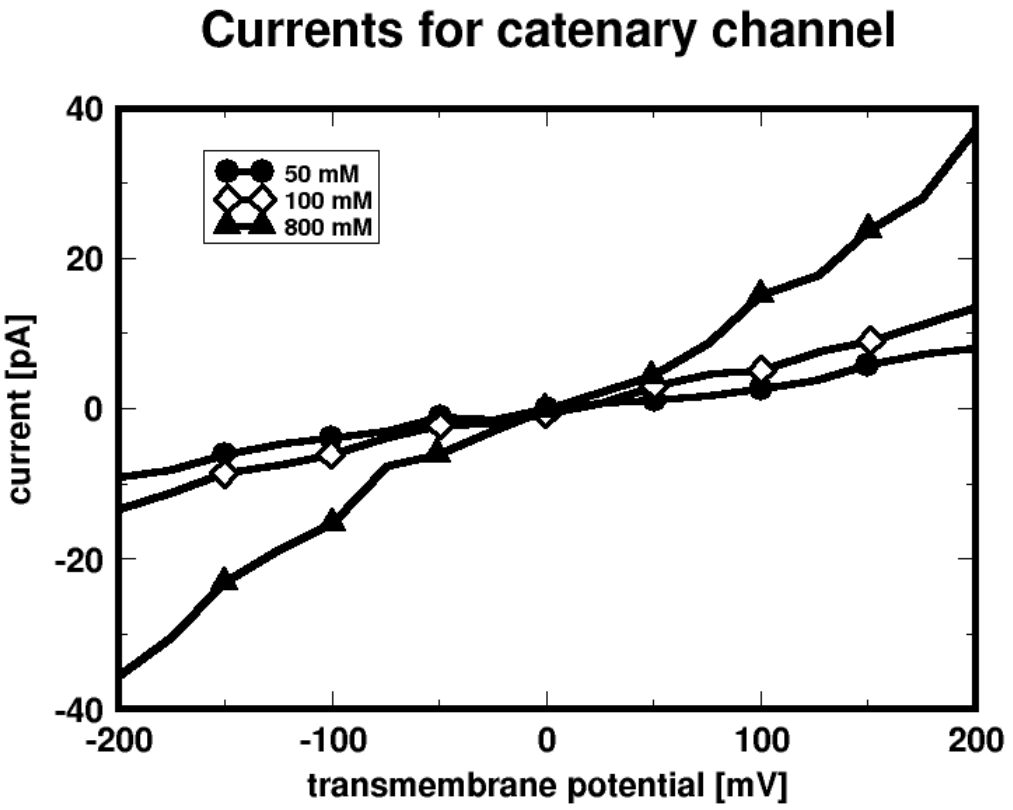

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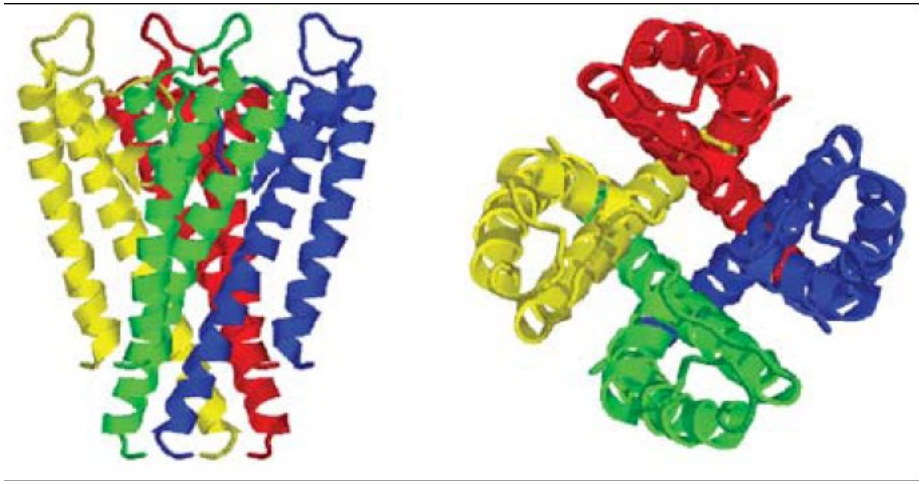
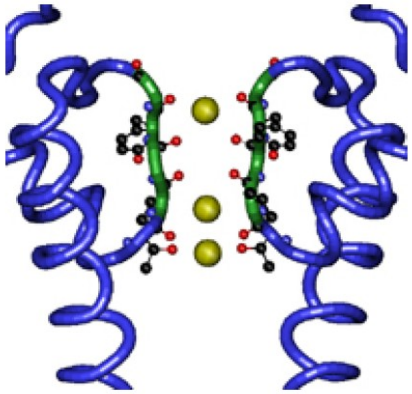
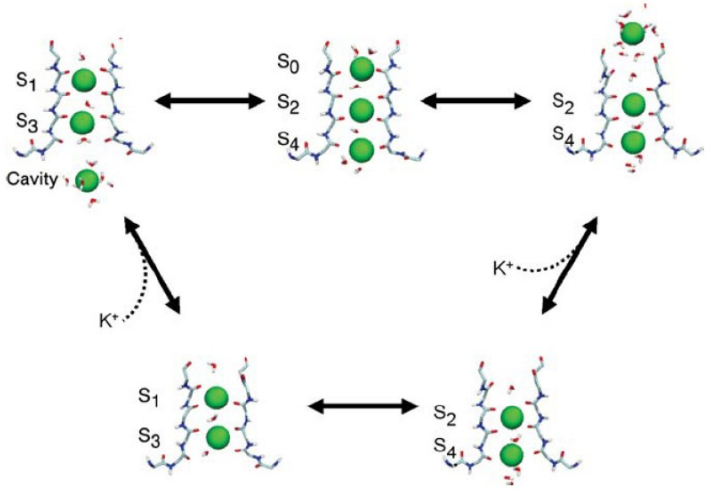
TEST CHANNELS – KcsA CHANNEL

- KcsA is a potassium channel of the bacterium *Streptomyces Lividans*



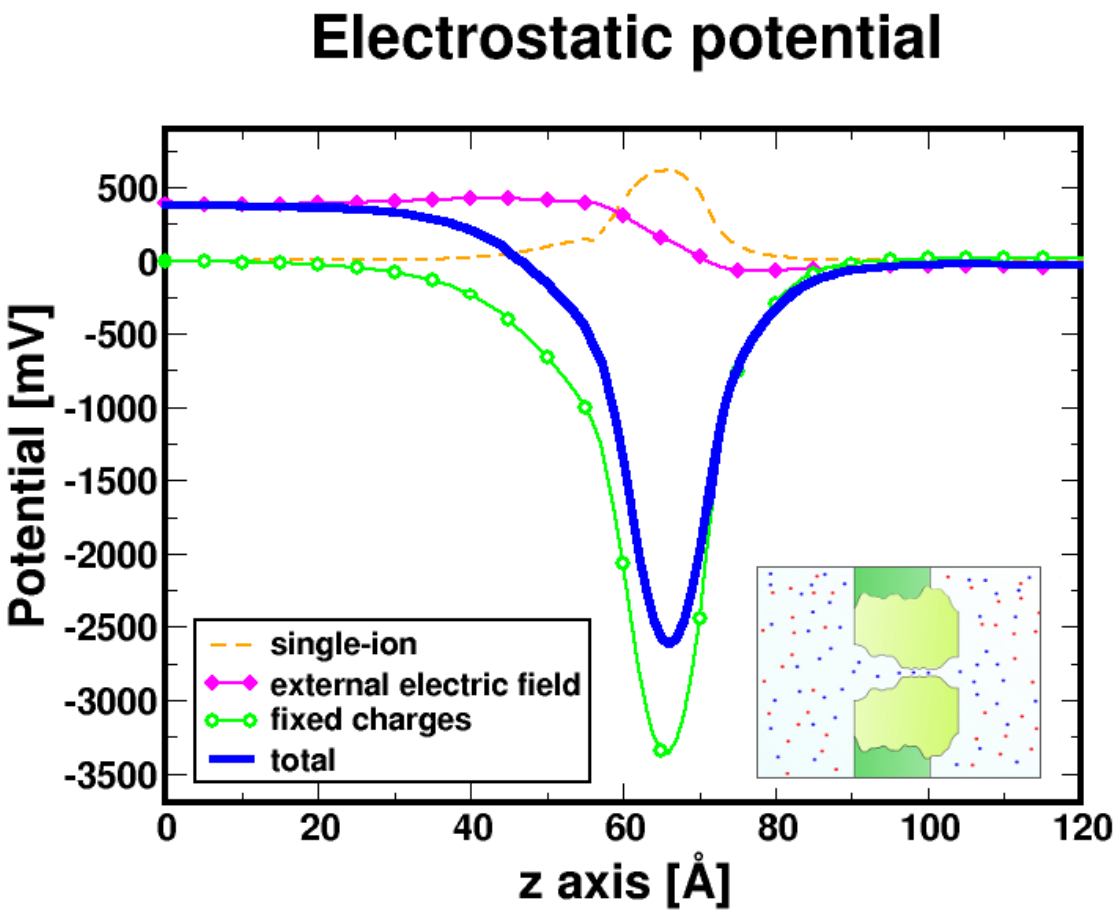
  - Highly selective
  - Highly permeable for K^+ ions





TEST CHANNELS – KcsA CHANNEL

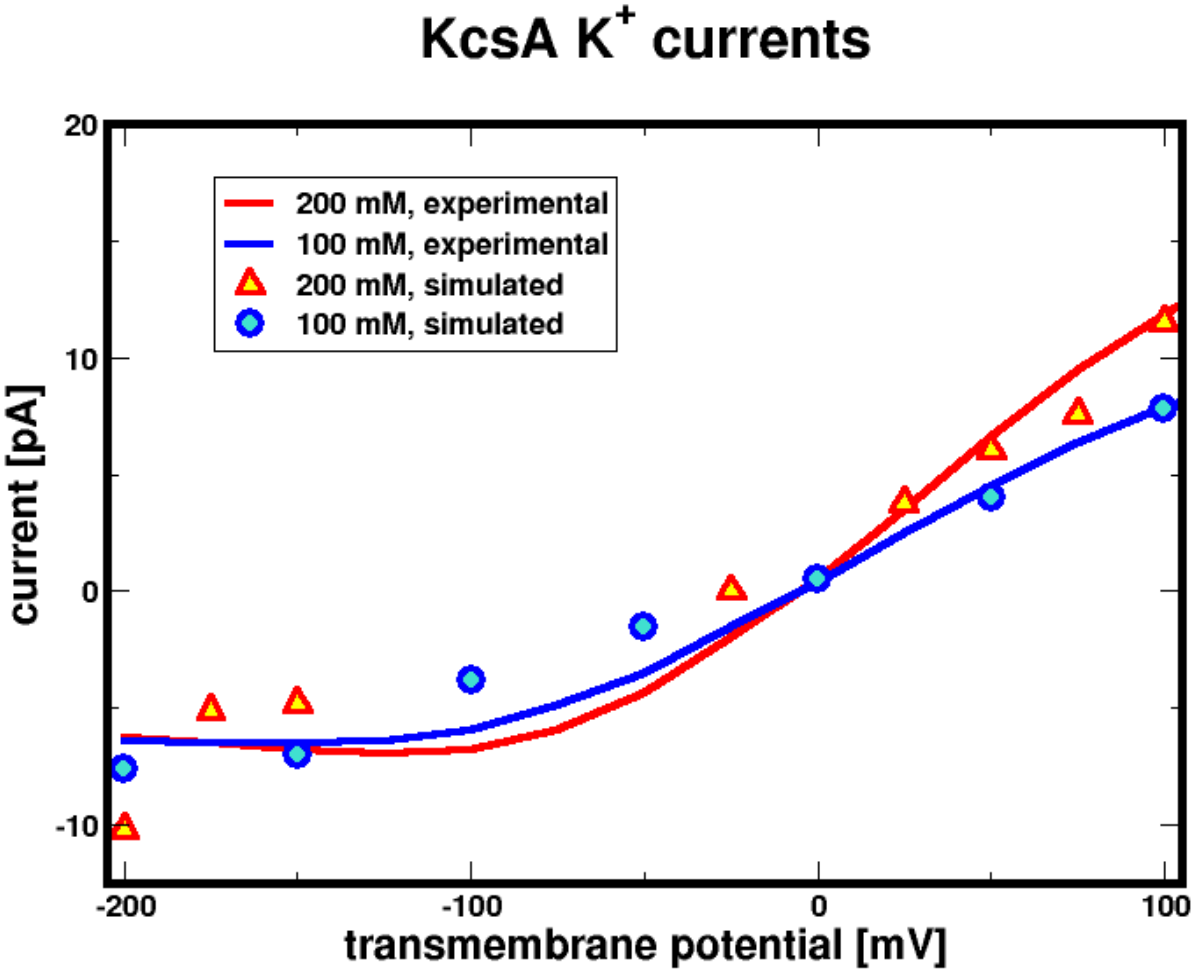
The potential profiles along the channel are in good agreement with those obtained by molecular Dynamics and Brownian Dynamics simulations [4]



[4] S.H. Chung et al., *Conducting-state properties of the KcsA potassium channel from ...* (Biophys. J. 82:628-645, 2002)

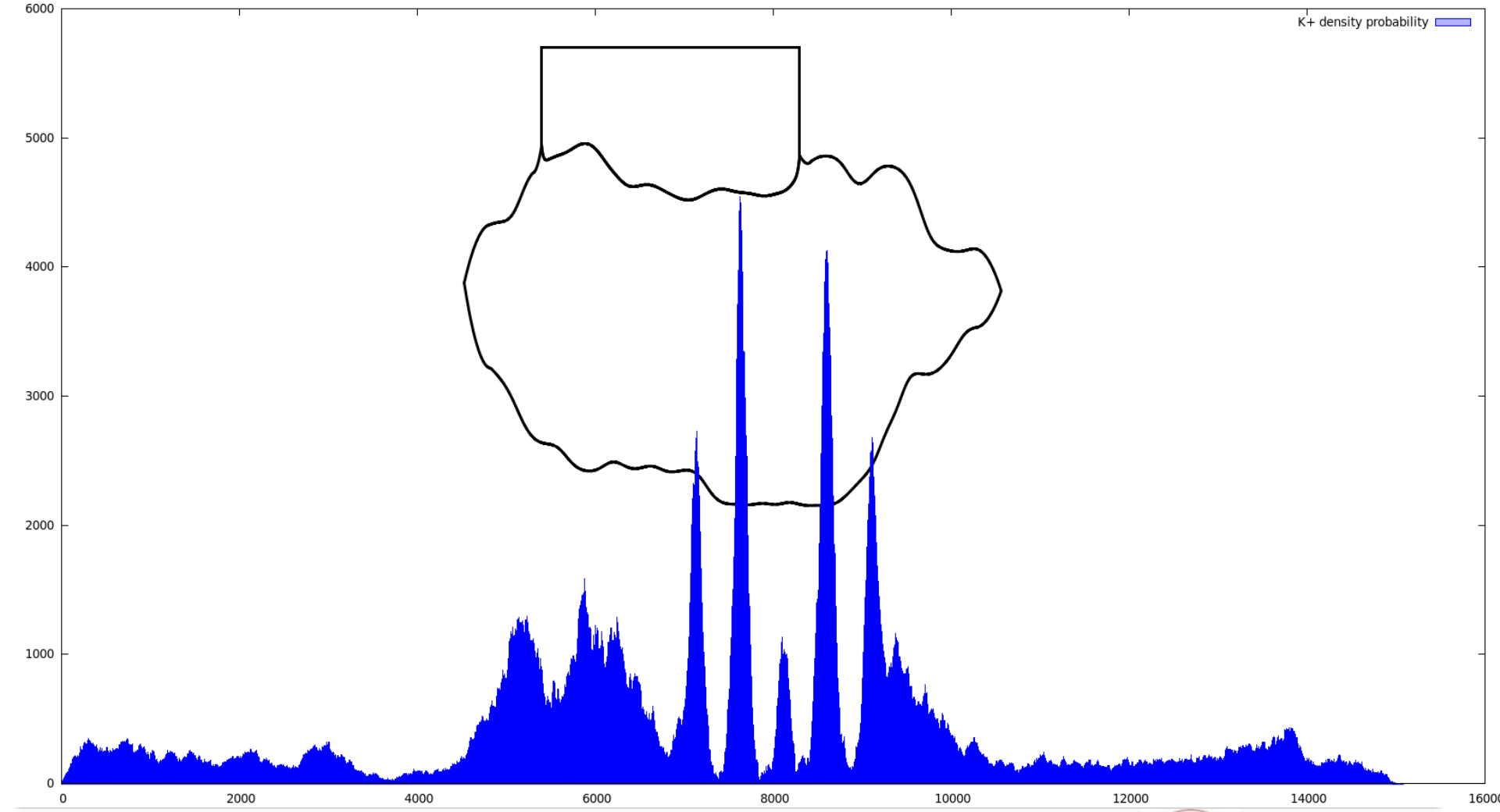
TEST CHANNELS – KcsA CHANNEL

- We compare our results with experimental data [5]



[5] M. LeMasurier et al., *KcsA: It's a potassium channel* (J. Gen. Physiol., 118:303-313, 2001)

MIXED BD-MC SIMULATOR



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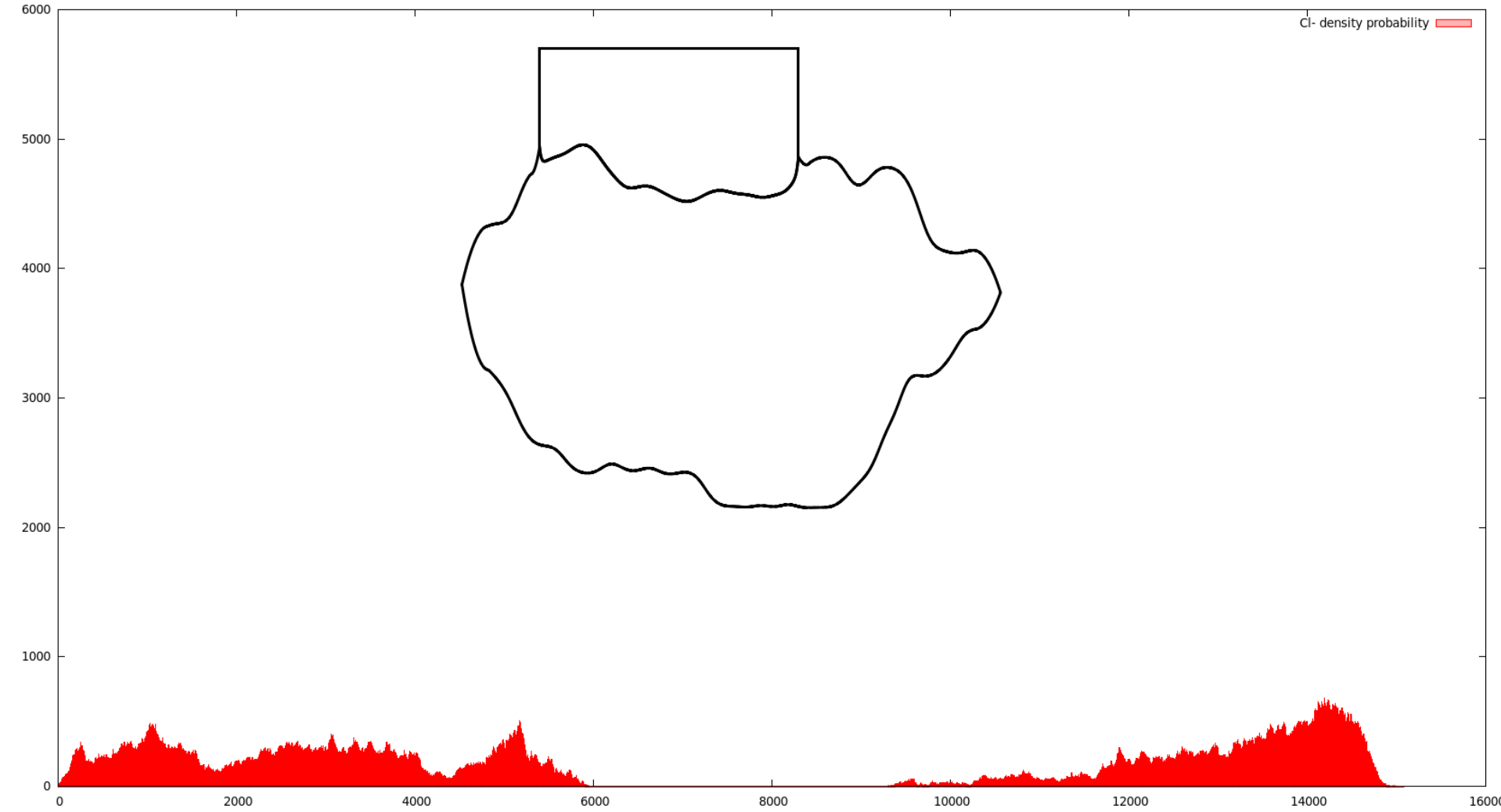

SYNTHETIC NANOPORES

- Solid-state nanopores are synthetic nanometer-scale pores located on an electrical-insulated membrane
- Adopted as single-molecule sensor
  - Fabrication methods determine geometry and dimensions of the nanopores
  - Detection principle is based on monitoring the variations of the ionic current flowing through the nanopore when a transmembrane potential is kept constant

Figures Removed due to copyright

Back to Silicon ……. New Opportunities

Figure Removed due to copyright

J. Li, D. Stein, C. McMullan, D. Branton, M. J. Aziz, and J. A. Golovchenko. Ion-beam sculpting at nanome- tre length scales. Nature, (412 (6843)):166{169, 2001

Conclusions

- Competences developed in the frame of CMOS Modeling and simulation can be easily re-used for different fields.
- Similarities in terms of mathematical formulation allowed to transfer the experience gained from the quantum-mechanical analysis of MOSFETs to the electromagnetic simulation of optoelectronic devices.
- Particle-based simulation (e.g. Monte Carlo simulation of MOSFETs) can be exploited for the analysis of nano-scale biological systems that can be integrated into silicon technology to provide new functionalities.