Supplementary Material

Access resistance in protein nanopores.

A structure-based computational approach

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Positioning of proteins in the membrane

The width and position of the membrane mimicking a low dielectric region have been obtained from the OPM database (https://opm.phar.umich.edu/). In the OPM database, each protein is positioned in a lipid bilayer of adjustable thickness by minimizing its transfer energy from water to the membrane. (see Lomize MA, Pogozheva ID, Joo H, Mosberg HI, Lomize AL. OPM database and PPM web server: resources for positioning of proteins in membranes. Nucleic Acids Res. 40 (2012) D370–D376. doi:10.1093/nar/gkr703)

Grid used for numerical solution of PNP equations

The cubic box used combines two different mesh sizes: a finer one of 1 Å for the protein region and a coarser one for the rest of the box. Figure S1 shows an example of the orthogonal mesh used for numerically solving Poisson-Nernst-Planck (PNP) equations for the OmpF protein channel embedded in a neutral membrane. The grid is shown for the membrane plane (XY plane). Analogous figures (not shown), except for the protein orientation, would appear for the XZ and YZ planes. The mesh is automatically build by a specific code calling the *gmsh* routine from within FiPy. We use a structured orthogonal mesh to get better accuracy in FiPy (see *https://www.ctcms.nist.gov/fipy/fipy/generated/meshes.numMesh.html* for details).

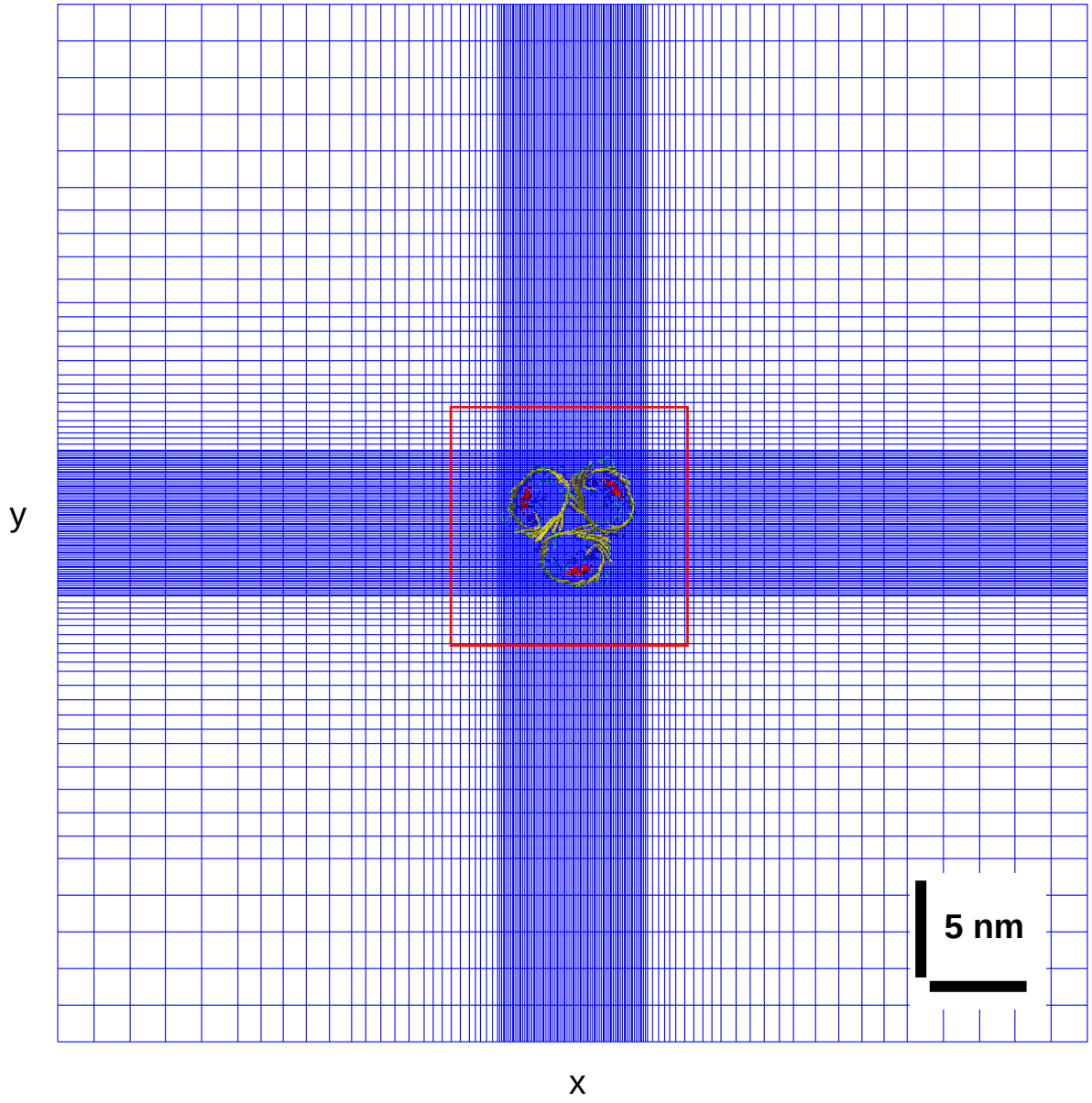

Figure S1. Orthogonal mesh used in the numerical solution of the PNP equations for the OmpF protein channel embedded in a neutral membrane. The region around the protein (centered in the box) has a smaller size (0.1 nm) and it gets coarser toward the boundaries up to a specified value (2 nm in the OmpF example shown). A detailed view of the region enclosed in the red rectangle is shown in Figure S2.

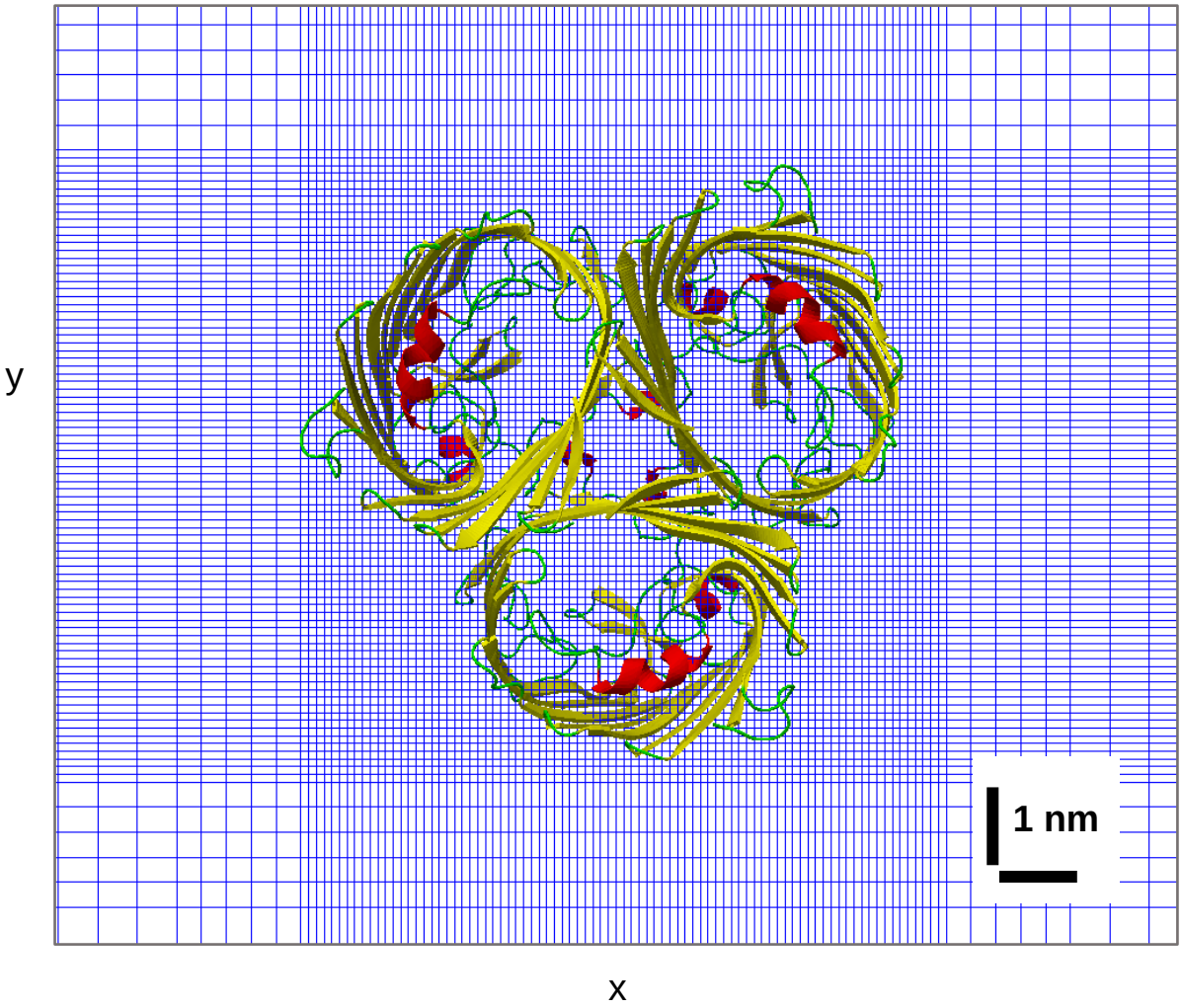

Figure S2. Detailed view of the mesh shown in the red rectangle of Figure S1.

Access resistance dependence on ion activities and concentrations

The range of concentrations explored in Access resistance (AR) measurements and calculations spans three orders of magnitude and goes from very diluted solutions (ideal solutions) to concentrated solutions where ion activity coefficients differ considerably from unity. Here we plot OmpF AR measurements in PC membranes (A. Alcaraz, M.L. López, M. Queralt-Martín, V.M. Aguilella, Ion Transport in Confined Geometries below the Nanoscale: Access Resistance Dominates Protein Channel Conductance in Diluted Solutions, ACS Nano. 11 (2017) 10392–10400) as a function of KCl concentration and activity. Except for the shift of the plot at high salt concentration, AR changes in a similar way and the difference in diluted solutions is

negligible. Since deviations from linearity occur at low concentrations where activity coefficients approach unity, they can hardly be attributed to the non-ideality of the solutions.

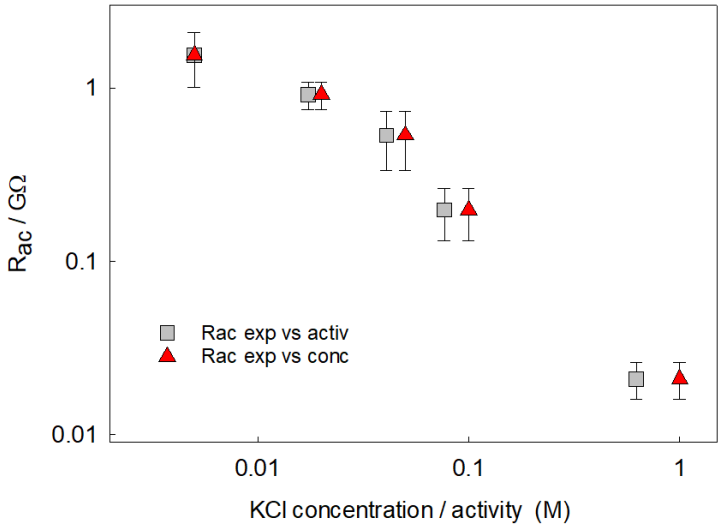

Figure S3. Access Resistance measurements in the OmpF channel for varying KCl concentrations and the corresponding activities.

In addition, the change of Access Resistance with activity according to Hall's equation $R_{ac} = (4\kappa a)^{-1}$ looks pretty similar to the corresponding plot vs. concentration. We copy below a plot of the inverse of KCl conductivity $1/\kappa$ by using measured conductivities in our laboratory for each KCl concentration (top line in red) and its corresponding activity (bottom line in blue).

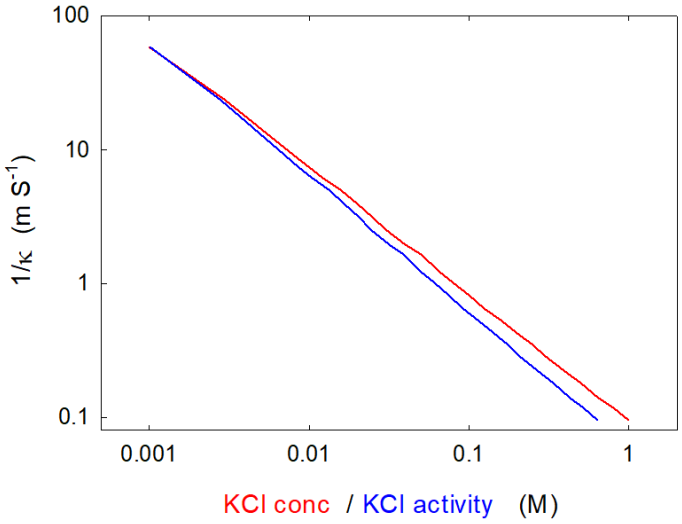

Figure S4. Measured inverse conductivity of KCl solutions as a function of their concentration and activity.