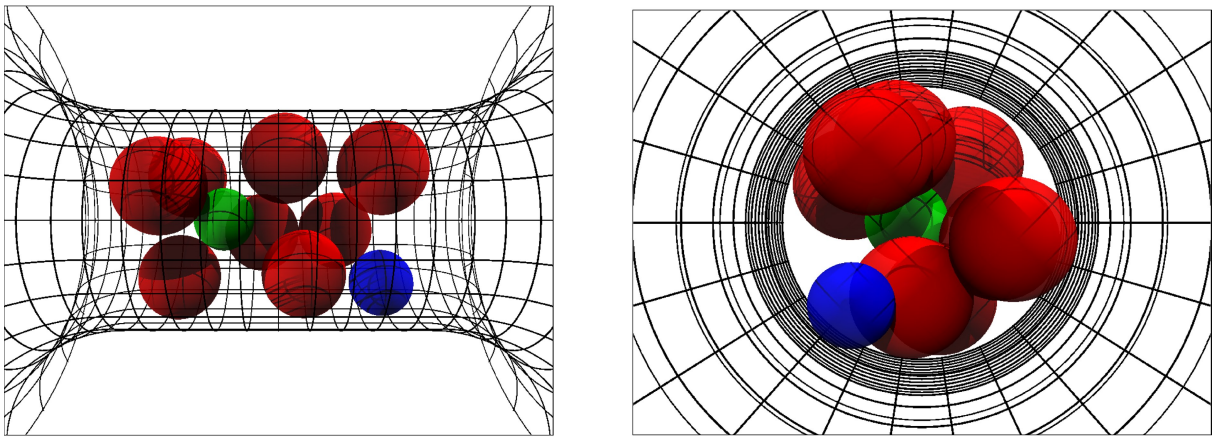
Ion Selectivity in Voltage-gated Biological Ion Channels

J. J. Finnerty[1], A. Peyser[2] and P. Carloni[2]

[1]*German Research School for Simulation Science, Jülich, Germany*
[2]*Forschungszentrum Jülich, Jülich, Germany*
E-mail: j.finnerty@grs-sim.de

We demonstrate that a combination of calculating the exact electrostatic potential and approximate volume exclusion within the sub-nanometer selectivity filter of a biological ion channel is critical for estimating the selectivity of the ion channel[1]. Biological membranes separate solutions of different ionic composition which can lead to significant transmembrane voltages and chemical potentials. Ion selective biological ion channels are used by nature to manage these potentials.



The high charge density within these ion channels requires computation of the electrostatic potential to consider induced charges on the dielectric boundary between the aqueous solution and the protein/membrane. Here, this is efficiently achieved by constraining the dielectric boundary to be constant, generating a set of surface elements, and pre-calculating a set of simultaneous equations that provides the induced charge of these elements in response to the external electric field.[2,3]

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References

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