Computing the Electrostatics

Charge density on external boundaries and internal dielectric boundaries is computed explicitly using the respective boundary conditions (Hoshi et al., J. Chem. Phys. 87, 1107(1987), Greenfield et al., Proc. SPIE Vol. 5025 (2003)). With the unknown boundary charges determined, the field/potential everywhere are given by Coulomb's law and superposition. The output quantities of interest including electrostatic energy and gating charge displacement are computed from the field.

For the numerical computation, surfaces are parcelled into elements (Fig.1). A linear relation connects the surface charge density of an element to the field/potential at the center of the element. For electrode elements, the surface charge sets the desired potential at the electrode. In isolating boundary elements, the surface charge nulls the (normal) electrical field just inside the boundary. The induced charge on dielectric elements creates the step in normal field strength that corresponds to the step in the dielectric coefficient.

The boundary conditions thus relate the unknown charge density of a surface element to the charges on the other surface elements, the source charges of the S4 model, and the externally set electrode potentials. These equations are solved simultaneously by linear algebra. The matrix elements of the system depend only on the configuration of the surface elements but not on the positions of source charges or electrode potential. Once the coefficient matrix has been inverted, many variations of the S4 position or electrode potential can be backsubstituted to solve the system repeatedly.

The charge displaced by S4 motion is computed from the electrical field at the dielectric boundaries. Due to the isolating boundary and Gauss' law, the total electrical displacement passing through each membrane face is identical to the displacement that reaches the respective electrode. The integrals of the displacement over each of the two dielectric boundaries give independent determinations of the displaced charge. In plots of displaced charge, the results of both determinations will be shown superimposed as a test of numerical consistency.

In a second control of numerical accuracy, we compute electrostatic energy by two different methods: (1) numerical integration of the force that acts on the S4 region being moved along a path, and (2) summation of the pairwise interactions of charges. The two results will also be shown as superpositions in the graphs.

The electrostatic analysis is **self-consistent**. Once the components of the model are defined, the accuracy of the results is exclusively a matter of the numerical accuracy of the chosen discretization of surfaces.