

Fig 1 Schematic of Computation Cell. We implement a reduced description of the S4 transmembrane domain, a rod of dielectric with embedded point charges. The S4 rod crosses the lipid membrane through a 'gating pore' that is tight in the center and widens into an atrium at each end (schematic is drawn to scale). The S4 rod and the membrane form one uniform dielectric that is separated by a sharp boundary from two aqueous bath regions. The baths and membrane form a cylindrical domain that is bounded by two conducting plates (Dirichlet boundaries, or 'electrodes', across which a voltage is applied) and an isolating (Neumann) boundary.

Dielectric and cell surfaces are discretized into surface elements for the computation of electrostatics (see text). The size of the surface elements is variable (illustrated by the dot graphs showing element centers); small elements are used where S4 charges or countercharges may approach a surface. About 4000 surface elements are used. S4 motion is computationally mimicked by moving S4 charges in the stationary S4 dielectric.