**Flux coupling by Kirchoff’s Law in a Branch Ion Channel**

Bob Eisenberg

June 1, 2013

Ion transporters are amongst the most important membrane molecules. Ion transporters are responsible for . Ion transporters are now defined, somewhat vaguely, by their structural characteristics, but that has not always been so. Ion transporters were originally defined by the coupling of fluxes characteristic of their function. The flux of one ion is proportional to the flux of another, with a quite constant proportionality constant in such systems. With suitable driving forces such coupling can transport one ion against the gradient of its own free energy or electrochemical potential. Flux coupling can produce actively transport one species at the expense of the passive transport of another.

The correlated motion that is flux coupling is usually explained by models of ion trajectories, often using the reciprocating mechanism first proposed, I believe, by Patlak. Here we show that flux coupling can arise in a branched channel as a simple consequence of Kirchoff’s current law in a fixed structure without reciprocating gates.

Kirchoff’s current law appears to be just another conservation law. It says that all currents that enter a node must leave it, and that the electrical current is the same everywhere in a single branch of a circuit.

But Kirchoff’s law is not just another conservation law, because it is about conservation of charge and current (the flow of charge) no matter what the physical nature of that current flow. Kirchoff’s law is in fact a form of Maxwell’s equations and thus much more general and accurate than many physical ‘laws’. Consider the system shown in Fig. 1. Here current flow in the wire is by electrons in a metal. In the semiconductor, current flow is by the movement of quasi particles holes and (what I like to call) semi-electrons, These in fact are mathematical constructs that bear faint resemblance to the electrons as taught in high school physics. Current flow in the cylinder of salt water is the movement of ions, say sodium and chloride. Current flow in the (vacuum) capacitor is by displacement current in a vacuum. No motion of mass is involved. Current flow in the polystyrene capacitor involves the displacement current accompanying the polarization of atoms as well as that in a vacuum.

What is remarkable is that the current flow in all these systems is equal to many significant figures even though the physical nature of the current is entirely different. The current flow is equal at all times and under all conditions no matter what carries the current. The motion of holes and semi-electrons is perfectly correlated (within the accuracy of Maxwell’s equations) with the motion of sodium and chloride (and everything else). The charge carried by atomic trajectories is perfectly correlated despite the bewilderingly complex shapes of the trajectories, that are nearly fractals reversing direction an uncountable number of times in any time interval (no matter how short) in Brownian motion. It is not clear how the laws that govern the trajectories can enforce Kirchoff’s current law. It is not clear how the physical properties of each system in Fig. 1 enforce Kirchoff’s current law. But they do.

The correlations arising from the inherent properties of the electric field can produce the phenomena of flux coupling in a branched channel, if the branches of the channel have different selectivity. Here I simply illustrate the point with a simplified model assuming selectivity. Obviously, the illustration needs to be expanded so selectivity is not assumed but rather is calculated as a consequence of the structure and properties of a real transporter. (This calculation is not as easy as it might seem, since it is not obvious that the usual programs of molecular dynamics satisfy Kirchoff’s current law, including displacement current: those programs calculate the electric field in complex ways and are not usually checked, as far as I know, to see if they compute displacement current correctly, or satisfy Maxwell’s equations.)

Consider a Y branch channel in which one slanted branch is sodium selective and current flow is only by the motion of sodium ions and the other slanted branch is calcium selective and current flow is only by the motion calcium ions. We assume (for simplicity) that current flow in the vertical branch is nonselective.

Obviously,



The corresponding (net) fluxes are  and the flux ratio is xxxx, yyyy.

Introduce conductance formulation.

Introduce unidirectional fluxes.

Fluxes are usually measured by their unidirectional components, so we must introduce these….. The ratio of unidirectional fluxes is then……

Comparison with the detailed properties of fluxes in real transporters is necessary.