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Presentation Abstract

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Abstract Title:	ENERGETIC VARIATIONAL ANALYSIS *EnVarA* OF IONS IN CALCIUM AND SODIUM CHANNELS.

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Abstract Body:

Selective binding in both calcium and sodium channels can be described (in many solutions and concentrations: Biophysical Journal (2007) 93:p.1960) by the same reduced model and unchanging two parameters (dielectric coefficient and diameter) despite the very different primary structure of the two proteins (Ca channel EEEA/EEEE; Na channel DEKA) and properties, even though amino-acid side-chains (E, D, etc.) are represented only as charged spheres. Monte Carlo *MC* simulations, reported in ~30 publications, work well (we think) because they do not specify structure as an input, independent of conditions. Rather, *MC* calculates the structure as an output, as a self-organized, induced fit of side-chains to ions (and vice-versa). **Structure is different in different solutions** in self-organized systems. Self-organized systems can be powerfully analyzed using the calculus of variations, specifically, energetic variational analysis (*EnVarA*). We optimize *both* action and dissipation integrals (Least Action and Maximum Dissipation Principles), motivated by Rayleigh, then Onsager who optimized just one, or the other. The resulting systems of coupled partial differential equations automatically satisfy the First and Second Laws of Thermodynamics and electrostatic Poisson equations, with physical

boundary conditions that can produce flow. *EnVarA* extends Navier-Stokes equations to complex fluids containing deformable droplets (Journal of Fluid Mechanics (2004) 515:p.293). ***EnVarA* provides a seamless extension of conservative Hamiltonian systems** (perhaps at thermodynamic equilibrium) **to dissipative systems.** *EnVarA* **is a** field theory of ions in channels and solutions with entropy, friction, and flow. *EnVarA* computes current where *MC* computes only binding. *EnVarA* applied to EEEE/DEKA channels gives binding like real calcium/sodium channels. Time dependent currents computed with *EnVarA* resemble time dependent currents in either voltage activated sodium or potassium (squid axon) channels (depending on parameters), **although the *EnVarA* model has only one unchanging conformation.**

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