**Mathematics and Molecular Biology**   
the engineering approach

# *Bob Eisenberg February 14 2016*

Life is different because it is inherited. All life comes from a blueprint (genes) that can only make proteins. Proteins are studied by more than one hundred thousand scientists and physicians every day because they are so important in health and disease. The function of proteins is on the macroscopic scale, but atomic details control that function, as is shown in a multitude of experiments. The structure of proteins is so important that governments spend billions studying them. Structures are known in exquisite detail determined by crystallographic measurement of more than 105 different proteins. **But the forces that govern the movement and function of proteins are not visible in the structure**. Mathematics is needed to compute both function and forces so comparison with experiment can be made. Experiments report numbers, typically sets of numbers in the form of graphs. Verbal models, however beautifully written in the biological tradition, do not provide numerical outputs, and so it is difficult to tell which verbal model better fits data.

The mathematics of molecular biology must be multiscale because atomic details control macroscopic function. The device approach of the engineering and English physiological tradition provides the dimensional reduction needed to solve the multiscale problem. Mathematical analysis of hundreds of experiments (reported in some fifty papers) has been successful in showing how some properties of an important class of proteins—ion channels— work. Ion channels are natural nanovalves as important to animals as Field Effect Transistors (FETs) are to computers. I will present the Fermi Poisson approach started by Jinn Liang Liu. The Fermi distribution is used to describe the saturation of space produced by crowded spherical ions. The Poisson equation (and continuity of current) is used to describe long range electrodynamics. Short range correlations are approximated by the Santangelo equation. A fully consistent mathematical description reproduces macroscopic properties of bulk solutions of sodium and calcium chloride solutions. It also describes several different channels (with quite different atomic detailed structures) quite well in a wide range of conditions using a handful of parameters never changed. It is not clear why the model works as well it does, nor is it clear how well the model will work on other channels, transporters or proteins.