Reliable Solution of the Poisson-Boltzmann Equation with Application to the SecYEG Membrane Channel

Johannes Kraus[1], Svetoslav Nakov[2], Sergey Repin[3]

[1] johannes.kraus@uni-due.de, University of Duisburg-Essen
[2] svetoslav.nakov@ricam.oeaw.ac.at, Johannes Kepler University, Linz
[3]sergey.s.repin@jyu.fi, V.A. Steklov Institute of Mathematics at St. Petersburg and University of Jyväskylä, Finland

We consider the Poisson-Boltzmann equation (PBE) which gives a mean field description of the electrostatic potential of a system of molecule(s) in ionic solution. The PBE is a semilinear elliptic equation with exponential nonlinearity and a measure right-hand side composed of a linear combination of delta distributions. Due to the irregular right-hand side it does not have a variational formulation involving H^1 spaces and thus existence and uniqueness of a solution is not straightforward. However, one can find a particular solution by employing a 2-term or 3-term splitting of the full potential. The regular part of this particular solution satisfies a variational formulation involving H^1 spaces and can be approximated by standard finite element methods.

We derive explicitly computable bounds on the error in energy norm for the regular H^1 component of the solution and obtain an analogue of Cea's lemma. A patchwise equilibrated flux reconstruction technique is used to obtain a conforming approximation of the dual variable. Thus, the evaluation of the error indicator in the adaptive algorithm can be realized in a very efficient manner in parallel.

This methodology is applied to study the electrostatic potential in the membrane channel SecYEG. The channel is located in the plasma membrane of bacteria and provides a lateral exit into the bilayer for membrane proteins, while simultaneously offering a pathway into the aqueous interior for secreted proteins. The system consists of 46 373 atoms, 9563 of which belong to the SecYEG. Moreover, an ion excluded layer with a thickness of $2\mathring{A}$ is added around the membrane and the SecYEG channel, and a variable dielectric coefficient is used for the aqueous media inside the channel.