RELIABLE ADAPTIVE METHOD FOR ELECTROSTATIC COMPUTATIONS IN BIOMOLECULAR SYSTEMS GOVERNED BY THE POISSON-BOLTZMANN EQUATION

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ABSTRACT

The Poisson-Boltzmann equation (PBE) gives a mean field description of the electrostatic potential in a system of molecule(s) and ionic solution. In this work, we derive explicitly computable bounds on the error in energy norm for the PBE

$$-\nabla\cdot\left(\epsilon(x)\nabla\tilde{\phi}\right)+k^2(x)\sinh\left(\tilde{\phi}\right) = \frac{4\pi e_c^2}{k_BT}\sum_{i=1}^{N} z_i\delta_{x_i}(x) \quad \text{in } \Omega_m\cup\Omega_s, \tag{1a}$$

$$\left[\tilde{\phi}\right]_\Gamma = 0, \tag{1b}$$

$$\left[\epsilon\nabla\tilde{\phi}\cdot n\right]_\Gamma = 0, \tag{1c}$$

$$\tilde{\phi} = g \quad \text{on } \partial\Omega, \tag{1d}$$

where $\tilde{\phi}$ is the unknown electrostatic potential, Γ is the interface between the domain Ω_m, occupied by the molecule(s), and the domain Ω_s, occupied by the ionic solution. In order to pose a standard weak formulation with a regular right hand side and a solution in $H^1(\Omega)$, two and three term splittings of $\tilde{\phi}$ are utilized [4].
This work is a continuation of [1] and the a posteriori error estimation analysis is based on the functional approach in [2]. The generality of this approach allows us to derive not only guaranteed bounds on the error, but also a near best approximation result for the regular component of the potential. Such a result is the basis for a finite element convergence analysis in energy norm. A patchwise equilibrated flux reconstruction technique ([3]) is used to obtain a conforming approximation of the dual variable. In this way, the error estimation part of the adaptive algorithm can be realized in a very efficient manner in parallel. We also present numerical examples performed on two sytems - Alexa 488 and Alexa 594, and an insulin protein with a PDB ID: 1RWE.

REFERENCES

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