

A Reduced Basis Method for the Nonlinear Poisson-Boltzmann Equation

Lijie Ji¹, Yanlai Chen^{2,*} and Zhenli Xu³

¹ School of Mathematical Sciences, Shanghai Jiao Tong University, Shanghai 200240, China

² Department of Mathematics, University of Massachusetts Dartmouth, 285 Old Westport Road, North Dartmouth, MA 02747, USA

³ School of Mathematical Sciences, Institute of Natural Sciences and Key Laboratory of Scientific and Engineering Computing (Ministry of Education), Shanghai Jiao Tong University, Shanghai 200240, China

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Abstract. In numerical simulations of many charged systems at the micro/nano scale, a common theme is the repeated resolution of the Poisson-Boltzmann equation. This task proves challenging, if not entirely infeasible, largely due to the nonlinearity of the equation and the high dimensionality of the physical and parametric domains with the latter emulating the system configuration. In this paper, we for the first time adapt a mathematically rigorous and computationally efficient model order reduction paradigm, the so-called reduced basis method (RBM), to mitigate this challenge. We adopt a finite difference method as the mandatory underlying scheme to produce the high-fidelity numerical solutions of the Poisson-Boltzmann equation upon which the fast RBM algorithm is built and its performance is measured against. Numerical tests presented in this paper demonstrate the high efficiency and accuracy of the fast algorithm, the reliability of its error estimation, as well as its capability in effectively capturing the boundary layer.

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1 Introduction

Fast numerical algorithms for solving parametrized partial differential equations (PDEs) have attracted wide-spread interest in recent years, particularly in engineering applications due to many control, optimization and design problems requiring repeated simulation of certain parametrized PDEs. Traditional numerical methods solve the equation

*Corresponding author.

Emails: sjtuidreamer@sjtu.edu.cn (L. J. Ji), yanlai.chen@umassd.edu (Y. L. Chen), xuzl@sjtu.edu.cn (Z. L. Xu)

for each necessary parameter value and thus obtaining the solution ensemble for the whole parameter space is potentially time-consuming if not entirely infeasible. This is an especially onerous task if the physical and/or parametric domain are of high dimensions. It is therefore imperative to design efficient and accurate reduced order modeling techniques for these scenarios capable of realizing negligible marginal (i.e., per parameter value) computational cost. The reduced basis method (RBM) provides a rigorous and highly efficient platform to achieve this exact goal. It was first introduced for nonlinear structure problem [1, 35] in 1970s and has been later analyzed and extended to solve many problems such as linear evolutionary equation [21], viscous Burgers equation [41], Navier-Stokes equations [14] and harmonic Maxwell's equation [10, 11] just to name a few. Interested readers are referred to the review papers [19, 37] and recent monographs [22, 36] for a systematic description of the RBM.

One such parametric scenario we are concerned in this paper is the simulation of the electrostatic interaction which is essential for many systems in physical, biological and materials sciences [16, 30, 42] at the nano/micro scale. These include, for example, biopolymers, colloidal suspensions and electrochemical energy devices. The Poisson-Boltzmann (PB) theory [3, 7, 15, 17] plays a fundamental role in understanding the electrostatic phenomenon in such systems. It subjects the electric potential of a charged system at the equilibrium state to a nonlinear elliptic equation with the Boltzmann distribution for the ionic densities. The numerical solution of the PB equation has been widely studied in literature [2, 34] and the numerical solvers are implemented in many popular software packages such as Delphi and APBS for practical simulations. However, one often needs to solve the PB equation repeatedly to determine certain physical quantities of interest (QoI) which are usually dependent on a wide range of parameters delineating e.g., the boundary voltage, the geometric length and the Debye length. Particular examples of such QoIs include the electrochemical capacitance, the current-voltage relation and the free-energy calculation etc.

In this work, we propose a reduced basis method for the parametrized nonlinear PB equation. Model order reduction for nonlinear equations is often realized by linearization techniques [44] or polynomial approximations, among others. One frequently-used tool is the empirical interpolation method (EIM) [5, 18] which is crucial to facilitate the offline-online decomposition, a hallmark feature of RBM to realize the negligible marginal computational cost. This paper extends the RBM for the nonlinear PB equation by approximating the nonlinear exponential term with a Taylor expansion form [39]. This leads to a linear equation in each calculation step. Realizing a partial offline-online decomposition, the method promises high accuracy due to the avoidance of the EIM error. It is noted that this work only focuses on the mean-field PB equation which is limited to describe phenomena when many-body interactions are important. The extension of our work to the modified PB equations such as those including correlation and steric effects (see, e.g., [32] and references therein) is of great interest due to the complex electrostatic phenomena they model and the drastically different nonlinearity contained therein. The successful application of the RBM will be reported in the future. We also note that Kweyu