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Existence, Uniqueness, and a Comparison of Nonintrusive Methods for the Stochastic Nonlinear Poisson–Boltzmann Equation*

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Abstract. The stochastic nonlinear Poisson–Boltzmann equation describes the electrostatic potential in a random environment in the presence of free charges and has applications in many fields. We show the existence and uniqueness of the solution of this nonlinear model equation and investigate its regularity with respect to a random parameter. Three popular nonintrusive methods, a stochastic Galerkin method, a discrete projection method, and a collocation method, are presented for its numerical solution. It is nonintrusive in the sense that solvers and preconditioners for the deterministic equation can be reused as they are. By comparing these methods, it is found that the stochastic Galerkin method and the discrete projection method require comparable computational effort and our results suggest that they outperform the collocation method.

Key words. stochastic partial differential equation, stochastic nonlinear Poisson–Boltzmann equation, existence, uniqueness, nonintrusive stochastic Galerkin method

AMS subject classifications. 34B08, 35B30, 60H25, 65K10, 65M70, 65J15

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1. Introduction.

Approximating the solutions of stochastic partial differential equations poses new challenges compared to partial differential equations (PDEs). One aspect that is also of great practical importance is the development of numerical methods that separate the spatial (physical) and the stochastic dimensions. Such methods have the advantage that both theory and implementations for the deterministic versions of the equations can be reused for discretizations of the spatial dimensions.

In recent years, the development of stochastic Galerkin methods has been of increasing interest [1, 2, 3, 4, 5, 6, 7]. In this paper, we apply three popular nonintrusive methods to the stochastic nonlinear Poisson–Boltzmann equation. A nonintrusive method is a method that makes it possible to reuse existing theory and implementations for the deterministic version of the equation, usually by separating the dimensions. Nonintrusive methods for parametric and stochastic equations were discussed recently in [8, 9, 10]. While it is commonly believed that Galerkin-type methods for stochastic partial differential equations always mix

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the spatial and stochastic dimensions necessitating the development of an entirely new theory and implementation, this is, however, not true in general.

The model equation considered here, the nonlinear Poisson–Boltzmann equation, is an important PDE in computational chemistry and related areas. It describes the electrostatic potential in all situations where free charge carriers are present and in equilibrium. As a nonlinear equation, it shows the generality of the numerical approach taken here. Linear elliptic equations are of course included as a special case.

We first show the existence and uniqueness of solutions in an appropriate function space for a class of stochastic elliptic partial differential equations including the stochastic Poisson–Boltzmann equation. Subsequently we discuss regularity properties of the solution of the stochastic Poisson–Boltzmann equation with respect to the random parameter. Recent work regarding the existence and regularity of linear elliptic, parabolic, and hyperbolic PDEs depending on countable random parameters includes [11, 12] as well as [13] for a class of semilinear elliptic PDEs, where the nonlinear term was modeled by a polynomial.

Then the numerical approach is developed. We have implemented these nonintrusive methods in one and two spatial (physical) dimensions and discuss various numerical examples, where both the operator and the forcing terms on the right-hand side are stochastic.

The rest of this work is organized as follows. Section 2 presents the model equation. The existence of a unique solution is shown. In section 3 we show that regularity of the data implies regularity of the solutions under certain assumptions. In section 4 we introduce nonintrusive methods for this equation, which can be generalized to other nonlinear stochastic partial differential equations. Section 5 tests and compares the Galerkin-type method to the projection method and the collocation method by applying them to examples in one and two spatial dimensions and up to three stochastic dimensions. We compare the methods by discussing their errors and computational expenses. Finally, conclusions are drawn in section 6.

2. The stochastic Poisson–Boltzmann equation.

We first discuss the model equation and then show the existence of a unique solution.

2.1. A physical model.

We consider a (spatial) domain $U \subset \mathbb{R}^d$, $d = 1, 2, 3$, which contains two species of free charge carriers, a positive and a negative one. The charge carriers may be anions and cations in a liquid or electrons and holes in a semiconductor. Certain parts of the domain are not accessible by the free charge carriers (see Figure 1), since they represent impenetrable molecules (when modeling a liquid) or dielectric materials (when modeling a semiconductor device).

The bulk concentrations of the two species of free charges are denoted by c_+ and c_-, and we make the physically reasonable assumption that $c_+ = c_-$. The charges of the single positive and negative charge carriers are denoted by q_+ and q_-, respectively, and we assume that $q_+ = -q_- =: q$. This case includes monovalent ions in liquids as well as electrons and holes in semiconductors. We also define the constant

$$c := c_+ + c_-.$$

The well-known Poisson equation is the elliptic equation

$$-\nabla \cdot (A(x)\nabla V(x)) = \rho(x), \tag{1}$$

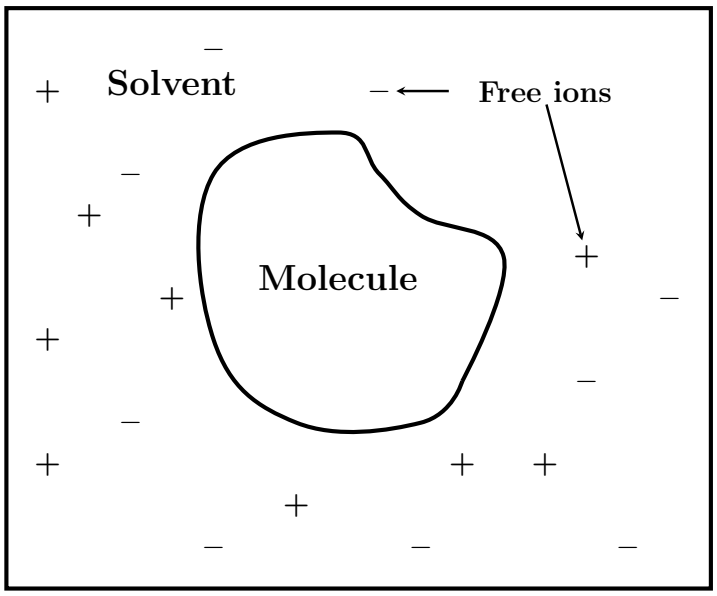

Figure 1. *A typical domain modeled by the Poisson–Boltzmann equation in two dimensions. The plus and minus signs indicate positive and negative charge carriers, and an impenetrable molecule is located in the center.*

where A is the dielectric constant or permittivity, V is the electrostatic potential, and ρ is the charge density of all charges in the system.

The charge density ρ of all charge carriers is the sum of the fixed charges ρ_{fixed} and the free charges ρ_{free}. The free charge carriers rearrange according to a Boltzmann distribution due to the electrostatic potential yielding

$$\rho_{\text{free}}(x) = c_+ \exp\left(-\frac{q_+ V(x)}{k_B T}\right) - c_- \exp\left(-\frac{q_- V(x)}{k_B T}\right), \tag{2}$$

where k_B is the Boltzmann constant and T is the absolute temperature [14]. In the monovalent case, this expression simplifies to

$$\rho_{\text{free}}(x) = -c \sinh\left(\frac{qV(x)}{k_B T}\right).$$

This physical model leads to the deterministic Poisson–Boltzmann equation

$$-\nabla \cdot (A(x)\nabla V(x)) = \rho_{\text{fixed}}(x) - c \sinh\left(\frac{qV(x)}{k_B T}\right). \tag{3}$$

The coefficient c may be replaced by a coefficient function $\kappa(x)$. Subdomains with vanishing κ cannot be accessed by the free ions, and therefore κ is often called the ion-accessibility function.

The stochastic generalization below of this deterministic equation describes—for example—physical systems where the fixed charges have probability distributions and hence the free

charges and the electrostatic potential V are stochastic as well. The different configurations of the fixed charges may be due to the movement of the molecules or binding and unbinding processes, for example, in biosensors [15, 16, 17, 18].

2.2. Existence of a unique solution. Let $U \subset \mathbb{R}^d$, $d = 1, 2, 3$, be an open, bounded domain with Lipschitz boundary and let $\mathcal{P} := (\Omega, \Sigma, \mathbb{P})$ be a probability space. The boundary of the domain U is partitioned into a Neumann boundary U_N and a nontrivial Dirichlet boundary U_D. We consider the stochastic semilinar elliptic boundary-value problem

$$-\nabla \cdot (A(x,\omega)\nabla u(x,\omega)) + b(x,\omega,u(x,\omega)) = f(x,\omega) \qquad \forall x \in U, \tag{4a}$$

$$u(x,\omega) = u_D(x,\omega) \qquad \forall x \in \partial U_D, \tag{4b}$$

$$\nu \cdot A(x,\omega)\nabla u(x,\omega) = 0 \qquad \forall x \in \partial U_N \tag{4c}$$

for almost all $\omega \in \Omega$. Here ν is an outward-pointing normal unit vector. This includes the stochastic nonlinear Poisson–Boltzmann equation

$$-\nabla \cdot (A(x,\omega)\nabla u(x,\omega)) + \kappa(x,\omega)\sinh(u(x,\omega)) = f(x,\omega) \qquad \forall x \in U, \tag{5a}$$

$$u(x,\omega) = u_D(x,\omega) \qquad \forall x \in \partial U_D, \tag{5b}$$

$$\nu \cdot A(x,\omega)\nabla u(x,\omega) = 0 \qquad \forall x \in \partial U_N \tag{5c}$$

for almost all $\omega \in \Omega$ as a special case.

In order to show the existence and uniqueness of a weak solution of (4) and hence (5), assumptions on the data are needed. Similar assumptions were used in [11, 13] and are physically reasonable [19].

Assumption 1.

1. *The coefficient matrix function* $A\colon U \times \Omega \to \mathbb{R}^{d\times d}$ *with entries* A_{ij} *for* $i, j \in \{1, \dots, d\}$ *is uniformly elliptic with constant* μ *and almost everywhere bounded with respect to* x *with constant* C_A*, both uniformly for almost all* $\omega \in \Omega$*.*
2. *We assume that the integral of* b *with respect to* u *exists and call it* B*, i.e.,*

$$B\colon \quad U \times \Omega \times \mathbb{R} \to \mathbb{R}, \quad (x,\omega,u) \mapsto \int_0^u b(x,\omega,t)\ \mathrm{d}t$$

   exists and is convex with respect to u *and bounded from below by* C_B*, both for almost all* $x \in U$ *and* $\omega \in \Omega$*.*
3. *The right-hand side* f *is in* $L^2(\mathcal{P}; L^2(U))$*.*
4. *Let the Dirichlet data* $u_D \in L^2(\mathcal{P}; H^{1/2}(\partial U_D))$ *and assume the existence of a linear, continuous extension operator* $\operatorname{ext}\colon H^{1/2}(\partial U_D) \to H^1(U)$*, such that* $\operatorname{tr}(\operatorname{ext}(\phi)) = \phi$ *holds on* ∂U_D *and* $\nu \cdot A\nabla \operatorname{ext}(\phi) = 0$ *holds on* ∂U_N *for almost all* $\omega \in \Omega$*. We may denote* $\operatorname{ext}(u_D)$ *by* $\bar{u}_D$*. Additionally, let* $\langle B(\bar{u}_D), 1\rangle_{L^2(U\times\Omega)}$ *be finite.*

Remark 2. *When we assume enough regularity of the Dirichlet and Neumann boundary, Assumption* 1.4 *is reasonable. Since then the trace operator* $\widehat{\operatorname{tr}}\colon H^1(U) \to H^{1/2}(\partial U_D)$ *is linear and continuous and can be extended to a linear, continuous operator* $\operatorname{tr}\colon L^2(\mathcal{P}; H^1(U)) \to L^2(\mathcal{P}; H^{1/2}(\partial U_D))$ *in a meaningful way. Analogously, we define the extension operator* $\widehat{\operatorname{ext}_0}\colon H^{1/2}(\partial U_D) \to H^1(U)$ *and its natural extension* $\operatorname{ext}_0\colon L^2(\mathcal{P}; H^{1/2}(\partial U_D)) \to L^2(\mathcal{P}; H^1(U))$*.*

One can define a continuous, linear extension operator $\operatorname{ext}\colon L^2(\mathcal{P}; H^{1/2}(\partial U_D)) \to L^2(\mathcal{P}; H^1(U))$ *such that* $\nu \cdot A\nabla \operatorname{ext}(v) = 0$ *holds on* ∂U_N *for almost all* $\omega \in \Omega$ *by defining* $\operatorname{ext}(\phi)$ *for* $\phi \in L^2(\mathcal{P}; H^{1/2}(\partial U_D))$ *as the sum of* $\operatorname{ext}_0(\phi)$ *and the solution of the following weak formulation:*

$$a(u + \operatorname{ext}_0(\phi), v) = 0 \quad \forall v \in L^2(\mathcal{P}; H^1_{0,D}(U)).$$

We define the spaces

$$\begin{aligned} G &:= L^2(\mathcal{P}; H^1(U)), \\ G_D &:= \{u \in G\colon \operatorname{tr}(u(\cdot,\omega)) = u_D(\cdot,\omega) \quad \mathbb{P}\text{-a.e.}\}, \\ H^1_{0,D}(U) &:= \{\varphi \in H^1(U)\colon \widehat{\operatorname{tr}}(\varphi) = 0 \text{ on } U_D\}, \\ G_0 &:= L^2(\mathcal{P}; H^1_{0,D}(U)) \end{aligned}$$

with the inner product

$$\langle v, w\rangle_G := \mathbb{E}(\langle v, w\rangle_{H^1(U)}).$$

We also define the bilinear form a as

$$a\colon \quad G \times G \to \mathbb{R}, \quad (u,v) \mapsto \mathbb{E}\left(\int_U A(x,\omega)\nabla u(x,\omega)\cdot\nabla v(x,\omega)\mathrm{d}x\right)$$

and the linear form F as

$$F\colon \quad G \to \mathbb{R}, \quad u \mapsto \mathbb{E}\left(\int_U f(x,\omega)u(x,\omega)\mathrm{d}x\right).$$

To shorten notation, we will occasionally skip the arguments x and ω, and write $b(u)$ and $B(u)$ instead of $b(x,\omega,u)$ and $B(x,\omega,u)$, respectively.

In order to include nonzero Dirichlet boundary conditions, we rewrite (4) using $\bar{u}_D$. The weak formulation then is to find $u_0 := u - \bar{u}_D \in G_0$ such that

$$a(u_0 + \bar{u}_D, v) + \langle b(u_0 + \bar{u}_D), v\rangle_{L^2(U\times\Omega)} = F(v) \qquad \forall v \in G_0 \tag{6}$$

holds.

We will use a variational formulation of the nonlinear problem (4) to show existence and uniqueness.

Theorem 3. *The stochastic semilinear elliptic boundary-value problem* (4) *has a unique weak solution in* G *under Assumption* 1.

Proof. To show the existence of a solution in G, we switch from the weak formulation 6 to the following variational formulation. We seek to minimize in G_0

$$J(u) := \frac{1}{2}a(u,u) + a(\bar{u}_D, u) + \langle B(u + \bar{u}_D), 1\rangle_{L^2(U\times\Omega)} - F(u). \tag{7}$$

By Assumption 1.2, we can bound $\langle B(u+\bar{u}_D), 1\rangle_{L^2(\mathcal{P};L^2(U))}$ from below with the constant C_B. Hence, we obtain that J is bounded from below on G

$$\begin{aligned} J(u) &\geq \frac{\mu}{2(1+C_P)^2}\|u\|_G^2 - C_A\|\bar{u}_D\|_G\|u\|_G + C_B - \|f\|_{L^2(\mathcal{P};L^2(U))}\|u\|_G \\ &\geq C_B - \frac{(1+C_P)^2}{2\mu}(\|f\|_{L^2(\mathcal{P};L^2(U))} + C_A\|\bar{u}_D\|_G)^2 > -\infty. \end{aligned}$$

Further, by Assumption 1.4 we deduce that $|J(0)| < \infty$. We may restrict the minimization onto the nonempty, convex set

$$C := \{u \in G_0 \colon \langle B(u+\bar{u}_D), 1\rangle_{L^2(U\times\Omega)} < \infty\}.$$

Thus, the minimum must be finite and we can find a minimizing sequence u_k in C such that

$$J(u_k) \to \min_{v\in G} J(v) \quad \text{for } k \to \infty.$$

Applying Young's inequality yields

$$J(u_k) \geq C_B + \left(\frac{\mu}{2(1+C_P)^2} - \epsilon\right)\|u_k\|_G^2 - \frac{1}{2\epsilon}\left(C_A^2\|\bar{u}_D\|_G^2 + \|f\|^2_{L^2(\mathcal{P};L^2(U))}\right).$$

As $J(u_k)$ is bounded, choosing ϵ sufficiently small implies that $\|u_k\|_G$ is bounded. By the Banach–Alaoglu theorem, the closed unit ball in G is compact with respect to the weak* topology which coincides here with the weak topology. Hence, we can extract a weakly convergent subsequence $(u_{k_n})_{n\in\mathbb{N}}$ and denote the limit by u. The map

$$u \mapsto \langle B(u+\bar{u}_D), 1\rangle_{L^2(U\times\Omega)}$$

is convex and continuous on C, and thus weakly lower semicontinuous; see [20, Theorem 1.2]. We infer weak lower semicontinuity of J and the minimality of u,

$$\inf_{u\in G} J(u) = \liminf_{n\in\mathbb{N}} J(u_{k_n}) \geq J(u).$$

Moreover, J is strictly convex, which the following computation for $u_1, u_2 \in C, u_1 \neq u_2$ and $t \in (0,1)$ shows,

$$tJ(u_1) + (1-t)J(u_2) - J(tu_1 + (1-t)u_2) \geq \frac{1}{2}t(1-t)a(u_1-u_2, u_1-u_2) > 0, \tag{8}$$

implying that u is the unique minimizer. ∎

From this general existence and uniqueness result for stochastic semilinear elliptic equations, the existence and uniqueness of solutions of the Poisson–Boltzmann equation (5) follows immediately. Note that the ion-accessibility function κ takes values between zero and the bulk ionic concentration, and is therefore nonnegative.

Corollary 4. *Let $\kappa \in L^2(\mathcal{P};L^2(U))$ be nonnegative and let $\bar{u}_D \in L^2(\mathcal{P};H^{1/2}(\partial U_D))$ be such that Assumption 1.4 is satisfied for $B(x,\omega,u) = \kappa(x,\omega)(\cosh(u)-1)$. Then the stochastic boundary-value problem (5) has a unique solution u in G.*

Proof. Assumption 1 is satisfied for the nonlinearity

$$b(x,\omega,u(x,\omega)) := \kappa(x,\omega)\sinh(u(x,\omega)). \tag{9}$$

The function b has an antiderivative $u \mapsto B(x,\omega,u)$ with respect to u, which is bounded from below and convex. Hence, Theorem 3 can be applied. ∎

3. Regularity and best approximation property. Our goal in this section is to prove regularity results for (5) as well as a best approximation property using the cut off deterministic weak formulation.

Lemma 5. *The weak solution u described by Theorem 3 satisfies the weak formulation of the deterministic version of (4) almost everywhere, i.e., there exists a set $\tilde{\Omega} \subseteq \Omega$ of full measure such that*

$$\int_U A(\omega)\nabla(u(\omega)) \cdot \nabla\phi + (b(\omega,u(\omega)) - f(\omega))\phi \, \mathrm{d}x = 0 \quad \forall\omega \in \tilde{\Omega}, \ \forall\phi \in H^1_{0,D}(U). \tag{10}$$

Proof. Since u is Bochner-measurable, we conclude for fixed $\phi \in H^1_{0,D}(U)$ the measurability of

$$\omega \mapsto \mathcal{Z}_\phi(\omega) := \int_U A(\omega)\nabla u(\omega) \cdot \nabla\phi + (b(\omega,u(\omega)) - f(\omega))\phi \, \mathrm{d}x.$$

Hence, for any $\phi \in H^1_{0,D}(U)$, we can split Ω into three disjoint, measurable sets

$$\Omega_0 := \mathcal{Z}_\phi^{-1}(\{0\}), \quad \Omega_+ := \mathcal{Z}_\phi^{-1}((0,\infty)), \quad \Omega_- := \mathcal{Z}_\phi^{-1}((-\infty,0)),$$

which lets us define the test function $v \in G_0$

$$v(x,\omega) := \begin{cases} \phi(x) & \omega \in \Omega_+, \\ -\phi(x) & \omega \in \Omega_-, \\ 0 & \text{else.} \end{cases}$$

By plugging v into the weak formulation, we obtain that

$$0 = \mathbb{E}\left[1_{\Lambda_+}\mathcal{Z}_\phi + \mathbb{1}_{\Lambda_-}\mathcal{Z}_{-\phi}\right],$$

where now the integrand is nonnegative. This implies the existence of a set $\Omega_\phi \subseteq \Omega$ of full measure such that

$$0 = \mathcal{Z}_\phi(\omega) \quad \forall\omega \in \Omega_\phi.$$

As $H^1_{0,D}(U)$ is separable, we may choose a countable, dense subset $\tilde{H}$ of $H^1_{0,D}(U)$. The set

$$\tilde{\Omega} := \bigcap_{\phi\in\tilde{H}} \Omega_\phi$$

is of full measure and satisfies (10) for all $\phi \in \tilde{H}$, and because $\tilde{H}$ is dense in $H^1_{0,D}(U)$ even for $\phi \in H^1_{0,D}(U)$. ∎

Henceforth we will restrict ourselves to the analysis of (5) even though under more restrictive assumptions the following techniques could also be applied to the more general setting of (4).

Proposition 6. *The solution u of (5) is in $L^\infty(\mathcal{P}; L^\infty(U))$ iff the solution of the associated stochastic linear elliptic boundary-value problem, i.e., (4) with vanishing function b, is in $L^\infty(\mathcal{P}; L^\infty(U))$.*

Proof. We denote by u_{lin} the solution of the stochastic linear elliptic boundary-value problem and define $w := u - u_{\text{lin}}$. Then, $w \in G_0$ satisfies the following weak formulation:

$$\mathbb{E}\left[\int A\nabla w \cdot \nabla v \mathrm{d}x\right] = \mathbb{E}\left[\int -\kappa \sinh(u) v \mathrm{d}x\right] \quad \forall v \in G_0. \tag{11}$$

First, we assume boundedness of u_{lin} and let $M := \|u_{\text{lin}}\|_{L^\infty(\mathcal{P};L^\infty(U))}$. By plugging $v := \max(w - M, 0)$ into (11) and using Poincaré's inequality, the uniform ellipticity of A, and Stampacchia's theorem, we obtain

$$\|\mathbb{1}_{w>M} w\|_G^2 \lesssim \mathbb{E}\left[\int A\nabla w \cdot \nabla v \mathrm{d}x\right] = \mathbb{E}\left[\int -\kappa \sinh(u) v \mathrm{d}x\right] \leq 0,$$

which implies that $w \leq M$ almost surely, and $u \leq 2M$ almost surely. By repeating the argument for $v := \max(w + M, 0)$, we obtain the desired boundedness of u. Due to symmetry reasons the reverse implication follows analogously. ∎

Remark 7. *By choosing $\mathcal{P}$ appropriately such that $\mathbb{P}$ is a Dirac measure and defining the coefficients in (5a) suitably, Proposition 6 can be applied to the deterministic case.*

To analyze the regularity of solutions with respect to the stochastic parameters, we want to avoid working on an abstract probability space $\mathcal{P}$, and hence we introduce a parameter space Λ endowed with a useful topology.

Assumption 8. *We assume that there is a random variable $\xi\colon \Omega \to \Lambda$ where the parameter space Λ is an open subset of $\mathbb{R}^n$, and that for almost all $x \in U$ and $\omega \in \Omega$*

$$A(x,\omega) = \tilde{A}(x, \xi(\omega)), \quad b(x,\omega,u) = \tilde{b}(x, \xi(\omega), u),$$
$$\kappa(x,\omega) = \tilde{\kappa}(x, \xi(\omega), \quad f(x,\omega) = \tilde{f}(x, \xi(\omega)).$$

Remark 9. *The general case where Λ is infinite-dimensional can be reduced to the finite-dimensional case by virtue of dimension reduction techniques such as the Karhunen–Loéve expansion* [21].

Instead of working on the abstract probability space $\mathcal{P}$, by applying Theorem 4 we may obtain a solution $\tilde{u}$ for the altered problem with permittivity $\tilde{A}$, nonlinearity $\tilde{b}$, and forcing term $\tilde{f}$ on the state space of ξ, $\mathcal{Q} := (\Lambda, \mathcal{B}(\Lambda), \xi_\# \mathbb{P})$, satisfying the weak formulation of (4). Moreover, $\tilde{u} \circ \xi$ satisfies the weak formulation of the initial problem and hence is the desired unique solution. By courtesy of Assumption 8 we are able to restrict ourselves to the associated problem on the parameter space $\mathcal{Q}$, where we can also study regularity of the solution with respect to that parameter. In the following, we will abuse notation and refer to $\tilde{A}$ by A, $\tilde{u}$ by u, and so forth.

Before we prove regularity results, we introduce a lemma that we will employ several times.

Lemma 10. *For $i \in \{1,2\}$, let $f_i\colon U \times \Lambda \to \mathbb{R}$ be measurable and uniformly bounded, i.e., $|f_i(x,p)| \le K$ almost everywhere in $U \times \Lambda$ for some $K > 0$. Let p_n be a sequence in Λ such that $f_i(p_n) \to 0$ in $L^2(U)$ as $n \to \infty$ and let $u_n \in H^1(U) \setminus \{0\}$. Then, for $w_i \in L^2(U)$, the sequence I_n defined as*

$$I_n := \frac{1}{\|u_n\|_{H^1(U)}} \left[\int_U f_1(p_n) u_n w_1 + f_2(p_n) \nabla u_n w_2 \, \mathrm{d}x \right] \tag{12}$$

satisfies $I_n \to 0$ as $n \to \infty$.

Proof. We show the claim by proving that every subsequence of I_n has a subsubsequence that converges to 0. To this end, we choose an arbitrary subsequence, for convenience again denoted by I_n. As $f_i(p_n) \to 0$ in $L^2(U)$ for $n \to \infty$, there is a subsequence n_k such that $f_i(x, p_{n_k}) \to 0$ for almost every $x \in U$. Using Cauchy–Schwartz, we find

$$|I_{n_k}| \le \left(\int_U f_1^2(p_{n_k}) w_1^2 \, \mathrm{d}x \right)^{1/2} + \left(\int_U f_2^2(p_{n_k}) w_2^2 \, \mathrm{d}x \right)^{1/2}.$$

As the integrands on the right-hand side are dominated by $K w_i^2 \in L^1(U)$ and converge to 0 pointwise a.e. in U, the dominated convergence theorem implies the claim. ∎

Theorem 11. *Additionally to Assumptions 1 and 8, if the data is continuous, i.e.,*

1. *$A_{ij} \in C(\Lambda; L^1(U))$ for $i,j \in \{1,\dots,d\}$ such that Assumption 1.1 holds pointwise for all $x \in U$ and $p \in \Lambda$,*
2. *$\kappa \in C(\Lambda; L^2(U))$ nonnegative,*
3. *$f \in C(\Lambda; L^2(U))$,*
4. *$u_D \in C(\Lambda; H^{1/2}(U))$,*
5. *for all $p \in \Lambda$, the unique (weak) solution of the deterministic equation*

$$-\nabla \cdot (A(x,p)\nabla u(x,p)) + \kappa(x,p)\sinh(u(x,p)) = f(x,p) \qquad \forall x \in U, \tag{13a}$$

$$u(x,p) = u_D(x,p) \qquad \forall x \in \partial U_D, \tag{13b}$$

$$\nu \cdot A(x,p)\nabla u(x,p) = 0 \qquad \forall x \in \partial U_N, \tag{13c}$$

satisfies $u(p) \in L^\infty(U)$,

then the solution u of the parametric boundary value problem (10) has a representative in $C(\Lambda; H^1(U))$.

Proof. The continuity of the data admits to pose the deterministic weak formulation pointwise for each $p \in \Lambda$ such that there is a unique solution $u(p) \in H^1(U)$ satisfying $\widehat{\mathrm{tr}}(u(p)) = u_D(p)$. We proceed to show that the map $p \mapsto u(p)$ is continuous from Λ to $H^1(U)$. Let $p, q \in \Lambda$ and write $u_0(p) := u(p) - u_D(p)$. The idea is to substract the weak formulations for $u(p)$ and $u(q)$ and linearize the resulting equation by applying the mean value theorem to the hyperbolic sine. Up to a perturbation term involving $A(p) - A(q)$, the resulting

weak formulation corresponds to that of a linear PDE, so standard estimation techniques can be applied. Substracting the weak formulations yields

$$\begin{aligned}\int_U A(p)\nabla(u_0(p)-u_0(q))\cdot\nabla\phi+\kappa(p)\cosh(\eta(u(p),u(q)))(u_0(p)-u_0(q))\phi\mathrm{d}x\\ =\int_U -A(p)\nabla(u_D(p)-u_D(q))\cdot\nabla\phi+(A(q)-A(p))\nabla(u_0(q)-u_D(q))\cdot\nabla\phi\\ +(\kappa(q)-\kappa(p))\sinh(u_0(q))\phi+(f(p)-f(q))\phi\mathrm{d}x\quad\forall\phi\in H_0^1(U),\end{aligned}$$

where $\eta:\mathbb{R}\times\mathbb{R}\to\mathbb{R}$ is a measurable selection of the set-valued map

$$\begin{aligned}&\Phi\colon\mathbb{R}\times\mathbb{R}\to\mathcal{B}(\mathbb{R}),\\ &\quad(x,y)\mapsto\{z\in[\min(x,y),\max(x,y)]\colon\ \cosh(z)(x-y)=\sinh(x)-\sinh(y)\}.\end{aligned}$$

Due to the continuity of sinh, cosh and the mean value theorem, Φ maps to closed, nonempty subsets of $\mathcal{B}(\mathbb{R})$ and is lower semicontinuous in the sense of set-valued maps. Utilizing Castaing's representation theorem [22, Theorem 6.6.8], we may choose η as the desired measurable selection.

By Poincaré's inequality, the uniform coercivity of A, and the positivity of κ and cosh, and by choosing $\phi=u_0(p)-u_0(q)$, we obtain

$$\begin{aligned}\|u_0(p)-u_0(q)\|_{H^1(U)}^2\lesssim\int_U(A(q)-A(p))\nabla u(q)\cdot\nabla(u_0(p)-u_0(q))\mathrm{d}x\\ +\left(\|u_D(p)-u_D(q)\|_{H^1(U)}+\|\kappa(p)-\kappa(q)\|_{L^2(U)}+\|f(p)-f(q)\|_{L^2(U)}\right)\|u_0(p)-u_0(q)\|_{H^1(U)}.\end{aligned}$$

Dividing this inequality by $\|u_0(p)-u_0(q)\|_{H^1(U)}$ and applying Lemma 10, we deduce that $u_0\in C(\Lambda,H^1(U))$. By the triangle inequality

$$\|u(p)-u(q)\|_{H^1(U)}\le\|u_0(p)-u_0(q)\|_{H^1(U)}+\|\bar{u}_D(p)-\bar{u}_D(q)\|_{H^1(U)},$$

we find that $p\mapsto u(p)\in C(\Lambda;H^1(U))$. By Lemma 5 and the uniqueness of the deterministic problem, the weak solution given by Theorem 3 agrees with $u(p)$ almost everywhere in Λ, which concludes the proof. ∎

Denote by $(e_i)_{i=1}^n$ the canonical basis of $\mathbb{R}^n$ and by ∂_{p_i} the partial derivative along e_i.

Theorem 12. *Additionally to Assumptions 1 and 8, we now consider the Dirichlet boundary-value problem. Let the data be continuously differentiable, i.e.,*

1. *$p\mapsto A_{ij}(x,p)\in C^1(\Lambda;\mathbb{R})$ for a.e. $x\in U$ and there is a $K_1>0$ such that*

$$\|\partial_{p_i}A(p)\|_{L^\infty(U\times\mathbb{R}^{d\times d})}\le K_1\ \forall p\in\Lambda$$

   and $i\in\{1,\dots,n\}$,
2. *$\kappa\in C_1(\Lambda;L^2(U))$ nonnegative,*
3. *$f\in C_1(\Lambda;L^2(U))$,*
4. *$u_D\in C_1(\Lambda;H^{1/2}(U))$,*

5. *there is a* $K_2 > 0$ *such that for all* $p \in \Lambda$ *the unique (weak) solution of the deterministic equation*

$$-\nabla \cdot (A(x,p)\nabla u(x,p)) + \kappa \sinh(u(x,p)) = f(x,p) \qquad \forall x \in U \tag{14a}$$
$$u(x,p) = u_D(x,p) \qquad \forall x \in \partial U, \tag{14b}$$

satisfies $\|u(p)\|_{L^\infty(U)} \leq K_2$,

then the solution u *of the parametric boundary value problem* (10) *has a representative in* $C^1(\Lambda; H^1(U))$.

Proof. As a first step, we identify a candidate w for the derivative by formally taking the derivative of the boundary-value problem (14) with respect to p_i.

$$\begin{aligned} \partial_{p_i}\left(-\nabla \cdot (A(x,p)\nabla u(x,p)) + \kappa(x,p)\sinh(u(x,p))\right) &= \partial_{p_i} f(x,p) && \forall x \in U, \\ \partial_{p_i} u(x,p) &= \partial_{p_i} u_D(x,p) && \forall x \in \partial U. \end{aligned}$$

For a given u, this yields a linear equation for the "derivative" w.

$$\begin{aligned} -\nabla \cdot (A\nabla w) + \kappa \cosh(u) w &= \partial_{p_i} f + \nabla \cdot (\partial_{p_i} A \nabla u) - \partial_{p_i} \kappa \sinh(u) && \text{on } U, \\ w &= \partial_{p_i} u_D && \text{on } \partial U. \end{aligned}$$

The existence, uniqueness, and continuity (in p) of the solution w of the parametric boundary value problem above follows from a similar reasoning as in the proof of Theorem 11. It remains to show that w is indeed the desired derivative of u with respect to p_i. To shorten notation, we denote the differential quotient for a function in p by

$$D_h^i u(p) := \frac{u(p + he_i) - u(p)}{h}.$$

For $h \neq 0$, we introduce the solution w_h of the auxiliary problem

$$\begin{aligned} -\nabla \cdot (A\nabla w_h) + \kappa \cosh(u) w_h &= \partial_{p_i} f + \nabla \cdot (\partial_{p_i} A \nabla u) - \partial_{p_i} \kappa \sinh(u) && \text{on } U, \\ w_h &= D_h^i u_D && \text{on } \partial U. \end{aligned}$$

Again, standard estimates for linear PDEs show that $w_h(p) \to w(p)$ in $H^1(U)$ as $h \to 0$ for each $p \in \Lambda$. By substracting the weak formulation at the points p and $p + he_i$, we obtain for $h \neq 0$ and $\phi \in H_0^1(U)$

$$\begin{aligned} \int_U \left[A(p+he_i)\nabla(D_h^i u(p)) + (D_h^i A(p))\nabla u(p)\right] \cdot \nabla \phi \\ + \left[\kappa(p+he_i) D_h^i \sinh(u)(p) + D_h^i \kappa(p) \sinh(u(p))\right] \phi \\ - [D_h^i f(p)]\phi \mathrm{d}x = 0. \end{aligned}$$

For $h \neq 0$, define

$$\begin{aligned}
\phi_h &:= \frac{u(p+he_i)-u(p)}{h} - w_h(p) \in H_0^1(U),\\
I_{0,h} &:= \int_U A(p+he_i)\nabla\phi_h \cdot \nabla\phi_h \,\mathrm{d}x,\\
I_{1,h} &:= \int_U \left[(A(p)-A(p+he_i))\nabla w(p) + (\partial_{p_i}A(p) - D_h^i A(p))\nabla u(p)\right]\cdot\nabla\phi_h\\
&\quad + (\kappa(p)-\kappa(p+he_i))\cosh(u(p))w(p)\phi_h \,\mathrm{d}x,\\
I_{2,h} &:= \int_U \left[\partial_{p_i}\kappa(p) - D_h^i\kappa(p))\sinh(u(p)) + (D_h^i f(p) - \partial_{p_i} f(p))\right]\phi_h \,\mathrm{d}x,\\
I_{3,h} &:= \int_U \kappa(p+he_i)(\cosh(u(p))w - D_h^i \sinh(u)(p))\phi_h \,\mathrm{d}x.
\end{aligned}$$

By computing the difference of the weak formulation of w and the differential quotient $D_h^i u$, and testing with $\phi = \phi_h$, we obtain

$$I_{0,h} = I_{1,h} + I_{2,h} + I_{3,h}.$$

The coercivity of A implies the estimate

$$\|\phi_h\|_{H^1(U)} \lesssim \frac{1}{\|\phi_h\|_{H^1(U)}}(I_{1,h} + I_{2,h} + I_{3,h}).$$

The mean value theorem together with the boundedness of $\partial_{p_i}A(p)$ shows that

$$|D_h^i A(x,p) - \partial_{p_i}A(x,p)| \leq 2\|\partial_{p_i}(A(p))\| \leq 2K_1$$

for almost every $x \in U$. Hence, we can apply Lemma 10 to show that the first term involving $I_{1,h}$ vanishes as $h \to 0$. Using the boundedness of u and Cauchy–Schwartz, the same follows for the term involving $I_{2,h}$. We rewrite the final term using the measurable selection η defined in the proof of Theorem 11 where we denote $\eta(u(p+he_i), u(p))$ by η_h

$$\begin{aligned}
I_{3,h} &= \int_U \kappa(p+he_i)\left[(\cosh(u(p))w - \cosh(\eta_h)D_h^i u(p)\right]\phi_h \,\mathrm{d}x\\
&= \int_U \kappa(p+he_i)\left([\cosh(u(p)) - \cosh(\eta_h)]\, w + \cosh(\eta_h)\left[(w-w_h) - \phi_h\right]\right)\phi_h \,\mathrm{d}x\\
&\leq \int_U \kappa(p+he_i)\left[\cosh(u(p)) - \cosh(\eta_h)\right] w\phi_h \,\mathrm{d}x\\
&\quad + \int_U \kappa(p+he_i)\cosh(\eta_h)(w-w_h)\phi_h \,\mathrm{d}x.
\end{aligned}$$

Again employing Lemma 10 and Cauchy–Schwartz, we see that $\frac{1}{\|\phi_h\|_{H^1(U)}} I_{3,h}$ vanishes as $h \to 0$. This implies that $\|\phi_h\|_{H^1(U)} \to 0$ as $h \to 0$, which in turn implies $D_h^i u(p) \to w(p)$ in $H^1(U)$ as $h \to 0$, completing the proof. ∎

The cut off function $b_\alpha \colon U \times \Omega \times \mathbb{R} \to \mathbb{R}$ is defined as

$$b_\alpha(x,\omega,u) = \begin{cases} \kappa(x,\omega)\sinh(-\alpha) & u \le -\alpha, \\ \kappa(x,\omega)\sinh(u) & -\alpha \le u \le \alpha, \\ \kappa(x,\omega)\sinh(\alpha) & \alpha \le u. \end{cases}$$

Since we assume $\kappa \in L^\infty(U \times \Omega)$, we obtain the Lipschitz continuity of b_α in u with Lipschitz constant L. Assume $u_0 \in G_0$ solves

$$a(u_0 + \bar{u}_D, v) + \langle b_\alpha(u_0 + \bar{u}_D), v\rangle_{L^2(U\times\Omega)} = \langle f, v\rangle_{L^2(\Omega\times U)} \qquad \forall v \in G_0, \tag{15}$$

where $\bar{u}_D$ is defined as in Assumption 1. Let V_h be a subspace of $H_0^1(U)$ and $u_h \in L^2(\mathcal{P}; V_h)$ the solution of

$$a(u_h + \bar{u}_D, v_h) + \langle b_\alpha(u_h + \bar{u}_D), v_h\rangle_{L^2(U\times\Omega)} = \langle f, v_h\rangle_{L^2(U\times\Omega)} \qquad \forall v_h \in L^2(\mathcal{P}; V_h), \tag{16}$$

then there holds the following best approximation property.

Theorem 13. *The cut off deterministic weak formulation satisfies the best approximation estimate*

$$\|u_0 - u_h\|_G \le \frac{(1+C_p)}{\mu}(C_A + L) \inf_{v_h \in L^2(\mathcal{P};V_h)} \|u_0 - v_h\|_G.$$

Proof. Because of the uniform ellipticity of A and monotonicity of b_α there holds

$$\mathbb{E}\left[\|\nabla u_0 - \nabla u_h\|^2_{L^2(U)}\right] \le \frac{1}{\mu} a(u_0 - u_h, u_0 - u_h) + \frac{1}{\mu}\langle b_\alpha(u_0) - b_\alpha(u_h), u_0 - u_h\rangle_{L^2(U\times\Omega)}. \tag{17}$$

By using the galerkin orthogonality of $u_0 - u_h$ we may exchange u_h with an arbitrary $v_h \in L^2(\mathcal{P}; V_h)$ to obtain

$$\mathbb{E}\left[\|\nabla u_0 - \nabla u_h\|^2_{L^2(U)}\right] \le \frac{1}{\mu} a(u_0 - u_h, u_0 - v_h) + \frac{1}{\mu}\langle b_\alpha(u_0) - b_\alpha(u_h), u_0 - v_h\rangle_{L^2(U\times\Omega)}. \tag{18}$$

Next we use the boundedness of a, the Lipschitz continuity of b_α, and the Poincaré inequality and divide by $\|u_0 - u_h\|_G$ to get

$$\|u - u_h\|_G \le \frac{1 + C_P}{\mu}\,(C_A + L)\,\|u - v_h\|_G. \tag{19}$$

Taking the infimum over all $v_h \in V_h$ and applying the Poincaré inequality concludes the proof. ∎

4. Stochastic Galerkin-type method.

In this section, a nonintrusive Galerkin discretization is presented for the stochastic Poisson–Boltzmann equation. This general Galerkin-type approach originates from [8].

Consider the following general setting: let $(H_i, \langle\cdot,\cdot\rangle_{H_i})$ for $i = 1, 2$ be Hilbert spaces, where H_1 represents the state space and H_2 represents some external influence. Their elements ϕ are

functions $\phi\colon U \to \mathbb{R}$. The operator $\mathcal{A}\colon H_1 \to H_2$ models the physics of the system depending on a parameter p such that the equation

$$\forall p \in \Lambda\colon \quad \mathcal{A}(p;\phi) = f(p) \tag{20}$$

holds for $f(p) \in H_2$. We require the problem (20) to be well-posed, meaning that for fixed $p \in \Lambda$ the operator $\phi \mapsto \mathcal{A}(p;\phi)$ is bijective and continuously invertible.

In the example of the Poisson–Boltzmann equation, we have $H_1 := H^1(U)$, $H_2 := L^2(U)$ and the operator $\mathcal{A}$ takes for $p \in \Lambda$ the following form:

$$\mathcal{A}(p;\phi) := -\nabla \cdot (A(p)\nabla(\phi + \bar{\phi}_D)) + \kappa(p)\sinh(\phi + \bar{\phi}_D),$$

where $\bar{\phi}_D$ is an appropriate function (depending on p) in $H^1(U)$ ensuring the boundary conditions. By passing over to the weak formulation, we conclude in the setting of Theorem 11 the well-posedness of the problem.

Furthermore, we require the existence of quadrature formulas on $\mathcal{Q}$, quadrature points $(q_z)_{z\in Z}$, and appropriate weights $(w_z)_{z\in Z}$, such that

$$\int_\Lambda g(p)\xi_\#\mathbb{P}(\mathrm{d}p) = \int_\Omega g(\xi(\omega))\mathbb{P}(\mathrm{d}\omega) \approx \sum_{z\in Z} w_z g(p_z).$$

Suppose that an iterative solver S for the deterministic problem, i.e., for the problem with fixed parameter p, is known, which converges pointwise for all $p \in \Lambda$, and may depend on the parameter p, the previous iteration $u^k(p)$, and the iteration count k.

As usual in the Galerkin setup, we define a set of linearly independent ansatz functions $(\psi_\alpha)_{\alpha\in\mathcal{I}}$ and a set of linearly independent test functions $(\tilde{\psi}_\alpha)_{\alpha\in\mathcal{I}}$, such that $\psi_\alpha, \tilde{\psi}_\alpha \in L^2(\mathcal{Q};\mathbb{R})$ for all α in the set of indices $\mathcal{I}$. For convenience, we may also assume that these sets form an orthonormal system in $L^2(\mathcal{Q};\mathbb{R})$ with $\psi_\alpha = \tilde{\psi}_\alpha$ for all $\alpha \in \mathcal{I}$, whereby the former is always possible due to Gram–Schmidt. For random variables with basic distributions, like uniform, gamma, or Gaussian distributions, or for general random variables, one considers the orthogonal polynomials associated with the (optimal) generalized polynomial chaos expansion [23, 24] of the random variable, respectively, the Askey scheme [25].

We strive to find an approximation $\tilde{u}$ of the solution u such that

$$\tilde{u} = \sum_{\alpha\in\mathcal{I}} u_\alpha \psi_\alpha, \quad u_\alpha \in \mathcal{H}, \tag{21}$$

$$\int_\Lambda (f(p) - A(p;\tilde{u}(p)))\phi_\alpha(p)\mathrm{d}\xi_\#\mathbb{P}(p) = 0 \quad \forall \alpha \in \mathcal{I}, \tag{22}$$

where we denote the residuum $f(p) - A(p,u(p))$ by $R(p,u)$. Based on a general parametric formulation, the following nonintrusive Galerkin-type Algorithm 1 was developed in [8]. We may represent the solution of this algorithm $\tilde{u}$ as a (finite) vector $\mathbf{u}$ of elements of $\mathcal{H}$.

Algorithm 1 Nonintrusive Galerkin-type block–Jacobi iteration.

Start with an initial guess $\mathbf{u}^{(0)} = [\dots, u_\alpha^{(0)}, \dots]^\top$.
$k \leftarrow 0$
while not converged **do**
  for $\alpha \in \mathcal{I}$ **do**
    $\Delta u_\alpha^{(k)} \leftarrow 0$
  end for
  for $z \in \mathcal{Z}$ **do**
    $\Delta u_z^{(k)} \leftarrow S(p_z; u^{(k)}(q_z)) - u^{(k)}(q_z)$
    $r_z \leftarrow w_z \Delta u_z^{(k)}$
    for $\alpha \in \mathcal{I}$ **do**
      $\Delta u_\alpha^{(k)} \leftarrow \Delta u_\alpha^{(k)} + r_z \psi_\alpha(q_z)$
    end for
  end for
  $\mathbf{u}^{(k+1)} \leftarrow \mathbf{u}^{(k)} + \boldsymbol{\Delta}\mathbf{u}^{(k)}$
  $k \leftarrow k + 1$
end while

In short, the algorithm starts with an initial guess $\mathbf{u}^{(0)}$. We initialize $\Delta u_\alpha^{(k)}$ with 0 and compute an approximation of $\Delta u_\alpha^{(k)}$ until convergence, namely,

$$\begin{aligned}\Delta u_\alpha^{(k)} &= \int_\Lambda (S(p; u^{(k)}(p)) - u^{(k)}(p))\psi_\alpha(p)\xi_\# \mathbb{P}(\mathrm{d}p) \\ &\approx \sum_{z\in\mathcal{Z}} w_z \underbrace{(S(q_z; u^{(k)}(q_z)) - u^{(k)}(q_z))}_{=:\Delta u_z^{(k)}} \psi_\alpha(q_z),\end{aligned}$$

by iterating through the set of indices of the interpolation points $\mathcal{Z}$. Adding up the previous approximation $\mathbf{u}^{(k)} = [\dots, u_\alpha^{(k)}, \dots]^\top$ and $\boldsymbol{\Delta}u^{(k)} := [\dots, \Delta u_\alpha^{(k)}, \dots]^\top$ yields the desired approximation $\mathbf{u}^{(k+1)}$. By construction and as discussed in [8], this method minimizes the residuum error.

4.1. Discrete projection. For comparison purposes, we introduce a discrete projection method [8, 26, 27]. As in the previous section, we want to find an approximative form of u such that

$$\tilde{u} = \sum_{\alpha\in\mathcal{I}} u_\alpha \psi_\alpha.$$

In the simplest form the algorithm can be summarized as the projection of u onto $\{\phi\psi_\alpha : \phi \in \mathcal{H}, \alpha \in \mathcal{I}\}$. Therefore, we compute the coefficient using quadrature

$$u_\alpha = \int_\Lambda u(p)\psi_\alpha(p)\xi_\# \mathbb{P}(\mathrm{d}p) \approx \sum_{z\in\mathcal{Z}} w_z u^{k_z}(q_z)\psi_\alpha(q_z).$$

Due to [8, Corollary 3.4], it is expected that the Galerkin-type method and the discrete projection method require a similar amount of solver calls to reach comparable accuracy if the

convergence speed of the solver S is linear. For further investigations of convergence speed we refer the reader to [8]. However, the additional calculations, which the Galerkin-type method requires, are not considered in this estimate. In each iteration, there are further additions and multiplications, which often can be regarded as insignificant compared to a solver call. We conclude that if the computational effort is measured in solver calls, then the block-Jacobi algorithm and the projection algorithm require comparable effort.

4.2. Stochastic collocation. Another nonintrusive method of interest is stochastic collocation methods as in [28]. Given a set of collocation nodes $\mathcal{N} \subseteq \Lambda$, we compute the solution u_β of the deterministic problem for each $\beta \in \mathcal{N}$ and obtain an approximation

$$\tilde{u}(p) = \sum_{\beta \in \mathcal{N}} u_\beta l_\beta(p),$$

where $(l_\beta)_{\beta \in \mathcal{N}}$ denotes the multivariate Lagrange basis at the collocation nodes $\mathcal{N}$. When we choose $\mathcal{N}$ as the set of interpolation points $\mathcal{Z}$ which are described above, the stochastic collocation method and the discrete projection method require the same amount of computations. Hence, they are directly comparable.

5. Implementation and numerical results. In this section, we apply the algorithms of the previous section to the stochastic nonlinear Poisson–Boltzmann equation introduced in section 2. To acquire an approximation of the solution u of (5), we solve pointwise for $p \in \Lambda$ the resulting deterministic equation by coupling low-order finite elements with Newton's method. The code was written in Julia. We use `gmsh`, an open-source mesh generation software, to create a triangulation of the spatial domain.

5.1. The physical domains. We consider two different geometries corresponding to the domain $U := [-1, 1]^d$, $d \in \{1, 2\}$, Figures 2 and 3. The position of a molecule (green) is uniformly distributed in the area, which is highlighted in grey. The solvent contain ions and electrons. Therefore $\kappa = \kappa_{\text{solvent}}$ is assumed to be positive and piecewise constant on this region, whereas there are no free charge carriers inside the molecule available, which yields that κ vanishes there.

The permittivity A is assumed to be piecewise constant on the different regions taking the values A_{solvent} and A_{molecule}. Further, the molecule is supposed to be charged yielding the system of equations (23). Let $p = (p_1, p_2) \in \Lambda := [-1, 1]^{n_1+n_2}$, where $n_1 \in \{1, 2\}$ and $n_2 = 1$

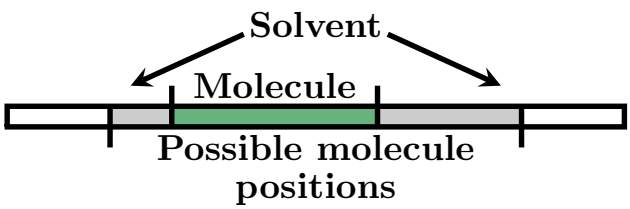

Figure 2. *First example—one dimension. The domain U contains a solvent. The area of possible molecule positions is shown grey. The green area represents a molecule.*

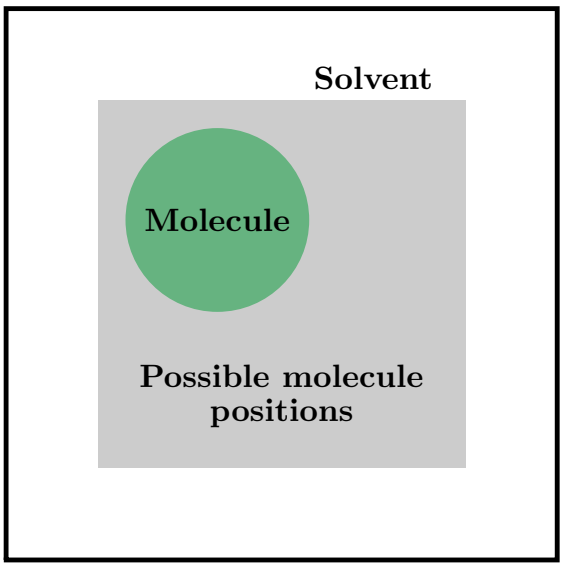

Figure 3. *Second example—two dimensions. The domain contains a solvent. The area of possible molecule positions is shown grey. The green circle represents a molecule.*

determine the position and size of the molecule, respectively. Let $K(p) := \{x \in U : \|x - p_1\| \leq r(p_2)\}$, where r is an affine function of p_2. We consider the problem

$$-\nabla \cdot (A(x,p)\nabla u(x,p)) + \kappa(x,p)\sinh(u(x,p)) = \mathbb{1}_{K(p)}(x) \quad \forall x \in U, \tag{23a}$$

$$u(x,p) = 0 \quad \forall x \in \partial U_D. \tag{23b}$$

In this setting, the assumptions of Theorem 3 are satisfied, implying the existence and uniqueness of the solution. Furthermore, we have $A \in C(\Lambda; L^1(U)^{d\times d}) \setminus C^1(\Lambda; L^1(U)^{d\times d})$ and $\kappa, f \in C(\Lambda; L^2(U)) \setminus C^1(\Lambda; L^2(U))$. We would like to apply Theorem 11 to obtain continuity in p of the solution, but it is not obvious whether $u(p) \in L^\infty(U)$ for every $p \in \Lambda$. In general, finding L^∞-bounds for solutions of semilinear elliptic equations seems to be delicate; see [29] for a survey. However, by virtue of Remark 7, we may prove pointwise boundedness for the deterministic semilinear problem (23) by considering the associated linear problem with $\kappa \equiv 0$. Applying Theorem 8.15 in [30] to the linear problem, we find that the assumptions of Theorem 11 are satisfied, yielding $u \in C(\Lambda; H^1_0(U))$. From now on we will only consider the FEM-discretization of (23). We will not distinguish between the exact solution u at parameter p and the computable FEM-approximation.

5.2. Numerical results. We set the $L^2(U)$-norm of the increment as a convergence criterion for the FEM-solver of the deterministic equation and the $L^2(\mathcal{P}; L^2(U))$-norm of the increment $\boldsymbol{\Delta}\mathbf{u}^{(k)}$ of the Galerkin-type method (cf. section 4).

To validate the numerical results, we use a quasi–Monte Carlo method, namely, the Sobol sequence [31], and a sufficiently large number of samples to calculate quantities of interest, like the expected value

$$\bar{u}(x) := \mathbb{E}[u(x,\xi)],$$

the residuum error

$$\mathrm{Res}(u_{\mathcal{I}}) := \mathbb{E}\big(\|R(\omega, u_{\mathcal{I}}(\omega))\|^2_{L^2(U)}\big)^{1/2},$$

and the root-mean-square error (RMSE)

$$\mathrm{RMSE}(u_{\mathcal{I}}) := \mathbb{E}\big(\|u - u_{\mathcal{I}}\|^2_{L^2(U)}\big)^{1/2}.$$

The sample size is chosen sufficiently large such that we have 99% confidence that the computational error is less than 1%.

To quantify the difficulty of the different test cases, we compute the coefficient of variation or the signal-to-noise ratio (SNR), namely, the quotient of mean value and standard deviation, in similar fashion. Then, the errors of the investigated stochastic approximation methods are compared. These results are visualized in tables and figures, where m denotes the maximal degree of the Legendre polynomials used and m_1 denotes the degree of the quadrature rule used, always satisfying $m \leq m_1$. In addition the quadrature nodes are used as collocation nodes for the stochastic collocation method.

5.2.1. The one-dimensional case. We investigated three different test cases in one dimension, $\kappa_{\text{solvent}} \in \{0, 1, 10^4\}$. In all test cases, the differences in RMSE and residuum error between the Galerkin and discrete projection methods were negligible, since the error of both methods agreed in the first 5–6 digits. Overall, the Galerkin method required up to $1/3$ more solver calls than the projection method.

Especially in the cases with higher SNR (2.8 and 2.5) where $\kappa_{\text{solvent}} = 0$ and $\kappa_{\text{solvent}} = 1$, increasing the amount of ansatz functions did not lead to an increase of accuracy as the solution is rather smooth and already well-approximated by low-order polynomials. Therefore, it was more effective to increase the precision of the used quadrature formula.

On the contrary, when the problem is more difficult, i.e., the SNR is lower (0.4) as in the case of $\kappa_{\text{solvent}} = 10^4$, increasing the amount of Ansatz functions as well as the precision of the quadrature formula is required to experience a substantial decrease of relative residuum error and RMSE. Here, it turned out that choosing as many ansatz functions as the quadrature formula permits proves as optimal.

Figure 4 shows oscillations of the approximative solutions which are caused by the used space of ansatz functions. Note that even though the exact solution is nonnegative, the approximations do not share this property.

5.2.2. The two-dimensional case. In this section, we consider the stochastic Poisson–Boltzmann equation (5) on the two-dimensional (2D) domain introduced in section 5.1. Here, we set the permittivity constant as $A = 1$ and $\kappa_{\text{solvent}} \in \{1, 10^3\}$. The SNR is 3.0 in the case of the weak nonlinearity ($\kappa_{\text{solvent}} = 1$). Choosing a stronger nonlinear term ($\kappa_{\text{solvent}} = 10^3$) in turn decreases the SNR to 0.9. Overall the different methods fare similar as in the 1D case. The investigated methods need a comparable amount of solver calls for convergence as in Table 1. Notably, the discrete projection and collocation methods require the same amount of solver calls whereas the Galerkin-type method needs more solver calls to reach convergence in the case of a smaller SNR. Varying the convergence criterion ϵ does not lead to different results in terms of relative residuum error and RMSE. This can be explained on the one hand

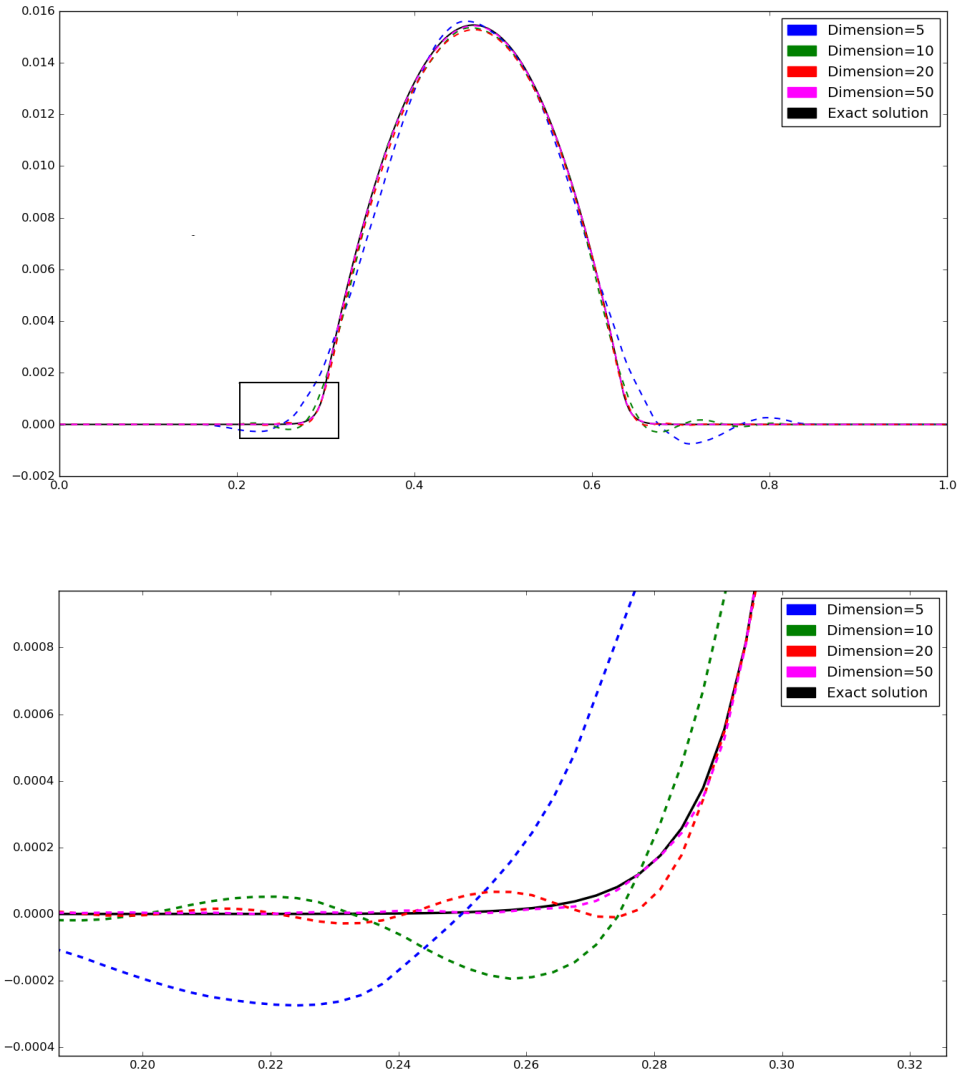

Figure 4. *1D problem.* $\kappa_{solvent} = 10^4$. *Solutions obtained by the Galerkin method compared to the exact solution for a certain parameter p with varying dimension of Ansatz space.*

Table 1

Comparison of required solver calls of Galerkin (G), discrete projection (P), and collocation method (C) for a given convergence criterion $\epsilon = 10^{-8}$ *to reach convergence.*

	$\kappa_{\text{solvent}} = 1$			$\kappa_{\text{solvent}} = 10^3$		
m	P	G	C	P	G	C
5	100	100	100	325	350	325
10	400	400	400	1299	1500	1299
15	900	900	900	2923	3600	2923
20	1600	1600	1600	5197	6800	5197
25	2500	2500	2500	8118	10625	8118
30	3600	3600	3600	11693	16200	11683

Table 2

Comparison of relative residuum error and RMSE of Galerkin (G), discrete projection (P), and collocation method (C) for $\kappa_{solvent} = 1$ and $m_1 = 2m - 1$.

	Rel. residuum error			Rel. RMSE		
m	P	G	C	P	G	C
5	$5.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$9.0 \cdot 10^{-3}$	$9.0 \cdot 10^{-3}$	$7.4 \cdot 10^{-3}$
10	$2.6 \cdot 10^{-3}$	$2.6 \cdot 10^{-3}$	$2.4 \cdot 10^{-3}$	$5.1 \cdot 10^{-3}$	$5.1 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$
15	$1.7 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$4.9 \cdot 10^{-3}$	$4.9 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$
20	$1.3 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$4.9 \cdot 10^{-3}$	$4.9 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$
25	$1.1 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$5.4 \cdot 10^{-3}$
30	$1.0 \cdot 10^{-3}$	$1.0 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$5.4 \cdot 10^{-3}$

Table 3

Comparison of relative residuum error and RMSE of Galerkin (G), discrete projection (P), and collocation method (C) for $\kappa_{solvent} = 10^3$ and $m_1 = 2m - 1$.

	Rel. residuum error			Rel. RMSE		
m	P	G	C	P	G	C
5	$1.9 \cdot 10^{-1}$	$1.9 \cdot 10^{-1}$	$1.7 \cdot 10^{-1}$	$9.4 \cdot 10^{-2}$	$9.4 \cdot 10^{-2}$	$7.3 \cdot 10^{-2}$
10	$8.6 \cdot 10^{-2}$	$8.4 \cdot 10^{-2}$	$7.6 \cdot 10^{-2}$	$3.8 \cdot 10^{-2}$	$4.1 \cdot 10^{-2}$	$3.6 \cdot 10^{-2}$
15	$5.4 \cdot 10^{-2}$	$5.3 \cdot 10^{-2}$	$4.9 \cdot 10^{-2}$	$3.2 \cdot 10^{-2}$	$3.5 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$
20	$4.0 \cdot 10^{-2}$	$3.9 \cdot 10^{-2}$	$3.8 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$3.4 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$
25	$3.3 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$	$3.4 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$	$3.2 \cdot 10^{-2}$
30	$2.9 \cdot 10^{-2}$	$2.9 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$3.1 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$	$3.2 \cdot 10^{-2}$

by the fast convergence of Newton's method and on the other hand by the dominant error caused by the chosen polynomial spaces and collocation nodes.

Tables 2 and 3 show a comparison of relative residuum error and RMSE of the different methods when varying m the amount of ansatz functions in both test cases. In the case of a moderate SNR (Table 2) the different methods need the same amount of solver calls. Additionally, the errors of the Galerkin and projection methods are not discernable. On the contrary the collocation method fares comparably better for smaller m, but soon stagnates especially when comparing relative RMSE. The case of less SNR (Table 3) shows the expected differences between the discrete projection method and the Galerkin: the former method performs better in terms of relative RMSE while the latter performs better in terms of relative residuum error.

5.2.3. The two-dimensional case—Additional randomness. looseness=1As a final example we choose $\kappa_{\text{solvent}} = 1$ and the permittivity A piecewise constant with values A_{solvent} and A_{molecule}. For additional randomness, we introduce the varying diameter of the molecule which we assume to be uniformly distributed on $[0, 1/3]$. Figures 5, 6, and 7 show the dependency of relative residuum error and error on the fineness h of the FEM-discretization. Since discrete projection and the Galerkin method behave similarly the latter one is not included in Figures 5 and 6. Interestingly enough, decreasing h leads to a significant improvement in terms of relative RMSE, required solver calls, and, more so, residuum error. Comparing the number of solver calls for small h is not very meaningful since the computation time for each solver call grows excessively fast as h goes to 0. Therefore it is also necessary to compare the overall computation time. For $h \in \{0.05, 0.045, \ldots, 0.03\}$, the computation time for one

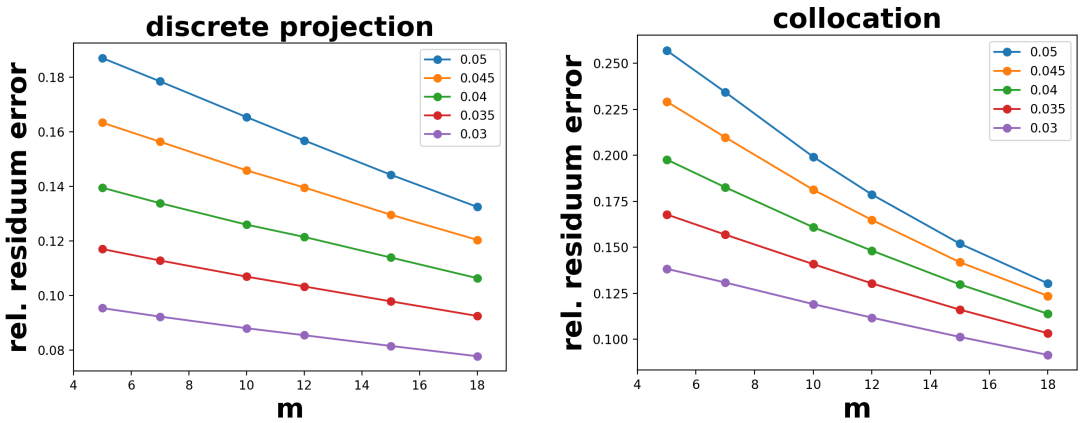

Figure 5. *Comparison of relative residuum error varying m, $m_1 = 2m - 1$ and fineness of the spatial discretization h, which is displayed in the legend. $A_{solvent} = 1$ and $A_{molecule} = 10$.*

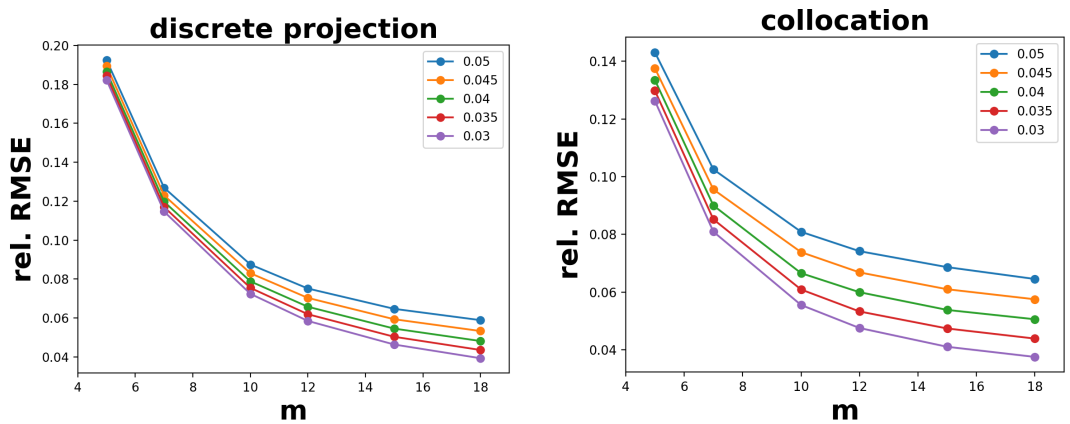

Figure 6. *Comparison of relative RMSE varying m, $m_1 = 2m - 1$ and fineness of the spatial discretization h, which is displayed in the legend. $A_{solvent} = 1$ and $A_{molecule} = 0.01$.*

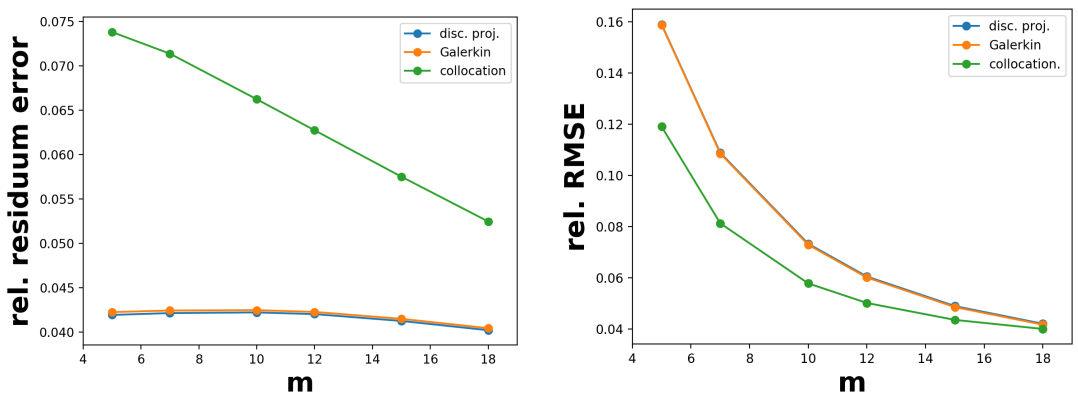

Figure 7. *Comparison of relative residuum error and RMSE of discrete projection and the collocation method varying m, $m_1 = 2m - 1$. $h = 0.03$, $A_{solvent} = 0.01$, and $A_{molecule} = 1$.*

solver call increases 1.5-fold when h decreases by 0.05. It becomes apparent for all three test cases and methods that decreasing the mesh size is more efficient in terms of residuum error, whereas increasing the amount of used ansatz functions (for fixed h) fares better in terms of RMSE. It is worth mentioning that since the permittivity A was dependent on the random parameter different stiffness matrices had to be computed. This turned out to be disadvantageous for the Galerkin-type method, as in each iteration of Algorithm 1 these matrices are required, which in turn leads either to increased computational overhead or excessive memory consumption.

6. Conclusions. We have proved the existence and uniqueness for solutions of the stochastic nonlinear Poisson–Boltzmann equation. Under additional assumptions regularity properties of the solution were shown. Apart from that, different nonintrusive stochastic approximation methods were implemented, using Legendre nodes and weights for numerical quadrature and interpolation. The great advantage of a nonintrusive approach is that it makes it possible to reuse any existing solvers for the deterministic equation. Analogous algorithms can immediately be used for other stochastic partial differential equations. We use Newton's method and low-order finite elements for solving the nonlinear deterministic equation.

Several test cases in one and two dimensions with varying coefficients (5) are discussed. The considered methods were investigated in view of relative residuum error and RMSE. This was done by varying the number of ansatz functions, precision of quadrature formulas, and fineness of spatial discretization. By comparing the Galerkin method to the discrete projection method, it was found that the Galerkin method is an alternative, which overall requires the same number of or slightly more solver calls to reach a comparable accuracy in both error notions. Particularly in the last test case, the structure of Algorithm 1 turned out to be a disadvantage for the Galerkin-type method. The collocation method outperformed the other methods when a smaller amount of ansatz functions and collocation nodes were used. Results seem to indicate that for more difficult problems with a higher-dimensional parameter space, the collocation method would prove to be more efficient, as in order to obtain convergence, the other methods require ansatz spaces which suffer distinctly from the curse of dimensionality. In order to reduce the effect of dimensional scaling, in the case where the randomness stems from many identical molecules, integration methods exploiting symmetry properties can be applied [32, 33]. Looking deeper into the results, one observes a numerical confirmation of the theoretical part of [8], concerning the convergence of the Galerkin-type method. Due to the fast convergence rate of Newton's method, it was not of great interest to look at different convergence criteria. The influence of the number of ansatz functions, of the number of quadrature nodes, and of different convergence criteria was investigated. Increasing the number of ansatz functions and quadrature nodes reduces relative residuum error and RMSE as expected. Our results suggest that decreasing the mesh size is more efficient in terms of residuum error, whereas increasing the amount of used ansatz functions (for fixed h) fares better in terms of RMSE.

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