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Abstract

Convergence of an adaptive collocation method for the stationary parametric diffusion equation with finite-dimensional affine coefficient is shown. The adaptive algorithm relies on a recently introduced residual-based reliable a posteriori error estimator. For the convergence proof, a strategy recently used for a stochastic Galerkin method with an hierarchical error estimator is transferred to the collocation setting.

1 Introduction

Collocation methods have become a mainstay for solving equations containing high-dimensional parameters such as arise in uncertainty quantification (UQ) analyses of ordinary or partial differential equations (ODE/PDE) with uncertain model coefficients [37, 45, 1]. It was realized early on that already moderately high-dimensional problems become tractable only when the approximations are based on sparse subspaces of the basic tensor product construction [42, 41, 10, 36, 9, 4].

Subsequent work established that, under mild conditions, certain classes of random PDEs are tractable even in presence of countably many parameter variables [15, 16, 44, 14, 14, 3, 46, 33, 2, 11, 25]. These results prove that *there exists* a sequence of converging approximation operators (be they of collocation or Galerkin/projection nature) and derive the corresponding convergence rates. Such sequence of converging approximation operators can be sometimes estimated a priori as in [46, 11, 25]. Another possible procedure is to rely instead on a posteriori adaptive strategies: the details of these strategies vary depending on the type of approximation operators (projection/collocation) and, moreover, these a posteriori adaptive strategies are often based on heuristics known to behave well in practice (even better than the a priori constructions) but for which a proof of convergence is lacking.

For projection approaches, adaptive stochastic Galerkin finite element methods (ASGFEM), which control the discretization of both physical and parametric variables, are well-studied. The extensive research activity in the last years comprises in particular residual-based error estimators [20, 24, 22, 23] and hierarchical error estimators [5, 8, 18, 6]. The setting in these works is similar to the one considered here, i.e., linear elliptic PDEs with affine parametric coefficients. However, there a countable infinite expansion is assumed, which makes an additional dimension adaptivity necessary. With the employed Legendre chaos discretization for the parameter space, only the margin of the active set of polynomials has to be considered in the error estimator. The developed error estimators are shown to be reliable and efficient, which for hierarchical estimators usually requires additional assumptions. Convergence of an ASGFEM algorithm was first shown in [24] for a residual estimator and, using a different argument, in [6] for a hierarchical estimator. A goal-oriented error estimator was presented in [7] and the more involved case of nonlinear coefficients and Gaussian parameters has only been considered recently in [21] with a low-rank hierarchical tensor discretization.

On the stochastic collocation side, the current literature discusses quite extensively algorithms for stochastic adaptivity, whereas much less attention has been devoted to (reliable) spatial adaptivity. To date, most adaptive sparse grid approximation schemes involve some variation of the basic procedure proposed by Gerstner and Griebel in [28], see also [32]. This algorithm drives adaptivity in the parameter variables by exploring at each iteration a certain number of admissible sparse subspaces to the approximation and then evaluating for each of these an *error indicator*; this requires solving a certain number of PDEs. The subspace with the largest error indicator is selected and added to the approximation, and a new set of admissible sparse subspaces for the next enrichment step is generated. Several error indicators and variations of the selection strategy have been considered, see e.g. [34, 29, 44, 14, 40, 27]. A crucial point is that these error indicators are *heuristics*. Conversely, the work by [31] proposes a variation of the Gerstner–Griebel algorithm based on a reliable residual-based error *estimator* which can control adaptivity in both the physical and parametric variables. Another significant difference compared with typical indicator-based adaptive algorithms is that in the procedure proposed in [31] evaluates the error estimator *without solving additional PDEs*. This allows significant computational savings with respect to the basic Gerstner–Griebel algorithm. For other works discussing spatial adaptivity in the context of stochastic collocation methods, see [43, 35].

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No convergence analysis is given in [31] for the proposed algorithm, and our contribution in this work is to close this gap. We do this by proving convergence of a slight modification of the algorithm in [31] thus establishing the first (to our knowledge) convergence result for an adaptive sparse collocation method. Our convergence analysis is based on a convergence theorem for abstract adaptive approximations (i.e., which covers both projection and collocation approximations, as well as other possible approximation strategies) w.r.t. the parameter variables. We derive this theorem by generalizing some results given in [6], which focused on convergence of adaptive stochastic Galerkin methods. This approach of proving convergence requires that the error estimator used have the propery of *reliability*. In [31] the authors already established this property for their error estimator, but only for a specific model problem, namely, an elliptic PDE whose diffusion coefficient depends linearly on a finite number of parameters. Moreover, we also require the underlying univariate sequence of collocation points to be nested in order that the sparse collocation construction is interpolatory. Hence, our particular convergence result is also tied to these assumptions on the underlying PDE and collocation points. However, we think that the general approach on establishing convergence of adaptive sparse collocation methods presented in this paper might be adapted to more general cases in the future. We note that our analysis considers adaptivity in the parameter variables only, i.e., we consider the semi-discrete setting.

The remainder of this paper is structured as follows. Sections 2 and 3 contain preliminary information: in particular, Section 2 states the model problem and recalls the results in [6] that will be instrumental for the rest of the work, while Section 3 gives details on the construction of adaptive sparse grid collocation schemes. Sections 4 and 5 contain our main results: Sections 4 contains the statement of the specific adaptive collocation algorithm, the associated convergence result, and some discussion on computational aspects, while Section 5 contains the proof of the convergence result. Finally, conclusions and future research directions are outlined in Section 6.

2 Preliminaries

In this section we specify the model problem under consideration and recall basic properties of its solution. Furthermore, we discuss general adaptive approximations w.r.t. the parameter variables and state an abstract convergence result which provides the basis of our convergence analysis for adaptive sparse grid collocation.

2.1 Model Problem

We consider a common model problem arising in uncertainty propagation via random differential equations, i.e., the stationary diffusion equation containing a coefficient function which depends linearly on a high-dimensional parameter. Specifically, we wish to solve the parametric elliptic boundary value problem

$$-\nabla \cdot (a(\boldsymbol{y})\nabla u(\boldsymbol{y})) = f, \qquad \text{on } D \subset \mathbb{R}^d \tag{1a}$$

$$u(\boldsymbol{y}) = 0, \qquad \text{on } \partial D. \tag{1b}$$

The domain $D \subset \mathbb{R}^d$ is assumed to be bounded and Lipschitz, $f \in L^2(D)$ and the coefficient $a(\boldsymbol{y}) \in L^\infty(D)$ is given by

$$a(\boldsymbol{x}, \boldsymbol{y}) = a_0(\boldsymbol{x}) + \sum_{m=1}^{M} a_m(\boldsymbol{x})\, y_m, \qquad \boldsymbol{y} \in \boldsymbol{\Gamma} := \Gamma^M,\ \Gamma := [-1, 1], \tag{2}$$

where $M \in \mathbb{N}$ is a finite number and $a_0, \dots, a_M \in L^\infty(D)$. Further, we assume that the functions $a_0, \dots, a_M \in L^\infty(D)$ satisfy the *uniform ellipticity condition*

$$\sum_{m=1}^{M} |a_m(\boldsymbol{x})| \le a_0(\boldsymbol{x}) - r, \qquad \forall x \in D, \tag{3}$$

for some $r > 0$. This implies that

$$a_{\min} := \min_{\boldsymbol{y} \in \boldsymbol{\Gamma}} \operatorname*{ess\,inf}_{\boldsymbol{x} \in D} a(\boldsymbol{x}, \boldsymbol{y}) \ge r > 0. \tag{4}$$

We then define the constant

$$\alpha := 1 - \frac{a_{\min}}{\inf_{x \in D} a_0(\boldsymbol{x})} \in (0, 1), \tag{5}$$

which will turn out to be important in Theorem 1 below. Due to the uniform ellipticity assumption, the weak solution $u(\boldsymbol{y}) \in \mathcal{H} = H_0^1(D)$ exists for any $\boldsymbol{y} \in \boldsymbol{\Gamma}$ and satisfies $u \in C(\boldsymbol{\Gamma}; \mathcal{H})$.

Polynomial expansions In order to approximate the solution u of (1), or rather the parameter-to-solution map $\boldsymbol{y} \mapsto u(\cdot, \boldsymbol{y}) \in \mathcal{H}$, we shall analyze polynomial expansions of u in the parameter $\boldsymbol{y} \in \boldsymbol{\Gamma}$,

$$u(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{k} \in \mathcal{F}} u_{\boldsymbol{k}}(\boldsymbol{x}) P_{\boldsymbol{k}}(\boldsymbol{y}), \qquad \mathcal{F} := \mathbb{N}_0^M, \quad u_{\boldsymbol{k}} \in \mathcal{H}, \tag{6}$$

where $P_{\boldsymbol{k}}(\boldsymbol{y}) = \prod_{m=1}^M P_{k_m}(y_m)$ is a finite product of univariate polynomials $P_k \colon \Gamma \to \mathbb{R}$ of degree k with $P_0 \equiv 1$. Two common choices for the basic polynomials P_k are

1 *Taylor polynomials:* $P_{\boldsymbol{k}}(\boldsymbol{y}) := \boldsymbol{y}^{\boldsymbol{k}} = \prod_{m=1}^M y_m^{k_m}$ where then

$$u_{\boldsymbol{k}}(\boldsymbol{x}) = t_{\boldsymbol{k}}(\boldsymbol{x}) := \frac{1}{\boldsymbol{k}!} \partial^{\boldsymbol{k}} u(\boldsymbol{x}, \boldsymbol{0}),$$

2 *Legendre polynomials:* $P_{\boldsymbol{k}}(\boldsymbol{y}) := L_{\boldsymbol{k}}(\boldsymbol{y}) = \prod_{m=1}^M L_{k_m}(y_m)$ with L_k denoting the kth $L^2_{\mu_1}$-normalized Legendre polynomial w.r.t. the uniform distribution $\mu_1(\mathrm{d}x) = \frac{\mathrm{d}y}{2}$ on $\Gamma = [-1, 1]$ and

$$u_{\boldsymbol{k}}(\boldsymbol{x}) := \int_{\boldsymbol{\Gamma}} u(\boldsymbol{x}, \boldsymbol{y}) L_{\boldsymbol{k}}(\boldsymbol{y}) \, \mu(\mathrm{d}\boldsymbol{y}).$$

Since $u \in C(\boldsymbol{\Gamma}; \mathcal{H}) \subset L^2_\mu(\boldsymbol{\Gamma}; \mathcal{H})$ we have that the expansion (6) using Legendre polynomials converges in $L^2_\mu(\boldsymbol{\Gamma}; \mathcal{H})$. The following result due to [3] establishes under suitable assumptions an ℓ^p-summability of both Taylor and Legendre coefficients which, for instance, implies that the Taylor expansion (6) of u converges in $L^\infty(\boldsymbol{\Gamma}; \mathcal{H})$.

Theorem 1 ([3, Theorem 2.2 & 3.1, Corollary 2.3 & 3.2])**.** *Let the condition* (3) *for* a *as in* (2) *be satisfied. Then a unique solution* u *of the corresponding elliptic problem* (1) *exists and belongs to* $C(\boldsymbol{\Gamma}; \mathcal{H})$*. Moreover, for any* $\boldsymbol{\rho} := (\rho_m)_{m=1}^M$ *with* $1 < \rho_m < \alpha^{-1}$ *with* α *as in* (5)

1 *the Taylor coefficients* $t_{\boldsymbol{k}} \in \mathcal{H}$ *of* u *satisfy* $(\boldsymbol{\rho}^{\boldsymbol{k}} \| t_{\boldsymbol{k}} \|_{\mathcal{H}})_{\boldsymbol{k} \in \mathcal{F}_M} \in \ell^2(\mathcal{F}_M)$*,*

2 *and the Legendre coefficients* $u_{\boldsymbol{k}} \in \mathcal{H}$ *of* u *satisfy* $(b_{\boldsymbol{k}}^{-1} \boldsymbol{\rho}^{\boldsymbol{k}} \| u_{\boldsymbol{k}} \|_{\mathcal{H}})_{\boldsymbol{k} \in \mathcal{F}_M} \in \ell^2(\mathcal{F}_M)$ *with* $b_{\boldsymbol{k}} := \prod_{m=1}^M \sqrt{1 + 2k_m}$*.*

Remark 2. *The authors of [3] actually consider the infinite-dimensional noise case, i.e., with* $M = \infty$ *in* (2)*, and prove the results stated in Theorem 1 under the assumption that*

$$\left\| \frac{\sum_{m=1}^\infty \rho_m |a_m|}{a_0} \right\|_{C(D)} < 1,$$

for a sequence $\boldsymbol{\rho} := (\rho_m)_{m \geq 1}$ *with* $\rho_m > 1$*. Hence, Theorem 1 can be derived easily from this general case by setting* $a_m(\boldsymbol{x}) \equiv 0$ *and* $\rho_m > 1$ *arbitrarily for* $m > M$*:*

$$\left\| \frac{\sum_{m=1}^\infty \rho_m |a_m|}{a_0} \right\|_{C(D)} = \left\| \frac{\sum_{m=1}^M \rho_m |a_m|}{a_0} \right\|_{C(D)} < \alpha^{-1} \left\| \frac{\sum_{m=1}^\infty |a_m|}{a_0} \right\|_{C(D)} \leq \alpha^{-1} \, (1 - a_{\min}) = 1.$$

2.2 Adaptive Polynomial Approximation

Given the decay rate stated in Theorem 1 for the norms of the coefficients $u_{\boldsymbol{k}}$ of the expansion (6), a polynomial approximation of u seems feasible. To this end, we consider the truncated expansions u_Λ based on a finite multi-index set $\Lambda \subset \mathcal{F}$,

$$u_\Lambda := S_\Lambda u = \sum_{\boldsymbol{k} \in \Lambda} \widehat{u}_{\boldsymbol{k}} P_{\boldsymbol{k}}, \qquad \widehat{u}_{\boldsymbol{k}} \in \mathcal{H},$$

where S_Λ denotes a suitable *approximation operator* and $\widehat{u}_{\boldsymbol{k}}$ are approximations to the true coefficients $u_{\boldsymbol{k}}$ of u (cf. (6)). For instance, S_Λ could be the operator associated with a Galerkin approach for approximating u using the finite-dimensional polynomial space

$$\mathcal{P}_\Lambda(\boldsymbol{\Gamma}) := \operatorname{span} \{ P_{\boldsymbol{k}} \colon \boldsymbol{k} \in \Lambda \},$$

or, as we in our case later, the operator associated to sparse grid collocation based on Λ. At this point we do not need to further specify S_Λ.

Algorithm 1 Generic adaptive algorithm

$\Lambda_0 = \{\mathbf{0}\}$
$u_0 := S_{\Lambda_0} u$
for $n \in \mathbb{N}_0$ **do**
  Choose a *candidate set* of multi-indices $\mathcal{C}_n \subset \mathcal{F} \setminus \Lambda_n$ for enriching Λ_n
  Evaluate estimates of the error contribution on the candidate set:

$$\eta_n(\boldsymbol{k}) = \eta(\boldsymbol{k}, u_n), \quad \boldsymbol{k} \in \mathcal{C}_n$$

  Determine *marked indices* $\mathcal{M}_n \subset \mathcal{C}_n$ (according to a given marking strategy based on $\eta_n(\boldsymbol{k})$);
  Set $\Lambda_{n+1} := \Lambda_n \cup \mathcal{M}_n$
  Set $u_{n+1} := S_{\Lambda_{n+1}} u$.
end for

We consider in particular an *adaptive approach* to compute such polynomial approximations u_Λ. More specifically, starting from an initial set $\Lambda_0 \subset \mathcal{F}$ we construct nested multiindex sets $\Lambda_n \subset \Lambda_{n+1}$, $n \in \mathbb{N}_0$, and compute the associated polynomial approximations $u_n := S_{\Lambda_n} u$ by the generic adaptive algorithm detailed in Algorithm 1. Again, we do not further specify how to compute the estimates $\eta_n(\boldsymbol{k}) = \eta(\boldsymbol{k}, u_n)$ at this point. Instead, we provide a fairly general convergence theorem for Algorithm 1, stating conditions on $\eta_n(\boldsymbol{k})$ that guarantee convergence of the algorithm.

The following theorem draws upon the work [6] on the convergence of adaptive stochastic Galerkin methods. Specifically, it is a compact summary of a way of proving for convergence for stochastic Galerkin outlined in detail in [6, Section 6 and 7], slightly modified to fit the application to adaptive sparse grid collocation. We state the theorem here and provide the proof at the end of the section.

Theorem 3 (cf. [6])**.** *Let u_n denote the approximations constructed via Algorithm 1. Assume that*

1 *the total error estimator $\eta_n := \sum_{\boldsymbol{k} \in \mathcal{C}_n} \eta_n(\boldsymbol{k})$ is reliable, i.e., there exists a constant $C < \infty$ independent of n such that*

$$\|u - u_n\| \leq C \eta_n,$$

where $\|\cdot\|$ denotes a suitable norm for functions $v \colon \boldsymbol{\Gamma} \to \mathcal{H}$,

2 *there exists a sequence of non-negative numbers $(\eta_\infty(\boldsymbol{k}))_{\boldsymbol{k} \in \mathcal{F}} \in \ell^1(\mathcal{F})$ such that for $(\widehat{\eta}_n(\boldsymbol{k}))_{\boldsymbol{k} \in \mathcal{F}}$ with $\widehat{\eta}_n(\boldsymbol{k}) := \eta_n(\boldsymbol{k})$ for $\boldsymbol{k} \in \mathcal{C}_n \cup \Lambda_n$ and $\widehat{\eta}_n(\boldsymbol{k}) = 0$ otherwise, we have*

$$\lim_{n \to \infty} \|\eta_\infty - \widehat{\eta}_n\|_{\ell^1} = 0,$$

3 *there exists a constant $c > 0$ independent of n such that for all $\boldsymbol{k} \in \mathcal{C}_n \setminus \mathcal{M}_n$ we have*

$$\eta_n(\boldsymbol{k}) \leq c \sum_{\boldsymbol{i} \in \mathcal{M}_n} \eta_n(\boldsymbol{i}).$$

From these assumptions it follows that

$$\lim_{n \to \infty} \|u - u_n\| = 0.$$

Remark 4. *Before we prove the theorem, we comment on the second and third assumption:*

1 *The third assumption is generally easily to satisfy. For instance, simply choosing $\mathcal{M}_n := \arg\max_{k \in \mathcal{C}_n} \eta_n(\boldsymbol{k})$ satisfies the assumption with $c = 1$.*

2 *For sparse grid collocation, the second assumption turns out to be the most difficult to verify. Moreover, it is probably the most cryptic assumption of the theorem. It can usually be verified as follows: assuming the sequence u_n has a limit u_∞ with corresponding error estimators $\eta_\infty(\boldsymbol{k}) := \eta(\boldsymbol{k}, u_\infty)$, conclude from $u_n \to u_\infty$ that $\|\eta_\infty - \widehat{\eta}_n\|_{\ell^1} \to 0$ by exploiting continuity properties of the error estimator $\eta(\boldsymbol{k}, u_n)$ w.r.t. u_n. Note that in principle u_∞ is just the limit of u_n, but does not necessarily coincide with the actual solution of the PDE (1). The fact that $u_\infty = u$ is the asesrtion of the theorem.*

3 As we will see in the proof of Theorem 3, the second assumption represents some kind of saturation of the reliable error estimators η_n: since $\|\eta_\infty - \widehat{\eta}_n\|_{\ell^1(\mathbb{N})} \to 0$ we have that

$$\eta_n \leq \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) + \sum_{\boldsymbol{k}\in\mathcal{C}_n} |\eta_n(\boldsymbol{k}) - \eta_\infty(\boldsymbol{k})| \leq \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) + \|\widehat{\eta}_n - \eta_\infty\|_{\ell^1(\mathbb{N})}$$

converges to zero if $\sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k})$ does. Since $\|\widehat{\eta}_n - \eta_\infty\|_{\ell^1(\mathbb{N})} < \infty$ we can expect $\eta_\infty(\boldsymbol{k})$ to decay for large multi-indices $\boldsymbol{k}$. Thus, if $\mathcal{C}_n$ tends to include increasingly larger multi-indices $\boldsymbol{k}$, then $\sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k})$ should decay to zero. This will be made rigorous in the subsequent proof.

The proof of Theorem 3 employs the following abstract lemma which was shown for the case $p = 2$ in [6, Lemma 15]. Since their proof can be generalized to arbitrary $1 \leq p < \infty$ without any significant modification we simply state the result and refer to [6, Lemma 15] for a detailed proof.

Lemma 5 (cf. [6, Lemma 15])**.** *Let $\boldsymbol{z} = (z_k)_{k\in\mathbb{N}} \in \ell^p(\mathbb{N})$, $p \in [1,\infty)$, and $\boldsymbol{z}^{(n)} = (z_k^{(n)})_{k\in\mathbb{N}} \in \ell^p(\mathbb{N})$, $n \in \mathbb{N}_0$, be sequences of non-negative numbers satisfying $\lim_{n\to\infty} \|\boldsymbol{z} - \boldsymbol{z}^{(n)}\|_{\ell^p} = 0$. Assume further that there exists a continuous function $g\colon [0,\infty) \to [0,\infty)$ with $g(0) = 0$ and a sequence of nested subsets $\mathcal{J}_n \subset \mathbb{N}$, i.e., $\mathcal{J}_n \subset \mathcal{J}_{n+1}$, such that*

$$\forall n \in \mathbb{N}_0\ \forall k \notin \mathcal{J}_{n+1}\colon\ z_k^{(n)} \leq g\left(\sum_{i\in\mathcal{J}_{n+1}\setminus\mathcal{J}_n} \left(z_i^{(n)}\right)^p\right).$$

Then $\lim_{n\to\infty} \sum_{k\notin\mathcal{J}_n} z_k^p = 0$.

Proof of Theorem 3. Since the error estimator is reliable, we only need to show that

$$\lim_{n\to\infty} \eta_n = \lim_{n\to\infty} \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_n(\boldsymbol{k}) = 0.$$

Due to

$$\sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_n(\boldsymbol{k}) \leq \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) + \sum_{\boldsymbol{k}\in\mathcal{C}_n} |\eta_n(\boldsymbol{k}) - \eta_\infty(\boldsymbol{k})| \leq \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) + \|\widehat{\eta}_n - \eta_\infty\|_{\ell^1(\mathbb{N})},$$

as well as $\|\widehat{\eta}_n - \eta_\infty\|_{\ell^1} \to 0$ by assumption, the statement of the theorem follows if

$$\lim_{n\to\infty} \sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) = 0.$$

In order to show this we apply Lemma 5 as follows: we identify the countable set $\mathcal{F}$ with $\mathbb{N}$, η_∞ with $\boldsymbol{z}$ and $\widehat{\eta}_n$ with $\boldsymbol{z}^{(n)}$. Recall that by assumption $\|\widehat{\eta}_n - \eta_\infty\|_{\ell^1} \to 0$. Thus, the first assumption of Lemma 5 is satisfied. Moreover, we identify the $\Lambda_n \subset \mathcal{F}$ with $\mathcal{J}_n \subset \mathbb{N}$. These sets are nested and $\mathcal{J}_{n+1} \setminus \mathcal{J}_n$ corresponds to $\mathcal{M}_n$. By our third assumption and the construction of $\widehat{\eta}_n$ there holds for each $n \in \mathbb{N}$

$$\widehat{\eta}_n(\boldsymbol{k}) \leq c \sum_{\boldsymbol{i}\in\mathcal{M}_n} \widehat{\eta}_n(\boldsymbol{i}) \qquad \forall \boldsymbol{k} \notin \Lambda_{n+1},$$

since $\widehat{\eta}_n(\boldsymbol{k}) = 0$ for $\boldsymbol{k} \notin \mathcal{C}_n \cup \Lambda_n$ and $(\mathcal{C}_n \cup \Lambda_n) \setminus \Lambda_{n+1} = \mathcal{C}_n \setminus \mathcal{M}_n$. Thus, the second assumption of Lemma 5 is also satisfied with $g(s) = cs$. Hence, we can apply Lemma 5 to $\boldsymbol{z} \simeq \eta_\infty$ and $\boldsymbol{z}_n \simeq \widehat{\eta}_n$ and obtain that

$$\lim_{n\to\infty} \sum_{\boldsymbol{k}\notin\Lambda_n} \eta_\infty(\boldsymbol{k}) = 0,$$

which by $\sum_{\boldsymbol{k}\in\mathcal{C}_n} \eta_\infty(\boldsymbol{k}) \leq \sum_{\boldsymbol{k}\notin\Lambda_n} \eta_\infty(\boldsymbol{k})$ concludes the proof. □

3 Adaptive Sparse Grid Collocation.

We now introduce the sparse grid collocation approach and discuss how adaptive sparse grids algorithms can be derived from the abstract Algorithm 1. In particular, we show how to obtain the classical a-posterior adaptive algorithm from [28], based on heuristic error *indicators* (as opposed to reliable error *estimators* as in [31]). As already discussed in the introduction, changing from indicators to estimators is key to prove convergence. Our version of the estimator-based algorithm and its convergence are then discussed in the next sections.

Leja sequences of points. The first ingredient for any sparse grid construction is the choice of the underlying univariate sequences of collocation points. In this work, we consider nested point sequences, and a particularly convenient construction is offered by Leja points. Leja sequences on $\Gamma = [-1,1]$ are defined recursively by first choosing $y_{(1)} \in \Gamma$ and then setting

$$y_{(i)} = \arg\max_{y\in\Gamma} \prod_{k=1}^{i-1} (y - y_{(k)}), \quad i \in \mathbb{N}_0, \tag{7}$$

see e.g. [12, 14, 13, 44, 38]. The standard choice is to set $y_1 = -1$: equation (7) then leads to

$$y_{(1)} = -1, \quad y_{(2)} = 1, \quad y_{(3)} = 0, \quad y_{(4)} \approx -0.57735, \quad y_{(5)} \approx 0.65871, \ \dots \ .$$

Another common sequence, referred to as *R-Leja* (real Leja) points, is obtained by carrying out the Leja construction on the upper unit circle in the complex plane in place of $\Gamma = [-1,1]$ and then projecting the results onto the real line. This results in (see e.g. [12] for a proof):

$$y_{(i)} = \cos\phi_{(i)} \quad i \in \mathbb{N}_0$$
$$\phi_{(1)} = 0, \quad \phi_{(2)} = \pi, \quad \phi_{(3)} = \pi/2, \quad \phi_{(2n+2)} = \frac{\phi_{(n+2)}}{2}, \quad \phi_{(2n+3)} = \phi_{(2n+2)} + \pi.$$

Sparse grid collocation. We consider *hierarchical* sparse grid collocation based on nested sequences of node sets, such as the Leja sequences just introduced. To this end, let $(y_{(i)})_{i\in\mathbb{N}_0} \subset [-1,1]$ denote a sequence of univariate interpolation nodes with associated node sets,

$$\mathcal{Y}_n := \{y_{(i)} : i = 0, \dots, n\} \subset \Gamma, \qquad n \in \mathbb{N}_0.$$

Moreover, let $\mathcal{P}_n(\Gamma)$ denote the set of all univariate polynomials on Γ of degree at most $n \in \mathbb{N}_0$. We can then define for any Hilbert space-valued continuous function $f : \Gamma \to \mathcal{H}$ two objects:

- a Lagrange interpolant $\mathcal{I}_n : C(\Gamma;\mathcal{H}) \to \mathcal{P}_n(\Gamma;\mathcal{H})$,
- a univariate *detail operator* $\Delta_n : C(\Gamma;\mathcal{H}) \to \mathcal{P}_n(\Gamma;\mathcal{H})$,

$$\Delta_0 = \mathcal{I}_0, \qquad \Delta_n := \mathcal{I}_n - \mathcal{I}_{n-1}, \quad n \in \mathbb{N}.$$

The detail operators may be conveniently expressed in terms of the sequence $(h_n)_{n\in\mathbb{N}_0}$ of *hierarchical Lagrange polynomials* associated with the nested sequence of node sets $(\mathcal{Y}_n)_{n\in\mathbb{N}}$ defined by

$$h_n(y) := \prod_{i=0}^{n-1} \frac{y - y_{(i)}}{y_{(n)} - y_{(i)}} \in \mathcal{P}_n, \qquad n \in \mathbb{N}_0. \tag{8}$$

The nth hierarchical Lagrange polynomial is simply the last of the $n+1$ Lagrange fundamental polynomials $(\ell_j^{(n)})_{j=0}^n$ associated with the node set $\mathcal{Y}_n$. As is easily verified by evaluating at the nodes of $\mathcal{Y}_n$, the interpolant $\mathcal{I}_n f$ of a function $f \in C(\Gamma;\mathcal{H})$ can be expressed recursively as

$$(\mathcal{I}_n f)(y) = (\mathcal{I}_{n-1} f)(y) + [f(y_{(n)}) - (\mathcal{I}_{n-1} f)(y_{(n)})] h_n(y), \qquad n \in \mathbb{N},$$

and therefore

$$\Delta_n f = \left[f(y_{(n)}) - (\mathcal{I}_{n-1} f)(y_{(n)})\right] h_n, \quad n \in \mathbb{N}.$$

The term $f(y_{(n)}) - \mathcal{I}_{n-1} f(y_{(n)}) = (f - \mathcal{I}_{n-1} f)(y_{(n)})$ is also called *hierarchical surplus*. Next, consider tensorized detail operators

$$\Delta_{\boldsymbol{i}} := \bigotimes_{m=1}^{M} \Delta_{i_m}.$$

Given a (finite) subset $\Lambda \subset \mathcal{F}$ we define the *sparse grid collocation operator* associated with the *sparse grid* $\mathcal{Y}_\Lambda$ by

$$S_\Lambda := \sum_{\boldsymbol{i}\in\Lambda} \Delta_{\boldsymbol{i}}, \qquad \mathcal{Y}_\Lambda := \bigcup_{\boldsymbol{i}\in\Lambda} \mathcal{Y}_{\boldsymbol{i}}, \quad \mathcal{Y}_{\boldsymbol{i}} := \mathcal{Y}_{i_1} \times \mathcal{Y}_{i_2} \times \ldots \times \mathcal{Y}_{i_M}.$$

We require the multi-index sets $\Lambda \subset \mathcal{F}$ to be *downward-closed* (or *monotone*), which is the property that

$$\boldsymbol{i} \in \Lambda \quad \text{implies} \quad \boldsymbol{i} - \boldsymbol{e}_m \in \Lambda,$$

where $\boldsymbol{e}_m$ denotes the mth canonical unit multi-index. Downward-closedness of Λ implies three facts (see e.g. [25]): First,

$$\mathcal{Y}_\Lambda = \{\boldsymbol{y}_{(\boldsymbol{i})} \colon \boldsymbol{i} \in \Lambda\}, \qquad \boldsymbol{y}_{(\boldsymbol{i})} := (y_{(i_1)}\ y_{(i_2)}\ \cdots\ y_{(i_M)}) \in \boldsymbol{\Gamma};$$

second, that the sparse grid collocation operator yields an approximation in $P_\Lambda(\boldsymbol{\Gamma};\mathcal{H})$,

$$S_\Lambda \colon C(\boldsymbol{\Gamma};\mathcal{H}) \to \mathcal{P}_\Lambda(\boldsymbol{\Gamma};\mathcal{H})$$

and third, together with the nestedness of the node sets, that S_Λ is *interpolatory*, i.e.,

$$S_\Lambda f(\boldsymbol{y}_{(\boldsymbol{i})}) = f(\boldsymbol{y}_{(\boldsymbol{i})}) \qquad \forall \boldsymbol{y}_{(\boldsymbol{i})} \in \mathcal{Y}_\Lambda.$$

Adaptive sparse grid collocation algorithms. Two ways to construct monotone multi-index sets Λ for (hierarchical) sparse grid collocation are the classical algorithm introduced by Gerstner & Griebel in [28] (as well as numerous variations mentioned in the literature survey in the introduction) and the alternative algorithm introduced by Guignard & Nobile in [31]. Both can be seen as specific instances of the generic Algorithm 1. We describe the former here and the latter (or rather, a slight variation of it) in the next section, together with a convergence analysis. To introduce these algorithms, we need to specify three "ingredients": the candidate set $\mathcal{C}_n$, a *marking strategy* for determining the marked set $\mathcal{M}_n \subset \mathcal{C}_n$, and corresponding estimates $\eta_n(\boldsymbol{k})$ for the error contribution of indices in the candidate set. To this end, we require the following definitions:

- The *margin* $\operatorname{Marg}(\Lambda) \subset \mathcal{F}$ of a multi-index set $\Lambda \subset \mathcal{F}$ is given by

$$\operatorname{Marg}(\Lambda) := \{\boldsymbol{k} \in \mathcal{F} \setminus \Lambda \colon \boldsymbol{k} - \boldsymbol{e}_m \in \Lambda \text{ for some } m \in \mathbb{N}\}.$$

- The *reduced margin* $\operatorname{R}(\Lambda) \subset \operatorname{Marg}(\Lambda)$ of a subset $\Lambda \subset \mathcal{F}$ is given by

$$\operatorname{R}(\Lambda) := \{\boldsymbol{k} \in \operatorname{Marg}(\Lambda) \colon \boldsymbol{k} - \boldsymbol{e}_m \in \Lambda \text{ for all } m \in \mathbb{N}\}.$$

- The *monotone envelope* $E_\Lambda(\boldsymbol{k}) \subset \operatorname{Marg}(\Lambda)$ of a multi-index $\boldsymbol{k} \in \operatorname{Marg}(\Lambda)$:

$$E_\Lambda(\boldsymbol{k}) := \bigcap \{E \subset \operatorname{Marg}(\Lambda) \colon \boldsymbol{k} \in E \text{ and } \Lambda \cup E \text{ is monotone}\}.$$

  Note that $E_\Lambda(\boldsymbol{k})$ is the smallest (in cardinality) monotone multi-index set containing $\Lambda \cup \{\boldsymbol{k}\}$ and that for $\boldsymbol{k} \in \operatorname{R}(\Lambda)$ we have $E_\Lambda(\boldsymbol{k}) = \{\boldsymbol{k}\}$ by construction.

The adaptive procedure in [28] now chooses

- as its candidate set the reduced margin of Λ_n, i.e. $\mathcal{C}_n = \operatorname{R}(\Lambda_n)$;
- and estimates the error contribution of $\boldsymbol{k} \in \mathcal{C}_n$ by the L^p-norm of the hierarchical surplus, i.e.,

$$\eta_n(\boldsymbol{k}) = \|\Delta_{\boldsymbol{k}} u\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}, \quad \boldsymbol{k} \in \operatorname{R}(\Lambda_n). \tag{9}$$

  Note that this is merely an error *indicator* and not a proper *estimator*, i.e., no proof of the properties required by Theorem 3 is available. A large body of literature, however, provides numerical evidence that this error indicator is quite robust and gives good results in practice;
- its marking strategy selects the index in the reduced margin for which the value of η_n is largest to comprise the marked set, i.e., $\mathcal{M}_n = \{\arg\max_{\boldsymbol{k} \in \operatorname{R}(\Lambda_n)} \eta_n(\boldsymbol{k})\}$. Another possibility would be to use a Dörfler marking strategy and mark e.g. the 50% of the indices in the reduced margin with the largest η_n, cf. [19].

Algorithm 2 summarizes the Gerstner–Griebel scheme as pseudocode. Note that, since S_Λ is interpolatory for $\mathcal{Y}_n$ nested and Λ monotone, we can efficiently compute η_n in Equation 9, and therefore $S_{\Lambda_{n+1}}$ based on S_{Λ_n}. For this, let $\boldsymbol{i} \in \operatorname{R}(\Lambda_n)$ and $\Lambda_{n+1} = \Lambda_n \cup \{\boldsymbol{i}\}$. Then,

$$\Delta_{\boldsymbol{i}} u = [u(\boldsymbol{y}_{(\boldsymbol{i})}) - (S_{\Lambda_n} u)(\boldsymbol{y}_{(\boldsymbol{i})})]\, h_{\boldsymbol{i}}, \qquad h_{\boldsymbol{i}}(\boldsymbol{y}) := \prod_{m \geq 1} h_{i_m}(y_m),$$

where the h_i are the univariate hierarchical Lagrange polynomials defined in (8), see, e.g., [14]. The main shortcoming of this approach is that the computation of $\Delta_{\boldsymbol{i}} u$ requires solving the PDE to evaluate $u(\boldsymbol{y}_{(\boldsymbol{i})})$, and for this reason one may

Algorithm 2 Adaptive sparse grid algorithm of Gerstner and Griebel [28]

$\Lambda_0 := \{\mathbf{0}\}$
$u_0 := S_{\Lambda_0} u$
for $n \in \mathbb{N}_0$ **do**
  Compute reduced margin $\mathrm{R}(\Lambda_n)$
  Compute error indicators (reduced margin): $\eta_n(\boldsymbol{k}) = \|\Delta_{\boldsymbol{k}} u\|_{L^p(\Gamma;L^2(D))}, \quad \boldsymbol{k} \in \mathrm{R}(\Lambda_n)$
  Choose $\boldsymbol{k}_n^* := \arg\max_{\boldsymbol{k}\in\mathrm{R}(\Lambda_n)} \eta_n(\boldsymbol{k})$
  Set $\Lambda_{n+1} := \Lambda_n \cup \{\boldsymbol{k}_n^*\}$
  Set $u_{n+1} := S_{\Lambda_{n+1}} u$.
end for

refer to this algorithm as *fully a posteriori*. If the reduced margin is large, this operation can be expensive. Moreover, as previously mentioned, the choice of η_n in (9) is a heuristic and no convergence proof for the adaptive algorithm is available. To overcome this issue, we introduce and analyze in the next Section another variation of Algorithm 1, for which we can prove convergence.

We close this section by pointing out that using a hierarchical basis is convenient but not necessary, and the standard (non-hierarchical) Lagrange basis can also be used to implement Algorithm 2. One would then need to resort to the so-called *combination technique* [30] to evaluate the detail operators $\Delta_{\boldsymbol{i}} u$ and the computation of needs to be adjusted accordingly, see e.g. [40, 31]; this has the advantage that non-nested sequences of node sets (such as zeros of orthogonal polynomials) can be used if desired, see e.g. [40, 25].

4 Adaptive Sparse Collocation for the Diffusion Problem

We now turn attention to the above-mentioned slight variation of the adaptive algorithm by Guignard & Nobile from [31]; see Remark 7 for a discussion on the difference between the two versions. This algorithm is based on the following error estimator, for which reliability is also established in [31].

Proposition 6 ([31, Proposition 4.3])**.** *Let u denote the solution of the random elliptic PDE given in equation* (1) *with linear diffusion coefficient as in* (2)*, and let $\Lambda \subset \mathcal{F}$ be a monotone subset such that the sparse grid collocation operator S_Λ as introduced in Section 3 is interpolatory. Then, for any $p \in [1,\infty]$ we have*

$$\|u - S_\Lambda u\|_{L^p_\mu(\mathbf{\Gamma};H^1_0(D))} \leq \frac{1}{a_{\min}} \sum_{\boldsymbol{k}\in\mathrm{Marg}(\Lambda)} \|\Delta_{\boldsymbol{k}}(a\nabla S_\Lambda u)\|_{L^p_\mu(\mathbf{\Gamma};L^2(D))}.$$

This proposition suggests to use $\|\Delta_{\boldsymbol{k}}(a\nabla S_{\Lambda_n} u)\|_{L^p_\mu(\mathbf{\Gamma};L^2(D))}$ as error estimators $\eta_n(\boldsymbol{k})$ for adaptively constructing the sparse grid approximations $u_n = S_{\Lambda_n} u_n$ and also to consider the whole margins $\mathrm{Marg}(\Lambda_n)$ as candidate sets. This yields Algorithm 3. Note here that the value $p \in [1,\infty]$ has to be chosen in advance and that $\mathcal{C}_n := \mathrm{Marg}(\Lambda_n) \subset \mathcal{F}$ is in fact finite for finite M. Moreover, we highlight that Proposition 6 implies that Algorithm 3 satisfies the first assumption (the reliable error estimate) of the abstract convergence result, Theorem 3. Besides that also the third assumption of Theorem 3 is satisfied by construction, i.e, by the marking strategy $\mathcal{M}_n := E_{\Lambda_n}(\boldsymbol{k}_n^*)$ and the choice of $\boldsymbol{k}_n^*$, cf. Remark 4.

Remark 7 (Adaptive algorithm in [31])**.** *The difference between Algorithm 3 and the version in [31] is that in [31] the following* profit indicators *are introduced instead of the error estimators $\eta_n(\boldsymbol{k})$ given in* (10)*:*

$$\pi_n(\boldsymbol{k}) := \frac{\sum_{\boldsymbol{i}\in E_{\Lambda_n}(\boldsymbol{k})} \eta_n(\boldsymbol{i})}{\sum_{\boldsymbol{i}\in E_{\Lambda_n}(\boldsymbol{k})} W(\boldsymbol{i})}, \qquad \boldsymbol{k} \in \mathrm{Marg}(\Lambda_n), \tag{11}$$

with $W(\boldsymbol{i})$ denoting the work contribution of the multi-index $\boldsymbol{i}$, i.e., the number of new grid points required to evaluate $\Delta_{\boldsymbol{i}}$. Then, $\boldsymbol{k}_n^*$ is chosen as

$$\boldsymbol{k}_n^* := \arg\max_{\boldsymbol{k}\in\mathcal{C}_n} \pi_n(\boldsymbol{k}), \qquad \mathcal{M}_n := E_{\Lambda_n}(\boldsymbol{k}_n^*). \tag{12}$$

In our case of linearly growing univariate node sets $|\mathcal{Y}_n| = n+1$ we have $W(\boldsymbol{i}) \equiv 1$, i.e., $\pi_n(\boldsymbol{k}) = \frac{1}{|E_{\Lambda_n}(\boldsymbol{k})|} \sum_{\boldsymbol{i}\in E_{\Lambda_n}(\boldsymbol{k})} \eta_n(\boldsymbol{i})$ corresponds to the average error estimator on the monotone envelope $E_{\Lambda_n}(\boldsymbol{k})$. This adaptive algorithm thus favors multi-indices belonging to the reduced margin. We provide a more detailed discussion on both versions of the adaptive algorithm for the elliptic problem in Section 4.2 with a focus on computational aspects.

Algorithm 3 Adaptive sparse grid algorithm for the diffusion problem (1)

$\Lambda_0 := \{\mathbf{0}\}$
$u_0 := S_{\Lambda_0} u$
for $n \in \mathbb{N}_0$ **do**
  Compute margin as candidate set $\mathcal{C}_n := \operatorname{Marg}(\Lambda_n)$
  Compute error estimators:

$$\eta_n(\boldsymbol{k}) := \|\Delta_{\boldsymbol{k}}(a\nabla u_n)\|_{L^p_\mu(\mathbf{\Gamma};L^2(D))}, \quad \boldsymbol{k} \in \operatorname{Marg}(\Lambda_n) \tag{10}$$

  choose $\boldsymbol{k}_n^* := \arg\max_{\boldsymbol{k}\in\mathcal{C}_n} \eta_n(\boldsymbol{k})$
  set $\mathcal{M}_n := E_{\Lambda_n}(\boldsymbol{k}_n^*)$
  set $\Lambda_{n+1} := \Lambda_n \cup \mathcal{M}_n$
  compute $u_{n+1} := S_{\Lambda_{n+1}} u$.
end for

We now turn to our main result stating the convergence of Algorithm 3 under rather mild assumptions on the employed univariate interpolation nodes. In particular, we assume an algebraic growth of the corresponding operator norm of univariate the detail operators

$$\|\Delta_k\|_\infty := \sup_{0\not\equiv f\in C(\Gamma;\mathbb{R})} \frac{\|\Delta_k f\|_{C(\Gamma;\mathbb{R})}}{\|f\|_{C(\Gamma;\mathbb{R})}}, \qquad k \in \mathbb{N}_0.$$

Theorem 8 (Convergence of Algorithm 3)**.** *Given the assumptions of Theorem 1 and assuming that there exist finite constants* $0 \le c, \theta < \infty$ *such that*

$$\|\Delta_k\|_\infty \le (1+ck)^\theta \qquad \forall k \in \mathbb{N}_0, \tag{13}$$

the approximations u_n *constructed by Algorithm 3 satisfy*

$$\lim_{n\to\infty} \|u - u_n\|_{L^p_\mu(\mathbf{\Gamma};H^1_0(D))} = 0.$$

We already discussed above that Algorithm 3 satisfies the first and third assumption of the abstract convergence theorem, Theorem 3. Thus, it remains to verify the second assumption. This turns out to be rather technical and is outlined in details in Section 5. We comment first on the additional assumption of Theorem 8.

Remark 9 (Leja sequences)**.** *The condition* (13) *on the "Lebesgue constant"*$\|\Delta_i\|_\infty$ *of the univariate detail operators is satisfied if the corresponding interpolation operators* $\mathcal{I}_n$ *possess an at most algebraically increasing Lebesgue constant*

$$\|\mathcal{I}_n\|_\infty := \sup_{0\not\equiv f\in C(\Gamma;\mathbb{R})} \frac{\|\mathcal{I}_n f\|_{C(\Gamma;\mathbb{R})}}{\|f\|_{C(\Gamma;\mathbb{R})}} \le \frac{c}{2} n^\theta \qquad \forall n \ge 1, \tag{14}$$

for finite constants $0 \le c, \theta < \infty$*. In fact,* (13) *is satisfied since for* $\Delta_0 = \mathcal{I}_0$ *we have* $\|\Delta_0\|_\infty = \|\mathcal{I}_0\|_\infty = 1$ *and* (14) *implies*

$$\|\Delta_i\|_\infty \le \|\mathcal{I}_i\|_\infty + \|\mathcal{I}_{i-1}\|_\infty \le c i^\theta \qquad \forall i \ge 1.$$

Note that the algebraic growth (14) *holds, for instance, for interpolation based on Leja and R-Leja nodes* $y^{(j)} \in [-1,1]$ *introduced earlier, see [12, 13, 39] and references therein.*

4.1 Extensions of Theorem 8

In this subsection we comment on two possible extensions of the convergence result in Theorem 8.

Extension to Clenshaw–Curtis nodes. Algorithm 3 as well as the proof of Theorem 8 can easily be extended to non-linearly growing nested univariate nodes sets

$$\mathcal{Y}_n = \{y^{(i)} \colon i = 0, \dots, g(n)\}, \qquad n \in \mathbb{N}_0,$$

where $g(\cdot)\colon \mathbb{N}_0 \to \mathbb{N}$ denotes the growth function with $m(0) = 1$. A common example for such node sets are the *Clenshaw–Curtis nodes* combined with the doubling rule $g(n) = 2^n + 1$ for $n \ge 1$. Note that the resulting univariate interpolation operators $\mathcal{I}_n$ satisfy condition (14) (see e.g. [39]) and therefore the assumptions of Theorem 8, cf. Remark 9.

Proving the convergence of the adaptive algorithm in [31]. As outlined in Remark 7 the adaptive algorithm proposed in [31] differs from Algorithm 3 only by the marking strategy, or to be more precise, by the choice of $\boldsymbol{k}_n^*$, see (12). Thus, in order to extend Theorem 8 to this algorithm it suffices to verify that the third assumption of the general Theorem 3 also holds for the marking strategy (12) w.r.t. to the error estimators η_n given in (10). This can be ensured by a mild additional assumption: there exists a constant $0 < c < \infty$ such that for any monotone multi-index set Λ we have

$$\max_{\boldsymbol{k}\in\mathrm{Marg}(\Lambda)} \eta_\Lambda(\boldsymbol{k}) \leq c \max_{\boldsymbol{k}\in\mathrm{R}(\Lambda)} \eta_\Lambda(\boldsymbol{k}), \qquad \eta_\Lambda(\boldsymbol{k}) := \|\Delta_{\boldsymbol{k}}(a\nabla S_\Lambda u)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}, \tag{15}$$

i.e., the largest error estimator in the *full margin* can be bounded by the constant times the largest error estimator in the *reduced margin*. Indeed, by construction of the profits π_n in (11) and of the marking strategy in (12) we always have

$$\max_{\boldsymbol{k}\in\mathrm{R}(\Lambda_n)} \eta_n(\boldsymbol{k}) \leq \sum_{\boldsymbol{i}\in\mathcal{M}_n} \eta_n(\boldsymbol{i}),$$

due to $\pi_n(\boldsymbol{k}) = \eta_n(\boldsymbol{k})$ for $\boldsymbol{k} \in \mathrm{R}(\Lambda_n)$. Condition (15) then guarantees that the third assumption of Theorem 3 is also satisfied for the marking strategy (12). We consider (15) as a plausible assumption in practice, although pathological counterexamples might possibly be constructed.

4.2 Computational Considerations

Having established the convergence of the adaptive Algorithm 3, we comment on the computational advantages and disadvantages of this algorithm compared to the classical Gerstner & Griebel adaptive sparse grid algorithm (GG algorithm for short in the following) as outlined in Section 3:

1 The GG algorithm considers candidate indices in the *reduced margin* instead of the *full margin*. This makes treating problems with high-dimensional parameters somewhat easier with the GG algorithm, since the size of the full margin grows substantially faster than the reduced margin.

2 However, as already mentioned, the GG algorithm is *fully a posteriori*: evaluating the error indicators involves actually evaluating u (i.e., solving additional PDEs) on the new collocation points $\mathcal{Y}_n^+(\boldsymbol{k}) = \mathcal{Y}_{\boldsymbol{k}} \setminus \mathcal{Y}_{\Lambda_n\cup\{\boldsymbol{k}\}}$ for each $\boldsymbol{k} \in \mathrm{R}(\Lambda_n)$, see (9) Algorithm 2. By contrast, Algorithm 3 computes its error estimator by evaluating *the current sparse grid interpolant* u_n at the new collocation points $\mathcal{Y}_n^+(\boldsymbol{k})$ for $\boldsymbol{k} \in \mathrm{Marg}(\Lambda_n)$. This is a significant advantage of the error estimator-based algorithms over the GG algorithm, in particular if solving the PDE for individual parameter values is computationally expensive.

3 On the other hand, because the error estimators are based on the current approximation, they have to be recomputed in each step of Algorithm 3, i.e., $\eta_n(\boldsymbol{k}) \neq \eta_{n+1}(\boldsymbol{k})$ for any $\boldsymbol{k} \in \mathrm{Marg}(\Lambda_n) \cap \mathrm{Marg}(\Lambda_{n+1})$. This is not required by the GG algorithm. Thus, the evaluation of the sparse grid interpolant u_n should be implemented in a very efficient way, since this operation is repeated at each iteration for an increasingly large number of multi-indices in the margin. In this sense, the hierarchical representation of the sparse grid interpolant via hierarchical Lagrange polynomials and hierarchical surpluses is to be preferred to the classical combination technique representation [30], since the former usually yields a faster evaluation—at the price of a higher offline-cost due to the computation of the surpluses.

4 The hierarchical sparse grid representation as well as the error estimators by [31] for the diffusion problem require nested univariate node sets—for an efficient implementation and reliability, respectively. Instead, the GG algorithm also works with non-nested nodes, see e.g. [40, 25, 26]. This might be a rather minor point, since suitable nested node families in form of Leja or Clenshaw-Curtis nodes are available.

As an extensive numerical study on the error estimator-based adaptive scheme has been already conducted in [31], we present no further numerical experiments here. For instance, in [31] the authors observed for several numerical test examples of the diffusion problem (1) that the error estimator stated in Proposition 6 is sharp. These test examples included different dimensions of the physical domain ($d = 1, 2$) as well as different numbers M of parameter variables and different expansion functions a_m in the definition of the diffusion coefficient. Besides this, a second set of experiments in [31] compared the performance of the error estimator-based algorithm and the GG algorithm: both showed a similar performance w.r.t. the number of grid points in the corresponding adaptively constructed sparse grids $\mathcal{Y}_{\Lambda_n}$ (recall that each sparse grid point corresponds to a PDE solve); however, if all PDE solves (i.e., also those necessary for evaluating the profits on the margin) are taken into account, than the GG algorithm performed significantly less effectively.

Although the setting and the algorithm in [31] slightly differs from the setting and Algorithm 3 considered here, these differences are negligible for the numerical performance for the following reasons:

- The version of Algorithm 3 considered in [31] considers normalized profit indicators π_n for the indices $\boldsymbol{k}$, see (11). However, previous numerical evidence for the GG algorithm suggests that whether error indicators or profit indicators are used does not play a major role for the convergence, see e.g. [40]. Therefore, for the same reasons, one can expect Algorithm 3 to exhibit similar numerical behavior as the adaptive algorithm in [31].
- Although the second set of results in [31] is for Clenshaw–Curtis collocation points only, it is well-known that in practice the performance of Leja and Clenshaw–Curtis points is quite similar for adaptive sparse grid collocation using the GG algorithm, see e.g. [38]. Thus, it is again reasonable to assume that similar results to those reported in [31] also hold for Algorithm 3 using Leja nodes.
- The tests in [31] are performed with $p = \infty$ only, both for the evaluation of the error and for the computation of the error indicator. Our theory covers any $p \in [1, \infty]$, and we expect that GG and Algorithm 3 would behave similarly also for $p \neq \infty$.

5 Proof of Convergence

We collect four auxiliary results required for the subsequent proof of our main result, Theorem 8. First, we recall a statement on the Lebesgue constant of the tensorized detail operators $\Delta_{\boldsymbol{i}}$ given in (13).

Proposition 10 ([14, Section 3])**.** *There holds for*

$$\|\Delta_{\boldsymbol{i}}\|_\infty := \sup_{0\neq f\in C(\boldsymbol{\Gamma};\mathbb{R})} \frac{\|\Delta_{\boldsymbol{i}} f\|_{C(\boldsymbol{\Gamma};\mathbb{R})}}{\|f\|_{C(\boldsymbol{\Gamma};\mathbb{R})}}, \qquad \boldsymbol{i} \in \mathcal{F},$$

that

$$\|\Delta_{\boldsymbol{i}}\|_\infty = \prod_{m=1}^{M} \|\Delta_{i_m}\|_\infty.$$

Next, we provide an estimate for the sparse grid collocation operator S_Λ applied to Taylor polynomials/multivariate monomials given an algebraically growing Lebesgue constant of the univariate detail operators. This result is similar to [25, Proposition 3.1].

Proposition 11. *Let there exist constants $1 < c < \infty$ and $\theta < \infty$ such that*

$$\|\Delta_i\|_\infty := \sup_{0\neq f\in C(\Gamma;\mathbb{R})} \frac{\|\Delta_i f\|_{C(\Gamma;\mathbb{R})}}{\|f\|_{C(\Gamma;\mathbb{R})}} \leq (1+ci)^\theta, \qquad \forall i \in \mathbb{N}.$$

Then for the Taylor polynomials $T_{\boldsymbol{k}}(\boldsymbol{y}) := \boldsymbol{y}^{\boldsymbol{k}}$, $\boldsymbol{k} \in \mathcal{F}$, and $\boldsymbol{\Gamma} = [-1,1]^M$ we have

$$\sup_{\Lambda\subseteq\mathcal{F}} \|S_\Lambda T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})} \leq \prod_{m=1}^{M} (1+ck_m)^{1+\theta}, \qquad \boldsymbol{k} \in \mathcal{F}.$$

Proof. First, notice that with $\mathcal{R}_{\boldsymbol{k}} := \{\boldsymbol{j} \in \mathcal{F} \colon j_m \leq k_m \ \forall m = 1,\dots,M\}$,

$$\sup_{\Lambda\subseteq\mathcal{F}} \|S_\Lambda T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})} = \max_{\Lambda\subseteq\mathcal{R}_{\boldsymbol{k}}} \|S_\Lambda T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})},$$

since $\Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} \equiv 0$ if for any m we have $i_m > k_m$. Moreover, the triangle inequality yields

$$\|S_\Lambda T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})} \leq \sum_{\boldsymbol{i}\in\Lambda} \|\Delta_{\boldsymbol{i}} T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})} \leq \sum_{\boldsymbol{i}\in\Lambda} \|\Delta_{\boldsymbol{i}}\|_\infty \, \|T_{\boldsymbol{k}}\|_{C(\boldsymbol{\Gamma};\mathbb{R})} \leq \sum_{\boldsymbol{i}\in\Lambda} \prod_{m=1}^{M} (1+ci_m)^\theta.$$

Since we are considering Λ to be a subset of $\mathcal{R}_{\boldsymbol{k}}$, we can further bound the last term as

$$\sum_{\boldsymbol{i}\in\Lambda} \prod_{m=1}^{M} (1+ci_m)^\theta \leq \sum_{\boldsymbol{i}\in\mathcal{R}_{\boldsymbol{k}}} \prod_{m=1}^{M} (1+ck_m)^\theta = |\mathcal{R}_{\boldsymbol{k}}| \prod_{m=1}^{M} (1+ck_m)^\theta = \prod_{m=1}^{M} (1+ck_m)^{1+\theta},$$

since $|\mathcal{R}_{\boldsymbol{k}}| = \prod_{m=1}^{M}(1+k_m)$. □

Furthermore, we require a rather general result on the summability of sequences on $\mathcal{F}$.

Lemma 12 ([17, Lemmas 2 & 3])**.** *For any $0 < q < 1$, one has*

$$\boldsymbol{\rho} \in \mathbb{R}^M \text{ and } \min_{m=1,\dots,M} |\rho_m| > 1 \quad \Longleftrightarrow \quad \left(\boldsymbol{\rho}^{-\boldsymbol{k}}\right)_{\boldsymbol{k}\in\mathcal{F}} \in \ell^q(\mathcal{F}).$$

Moreover, for any $0 < q < 1$ and any algebraic factor

$$\beta(\boldsymbol{k}) := \prod_{m=1}^{M} (1 + ck_m)^\theta, \qquad \boldsymbol{k} \in \mathcal{F},$$

with finite $c, \theta \geq 0$, one has

$$\boldsymbol{\rho} \in \mathbb{R}^M \text{ and } \min_{m=1,\dots,M} |\rho_m| > 1 \quad \Longleftrightarrow \quad \left(\beta(\boldsymbol{k})\, \boldsymbol{\rho}^{-\boldsymbol{k}}\right)_{\boldsymbol{k}\in\mathcal{F}} \in \ell^q(\mathcal{F}).$$

Note that the original statement in [17, Lemmas 2 & 3] is for the case of countable sequences $\boldsymbol{\rho} = (\rho_m)_{m\in\mathbb{N}} \in \ell^q(\mathbb{N})$.

The last auxiliary result provides a simple estimate for the tails of converging series of the same form $\left(\beta(\boldsymbol{k})\, \boldsymbol{\rho}^{-\boldsymbol{k}}\right)_{\boldsymbol{k}\in\mathcal{F}}$ as considered in the previous lemma.

Proposition 13. *Let $\boldsymbol{\rho} \in \mathbb{R}^M$ be a vector of numbers $\rho_m > 1$, $m = 1, \dots, M$, and*

$$\beta(\boldsymbol{k}) := \prod_{m=1}^{M} (1 + ck_m)^\theta, \qquad \boldsymbol{k} \in \mathcal{F},$$

an algebraic factor with finite $c, \theta \geq 0$ such that

$$C := \sum_{\boldsymbol{k}\in\mathcal{F}} \beta(\boldsymbol{k})\boldsymbol{\rho}^{-\boldsymbol{k}} < \infty. \tag{16}$$

Then, we have for any $\boldsymbol{k} \in \mathcal{F}$

$$\sum_{\boldsymbol{j}\geq\boldsymbol{k}} \beta(\boldsymbol{j})\boldsymbol{\rho}^{-\boldsymbol{j}} \leq C\, \beta(\boldsymbol{k})\boldsymbol{\rho}^{-\boldsymbol{k}}. \tag{17}$$

Proof. By refactoring, we have

$$\sum_{\boldsymbol{j}\geq\boldsymbol{k}} \beta(\boldsymbol{j})\boldsymbol{\rho}^{-\boldsymbol{j}} = \sum_{\boldsymbol{j}\geq\boldsymbol{k}} \prod_{m=1}^{M} (1 + cj_m)^\theta \rho_m^{-j_m} = \prod_{m=1}^{M} \left(\sum_{j_m\geq k_m} (1 + cj_m)^\theta \rho_m^{-j_m} \right).$$

We then obtain for each $m = 1, \dots, M$,

$$\begin{aligned} \sum_{j_m\geq k_m} (1 + cj_m)^\theta \rho_m^{-j_m} &= (1 + ck_m)^\theta\, \rho_m^{-k_m} \sum_{j=0}^{\infty} \left(\frac{1 + cj + ck_m}{1 + ck_m} \right)^\theta \rho_m^{-j} \\ &\leq (1 + ck_m)^\theta\, \rho_m^{-k_m} \sum_{j=0}^{\infty} (1 + cj)^\theta\, \rho_m^{-j}. \end{aligned}$$

Thus, the refactoring argument can be continued as

$$\begin{aligned} \sum_{\boldsymbol{j}\geq\boldsymbol{k}} \beta(\boldsymbol{j})\boldsymbol{\rho}^{-\boldsymbol{j}} = \sum_{\boldsymbol{j}\geq\boldsymbol{k}} \prod_{m=1}^{M} (1 + cj_m)^\theta \rho_m^{-j_m} &\leq \prod_{m=1}^{M} \left((1 + ck_m)^\theta\, \rho_m^{-k_m} \sum_{j_m\geq 0} (1 + cj_m)^\theta \rho_m^{-j_m} \right) \\ &= \beta(\boldsymbol{k})\boldsymbol{\rho}^{-\boldsymbol{k}} \sum_{\boldsymbol{j}\geq 0} \prod_{m=1}^{M} (1 + cj_m)^\theta \rho_m^{-j_m} = C\, \beta(\boldsymbol{k})\boldsymbol{\rho}^{-\boldsymbol{k}}, \end{aligned}$$

with C as in Equation (16). □

5.1 Proof of Theorem 8

Proof. We prove Theorem 8 by applying Theorem 3. To this end, we need to verify the three assumptions of Theorem 3. The first holds due to Proposition 6 and the third by construction, cf. Remark 4. Hence, it remains to verify the second assumption. To this end, we set

$$\widehat{\eta}_n(\boldsymbol{k}) := \begin{cases} \|\Delta_{\boldsymbol{k}}(a\nabla S_{\Lambda_n} u)\|_{L^p_\mu(\Gamma;L^2(D))}, & \boldsymbol{k} \in \Lambda_n \cup \mathcal{C}_n \\ 0, & \text{otherwise,} \end{cases} \tag{18}$$

and proceed in two steps (see also Remark 4):

1 We define the (formal) limit

$$u_\infty := \sum_{\boldsymbol{k}\in\Lambda_\infty} \Delta_{\boldsymbol{k}} u, \qquad \Lambda_\infty := \bigcup_{n\in\mathbb{N}} \Lambda_n, \tag{19}$$

and verify in Lemma 14 below that $u_\infty \in C(\mathbf{\Gamma}; H^1_0(D))$ as well as

$$\lim_{n\to\infty} \|u_\infty - u_n\|_{C(\mathbf{\Gamma};H^1_0(D))} = 0.$$

2 We then set

$$\eta_\infty(\boldsymbol{k}) := \begin{cases} \|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\Gamma;L^2(D))}, & \boldsymbol{k} \in \Lambda_\infty \cup \operatorname{Marg}(\Lambda_\infty), \\ 0, & \text{otherwise,} \end{cases} \tag{20}$$

and show in Lemma 16 that

$$\lim_{n\to\infty} \|\eta_\infty - \widehat{\eta}_n\|_{\ell^1} = 0,$$

which concludes the proof. □

Lemma 14. *Given the assumptions of Theorem 8, the function u_∞ in* (19) *is well-defined in $C(\mathbf{\Gamma}; H^1_0(D))$, i.e., $u_\infty \in C(\mathbf{\Gamma}; H^1_0(D))$, and satisfies*

$$\lim_{n\to\infty} \|u_\infty - u_n\|_{C(\mathbf{\Gamma};H^1_0(D))} = 0.$$

Proof. We abbreviate the norms in $C(\mathbf{\Gamma}; H^1_0(D))$ and $C(\mathbf{\Gamma};\mathbb{R})$ by $\|\cdot\|_C$. Furthermore, let $\boldsymbol{\rho} \in \mathbb{R}^M$ be such that $1 < \rho_m < \alpha^{-1}$ as in equation (5). Then, with $T_{\boldsymbol{k}}$, $\boldsymbol{k} \in \mathcal{F}$, denoting the multivariate Taylor polynomials and $t_{\boldsymbol{k}}$ the corresponding Taylor coefficients of u, we obtain

$$\begin{aligned} \|u_\infty\|_C &= \left\| \sum_{\boldsymbol{i}\in\Lambda_\infty} \Delta_{\boldsymbol{i}} u \right\|_C = \left\| \sum_{\boldsymbol{i}\in\Lambda_\infty} \sum_{\boldsymbol{k}\in\mathcal{F}} t_{\boldsymbol{k}} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} \right\|_C = \left\| \sum_{\boldsymbol{k}\in\mathcal{F}} t_{\boldsymbol{k}} \sum_{\boldsymbol{i}\in\Lambda_\infty} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} \right\|_C \\ &\le \sum_{\boldsymbol{k}\in\mathcal{F}} \|t_{\boldsymbol{k}}\|_{\mathcal{H}} \, \|S_{\Lambda_\infty} T_{\boldsymbol{k}}\|_C \le \sum_{\boldsymbol{k}\in\mathcal{F}} \|t_{\boldsymbol{k}}\|_{\mathcal{H}} \beta(\boldsymbol{k}) \\ &\le \left(\sum_{\boldsymbol{k}\in\mathcal{F}} \boldsymbol{\rho}^{2\boldsymbol{k}} \, \|t_{\boldsymbol{k}}\|^2_{\mathcal{H}} \right)^{1/2} \left(\sum_{\boldsymbol{k}\in\mathcal{F}} \beta(\boldsymbol{k})^2 \, \boldsymbol{\rho}^{-2\boldsymbol{k}} \right)^{1/2}, \end{aligned}$$

where

$$\beta(\boldsymbol{k}) := \prod_{m=1}^{M} (1 + c k_m)^{1+\theta}, \qquad \boldsymbol{k} \in \mathcal{F}. \tag{21}$$

Here, we used Proposition 11 in the second inequality in the second line. By Theorem 1 we know that

$$C_{u,\boldsymbol{\rho}} := \left(\sum_{\boldsymbol{k}\in\mathcal{F}} \boldsymbol{\rho}^{2\boldsymbol{k}} \, \|t_{\boldsymbol{k}}\|^2_{\mathcal{H}} \right)^{1/2} < \infty, \tag{22}$$

and by Lemma 12 that $\left(\beta(\boldsymbol{k})^2 \, \boldsymbol{\rho}^{-2\boldsymbol{k}}\right)_{\boldsymbol{k}\in\mathcal{F}} \in \ell^1(\mathcal{F})$. Thus, we can conclude that $\|u_\infty\|_C < \infty$. Note that interchanging the series with respect to $\boldsymbol{i} \in \Lambda_\infty$ and $\boldsymbol{k} \in \mathcal{F}$ in the first line above could be made rigorous by first considering only finite subsets $\mathcal{R}_{\boldsymbol{j}} := \{\boldsymbol{k} \in \mathcal{F} \colon k_m \le j_m\} \subset \mathcal{F}$ and then taking the limit $\boldsymbol{j} \to \infty$.

Next, the continuity of u_∞ with respect to $\boldsymbol{y}$ can be concluded from the continuity of u_n with respect to $\boldsymbol{y}$ and the subsequently proved convergence of $u_n \to u_\infty$ in $C(\boldsymbol{\Gamma};\mathcal{H})$. To this end, we apply Lebesgue's dominated convergence theorem. We have

$$u_\infty - u_n = \sum_{\boldsymbol{i}\in\Lambda_\infty\setminus\Lambda_n} \Delta_{\boldsymbol{i}} u = \sum_{\boldsymbol{k}\in\mathcal{F}} t_{\boldsymbol{k}} \sum_{\boldsymbol{i}\in\Lambda_\infty\setminus\Lambda_n} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}},$$

and by the triangle and Cauchy–Schwarz inequalities we obtain

$$\|u_\infty - u_n\|_C \le C_{u,\boldsymbol{\rho}} \left(\sum_{\boldsymbol{k}\in\mathcal{F}} \boldsymbol{\rho}^{-2\boldsymbol{k}}\, g_n^2(\boldsymbol{k})\right)^{1/2}, \qquad g_n(\boldsymbol{k}) := \left\| \sum_{\boldsymbol{i}\in\Lambda_\infty\setminus\Lambda_n} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} \right\|_C. \tag{23}$$

Now, for any $\boldsymbol{k}\in\mathcal{F}$ and with $\mathcal{R}_{\boldsymbol{k}} = \{\boldsymbol{i}\in\mathcal{F}\colon \boldsymbol{i}\le\boldsymbol{k}\}$ it holds that

$$\sum_{\boldsymbol{i}\in\Lambda_\infty\setminus\Lambda_n} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} = \sum_{\boldsymbol{i}\in(\Lambda_\infty\cap\mathcal{R}_{\boldsymbol{k}})\setminus\Lambda_n} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}},$$

where the right-hand side is a finite sum. Since for any of the finitely many $\boldsymbol{i}\in\Lambda_\infty\cap\mathcal{R}_{\boldsymbol{k}}$ there exists an $n_0\in\mathbb{N}$ such that $\boldsymbol{i}\in\Lambda_n$ for all $n\ge n_0$, we obtain

$$\lim_{n\to\infty} g_n(\boldsymbol{k}) = 0 \qquad \forall \boldsymbol{k}\in\mathcal{F}.$$

The final step is to apply the dominated convergence theorem and exchange the limit and the sum in (23), to obtain

$$\lim_{n\to\infty} \|u_\infty - u_n\|_C \le C_{u,\boldsymbol{\rho}} \lim_{n\to\infty} \left(\sum_{k\in\mathcal{F}} g_n^2(\boldsymbol{k})\, \boldsymbol{\rho}^{-2\boldsymbol{k}}\right) = C_{u,\boldsymbol{\rho}} \sum_{k\in\mathcal{F}} \boldsymbol{\rho}^{-2\boldsymbol{k}} \left(\lim_{n\to\infty} g_n^2(\boldsymbol{k})\right) = 0.$$

To this end, we need to show the existence of some $g\colon \mathcal{F}\to\mathbb{R}$ such that

$$g_n(\boldsymbol{k}) \le g(\boldsymbol{k}) \quad \forall \boldsymbol{k}\in\mathcal{F} \qquad \text{and} \qquad \sum_{\boldsymbol{k}\in\mathcal{F}} \boldsymbol{\rho}^{-2\boldsymbol{k}} g^2(\boldsymbol{k}) < \infty.$$

This is obtained by

$$g_n(\boldsymbol{k}) = \left\| \sum_{\boldsymbol{i}\in(\Lambda_\infty\cap\mathcal{R}_{\boldsymbol{k}})\setminus\Lambda_n} \Delta_{\boldsymbol{i}} T_{\boldsymbol{k}} \right\|_C \le \beta(\boldsymbol{k}) = \prod_{m\in\mathbb{N}} (1+ck_m)^{\theta+1} =: g(\boldsymbol{k}),$$

since $\left(\beta(\boldsymbol{k})^2\, \boldsymbol{\rho}^{-2\boldsymbol{k}}\right)_{\boldsymbol{k}\in\mathcal{F}} \in \ell^1(\mathcal{F})$, see above. □

For the second step of the proof, we first state an important lemma concerning the decay of the error estimators.

Lemma 15. *Let the assumptions of Theorem 8 be satisfied and let $\Lambda\subset\mathcal{F}$ be an arbitrary monotone subset. Then, there exists a constant $C = C(M,\boldsymbol{\rho},c,\theta,a) < \infty$ such that for*

$$\eta(\boldsymbol{k}, S_\Lambda u) := \|\Delta_{\boldsymbol{k}}(a\nabla S_\Lambda u)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}, \qquad \boldsymbol{k}\in\mathcal{F},$$

we have for any $\boldsymbol{k}\in\mathcal{F}$

$$\eta(\boldsymbol{k}, S_\Lambda u) \le C\, g(\boldsymbol{k}), \qquad g(\boldsymbol{k}) := \left(\prod_{m=1}^{M} (1+ck_m)^{2\theta+1}\right) \boldsymbol{\rho}^{-\boldsymbol{k}}.$$

Proof. Set $u_\Lambda := S_\Lambda u$. By linearity $\Delta_{\boldsymbol{k}}(a\nabla u_\Lambda)$ for $\boldsymbol{k}\in\mathcal{F}$ can be written as

$$\Delta_{\boldsymbol{k}}\left[a\nabla u_\Lambda\right] = \Delta_{\boldsymbol{k}}\left[a\sum_{\boldsymbol{i}\in\Lambda} \Delta_{\boldsymbol{i}}\nabla u\right] = \sum_{\boldsymbol{i}\in\Lambda} \Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}\nabla u\right].$$

Moreover, using the Taylor expansion of the solution u we deduce that

$$\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}\nabla u\right] = \Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}\sum_{j\in\mathcal{F}} (\nabla t_j)\, T_j\right] = \sum_{j\in\mathcal{F}} (\nabla t_j)\, \Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}} T_j\right]. \tag{24}$$

We observe that for certain combinations of $\boldsymbol{i}$, $\boldsymbol{j}$, and $\boldsymbol{k}$ it holds $\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}}\right] \equiv 0$. First of all,

$$\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}} = \prod_{m=1}^{M}\left(\Delta_{i_m}T_{j_m}\right) \equiv 0 \qquad \text{if } \exists m\colon j_m < i_m,$$

since then $\Delta_{i_{m'}}T_{j_{m'}} \equiv 0$. Second, the function $a\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}}$ is a polynomial in $\boldsymbol{y}$ belonging to the space

$$\mathcal{P}_{\boldsymbol{i}+\boldsymbol{1}} := \operatorname{span}\left\{\boldsymbol{y}^{\boldsymbol{p}}\colon p_m \le i_m + 1 \text{ for } m = 1,\dots,M\right\},$$

since a is affine in $\boldsymbol{y}$. Hence,

$$\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}}\right] \equiv 0 \qquad \text{if } \exists m\colon i_m + 1 < k_m.$$

Combining both conditions $\boldsymbol{j} \ge \boldsymbol{i}$ and $\boldsymbol{i} \ge \boldsymbol{k} - \boldsymbol{1}$, and introducing the notation $[\boldsymbol{k}-\boldsymbol{1}]_+ := (\max\{k_m - 1, 0\})_{m=1}^M$, the sum (24) reduces to

$$\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}u\right] = \sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left(\nabla t_{\boldsymbol{j}}\right)\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}}\right].$$

Thus, reverting the interchange of the series yields

$$\begin{aligned}\left\|\Delta_{\boldsymbol{k}}(a\nabla u_\Lambda)\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))} &= \left\|\sum_{\boldsymbol{i}\in\Lambda}\Delta_{\boldsymbol{k}}(a\Delta_{\boldsymbol{i}}\nabla u_\Lambda)\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))} = \left\|\sum_{\boldsymbol{i}\in\Lambda}\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left(\nabla t_{\boldsymbol{j}}\right)\Delta_{\boldsymbol{k}}\left[a\Delta_{\boldsymbol{i}}T_{\boldsymbol{j}}\right]\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}\\ &= \left\|\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left(\nabla t_{\boldsymbol{j}}\right)\Delta_{\boldsymbol{k}}\left[aS_\Lambda T_{\boldsymbol{j}}\right]\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}.\end{aligned}$$

We now set $\beta(\boldsymbol{k}) := \prod_{m=1}^M (1+ck_m)^\theta$ as well as

$$a_{\max} := \sup_{y\in\boldsymbol{\Gamma}}\sup_{\boldsymbol{x}\in D}|a(\boldsymbol{x},\boldsymbol{y})| < \infty. \tag{25}$$

By using the triangular inequality, Proposition 10 and Proposition 11 we deduce

$$\begin{aligned}\left\|\Delta_{\boldsymbol{k}}(a\nabla u_\Lambda)\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))} &= \left\|\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left(\nabla t_{\boldsymbol{j}}\right)\Delta_{\boldsymbol{k}}\left[aS_\Lambda T_{\boldsymbol{j}}\right]\right\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}\\ &\le \sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left\|\left(\nabla t_{\boldsymbol{j}}\right)\right\|_{L^2(D)}\ \left\|\Delta_{\boldsymbol{k}}\left[aS_\Lambda T_{\boldsymbol{j}}\right]\right\|_{C(\boldsymbol{\Gamma};\mathbb{R})}\\ &\le \sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left\|t_{\boldsymbol{j}}\right\|_{\mathcal{H}}\beta(\boldsymbol{k})\ \left\|aS_\Lambda T_{\boldsymbol{j}}\right\|_{C(\boldsymbol{\Gamma};\mathbb{R})}\\ &\le \sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left\|t_{\boldsymbol{j}}\right\|_{\mathcal{H}}\beta(\boldsymbol{k})\,a_{\max}\left\|S_\Lambda T_{\boldsymbol{j}}\right\|_{C(\boldsymbol{\Gamma};\mathbb{R})}\\ &\le a_{\max}\,\beta(\boldsymbol{k})\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left\|t_{\boldsymbol{j}}\right\|_{\mathcal{H}}\gamma(\boldsymbol{j}),\end{aligned}$$

where we set $\gamma(\boldsymbol{j}) := \prod_{m=1}^M (1+cj_m)^{1+\theta}$. By the Cauchy–Schwarz inequality we obtain

$$\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\left\|t_{\boldsymbol{j}}\right\|_{\mathcal{H}}\gamma(\boldsymbol{j}) \le C_{u,\boldsymbol{\rho}}\left(\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\boldsymbol{\rho}^{-2\boldsymbol{j}}\,\gamma(\boldsymbol{j})^2\right)^{1/2},$$

with $\boldsymbol{\rho}$ as in Theorem 1 and $C_{u,\boldsymbol{\rho}}$ as in (22). We can then apply Proposition 13 to bound $\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\boldsymbol{\rho}^{-2\boldsymbol{j}}\,\gamma(\boldsymbol{j})^2$. More specifically, Proposition 13 yields the existence of a constant $C_{\boldsymbol{\rho},c,\theta} < \infty$ such that it holds

$$\sum_{\boldsymbol{j}\ge[\boldsymbol{k}-\boldsymbol{1}]_+}\boldsymbol{\rho}^{-2\boldsymbol{j}}\,\gamma(\boldsymbol{j})^2 \le C_{\boldsymbol{\rho},c,\theta}\,\boldsymbol{\rho}^{-2[\boldsymbol{k}-\boldsymbol{1}]_+}\,\gamma([\boldsymbol{k}-\boldsymbol{1}]_+)^2 \le C_{\boldsymbol{\rho},c,\theta}\left(\prod_{m=1}^M\rho_m^2\right)\boldsymbol{\rho}^{-2\boldsymbol{k}}\,\gamma(\boldsymbol{k})^2,$$

since γ is increasing and $\rho_m > 1$ for each m. Thus, for any $\boldsymbol{k} \in \mathcal{F}$ we get

$$\|\Delta_{\boldsymbol{k}}(a\nabla u_\Lambda)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))} \leq a_{\max}\, C_{u,\boldsymbol{\rho}}\, \beta(\boldsymbol{k})\, C^{1/2}_{\boldsymbol{\rho},c,\theta} \left(\prod_{m=1}^{M} \rho_m\right) \gamma(\boldsymbol{k})\, \boldsymbol{\rho}^{-\boldsymbol{k}}.$$

The statement follows with

$$C := a_{\max}\, C_{u,\boldsymbol{\rho}}\, C^{1/2}_{\boldsymbol{\rho},c,\theta} \left(\prod_{m=1}^{M} \rho_m\right), \tag{26}$$

since $g(\boldsymbol{k}) = \beta(\boldsymbol{k})\gamma(\boldsymbol{k})\, \boldsymbol{\rho}^{-\boldsymbol{k}}$. □

This bound of the error indicators is now used to proceed with the second step of the proof to verify the second assumption of Theorem 3.

Lemma 16. *Given the assumptions of Theorem 8 we have for η_∞ as in* (20) *and $\widehat{\eta}_n$ as in* (18) *that*

$$\lim_{n\to\infty} \|\eta_\infty - \widehat{\eta}_n\|_{\ell^1(\mathcal{F})} = 0.$$

Proof. We introduce the short-hand notation

$$\Lambda^+ := \Lambda \cup \operatorname{Marg}(\Lambda), \qquad \Lambda \subseteq \mathcal{F},$$

and notice that consequently $\Lambda^+_\infty \subseteq \bigcup_{n\in\mathbb{N}} \Lambda^+_n$. Moreover, we have

$$|\eta_\infty(\boldsymbol{k}) - \widehat{\eta}_n(\boldsymbol{k})| \leq \begin{cases} \|\Delta_{\boldsymbol{k}}(a\nabla(u_\infty - u_n))\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}, & \boldsymbol{k} \in \Lambda^+_n \subset \Lambda^+_\infty, \\ \|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}, & \boldsymbol{k} \in \Lambda^+_\infty \setminus \Lambda^+_n, \\ 0, & \boldsymbol{k} \in \mathcal{F} \setminus \Lambda^+_\infty. \end{cases}$$

Hence,

$$\|\eta_\infty - \widehat{\eta}_n\|_{\ell^1(\mathcal{F})} \leq \underbrace{\sum_{\boldsymbol{k}\in\Lambda^+_\infty} \|\Delta_{\boldsymbol{k}}(a\nabla(u_\infty - u_n))\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}}_{\text{term I}} + \underbrace{\sum_{\boldsymbol{k}\in\Lambda^+_\infty\setminus\Lambda^+_n} \|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))}}_{\text{term II}}.$$

We would like to take the limit at both sides, and verify that the two terms on the right-hand side tend to zero, which we analyze separately in the following.

Term I. Assuming for a moment that we can apply the dominated convergence theorem to exchange the sum and the limit, we would get

$$\begin{aligned}
&\lim_{n\to\infty} \sum_{\boldsymbol{k}\in\Lambda^+_\infty} \|\Delta_{\boldsymbol{k}}(a\nabla(u_\infty - u_n))\|_{L^p_\mu(\Gamma;L^2(D))} \\
&= \sum_{\boldsymbol{k}\in\Lambda^+_\infty} \lim_{n\to\infty} \|\Delta_{\boldsymbol{k}}(a\nabla(u_\infty - u_n))\|_{L^p_\mu(\Gamma;L^2(D))} && \text{by dominated convergence} \\
&\leq \sum_{\boldsymbol{k}\in\Lambda^+_\infty} \lim_{n\to\infty} \beta(\boldsymbol{k}) \|a\nabla(u_\infty - u_n)\|_{C(\boldsymbol{\Gamma};L^2(D))} && \text{by Prop. 10 with } \beta(\boldsymbol{k}) := \textstyle\prod_{m=1}^{M}(1+ck_m)^\theta \\
&\leq \sum_{\boldsymbol{k}\in\Lambda^+_\infty} \lim_{n\to\infty} \beta(\boldsymbol{k}) a_{\max} \|u_\infty - u_n\|_{C(\boldsymbol{\Gamma};H^1_0(D))} && \text{recalling the definition of } a_{\max} \text{ in (25)} \\
&= 0 && \text{by Lemma 14.}
\end{aligned}$$

In order to apply Lebesgue's dominated convergence, we need to check that there exists a function $g\colon \mathcal{F} \to [0,\infty)$ such that, for all $n \in \mathbb{N}$ and $\boldsymbol{k} \in \Lambda^+_\infty$,

$$\|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\Gamma;L^2(D))} + \|\Delta_{\boldsymbol{k}}(a\nabla u_n)\|_{L^p_\mu(\Gamma;L^2(D))} \leq g(\boldsymbol{k}) \quad \text{and} \quad \sum_{\boldsymbol{k}\in\Lambda^+_\infty} g(\boldsymbol{k}) < \infty. \tag{27}$$

The bounding function g is obtained by Lemma 15: there exists a constant $C < \infty$ such that

$$\|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\Gamma;L^2(D))} + \|\Delta_{\boldsymbol{k}}(a\nabla u_n)\|_{L^p_\mu(\Gamma;L^2(D))} \leq 2C\, g(\boldsymbol{k}),$$

with

$$g(\boldsymbol{k}) := \left(\prod_{m=1}^{M}(1+ck_m)^{2\theta+1}\right)\boldsymbol{\rho}^{-\boldsymbol{k}}.$$

The required summability of g is derived by Lemma 12, i.e.,

$$\sum_{\boldsymbol{k}\in\Lambda^+_\infty} 2C\, g(\boldsymbol{k}) \leq 2C \sum_{\boldsymbol{k}\in\mathcal{F}} \left(\prod_{m=1}^{M}(1+ck_m)^{2\theta+1}\right)\boldsymbol{\rho}^{-\boldsymbol{k}} < \infty.$$

Term II. To verify that the limit of the second term is also zero, observe that the dominated convergence theorem in (27) implies

$$\sum_{\boldsymbol{k}\in\Lambda^+_\infty} \|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\boldsymbol{\Gamma};L^2(D))\cdot} < \infty$$

Together with the fact that $\Lambda^+_\infty \subseteq \bigcup_{n\in\mathbb{N}} \Lambda^+_n$, this implies the final result

$$\lim_{n\to\infty} \sum_{\boldsymbol{k}\in\Lambda^+_\infty\setminus\Lambda^+_n} \|\Delta_{\boldsymbol{k}}(a\nabla u_\infty)\|_{L^p_\mu(\Gamma;L^2(D))} = 0. \qquad \square$$

By Lemma 16, the three assumptions of Theorem 3 have been verified, proving convergence of the described adaptive algorithm.

6 Conclusions

We have proved convergence of an adaptive sparse grid collocation algorithm for approximating the solution of an elliptic PDE with a multi-dimensional parameter applying the analysis technique from [6], developed for the stochastic Galerkin FEM, to a slight variation of the algorithm proposed in [31]. In this sense, our work can be seen as an extension or follow-up of [31], where a very close variant of the algorithm considered here was presented and analyzed numerically, but without convergence proof.

The algorithm we consider here and in [31] is a modification of the well-known dimension-adaptive sparse grid algorithm due to Gerstner and Griebel, and it is based on a replacing the hierarchical surplus error indicators with a rigorous residual-based error estimator. The convergence proof is tailored to the specific problem, i.e., an elliptic PDE with parametric diffusion coefficient depending affinely on a finite number of variables. Because the algorithm is based on a residual-based error estimator, the analysis is problem-specific and must be repeated for each PDE at hand as well as for other forms of the random diffusion coefficient. However, we expect that a large part of the machinery proves valid or at least extensible in a straightforward way. Particularly, if reliable error estimators (for the approximation error w.r.t. the parameter variables) are available, simply a stability condition of these estimators w.r.t. u_n has to been established in order to verify the crucial second hypothesis of the general convergence Theorem 3. Our analysis in Section 5.1 might serve as a blueprint for doing so.

Regarding possible extensions of this work, we point out that the convergence analysis we have presented proves convergence but does not provide a rate. This might be achieved by a saturation assumption following again the line of proof in [6] for adaptive stochastic Galerkin FEM. Conversely, the extension of the specific model problem to the important case of the diffusion coefficient resulting from the parametrization of a log-normal random field is deemed to be more challenging. Another important yet challenging addition to our work would be to extend the convergence result to the infinite-dimensional case, i.e., to consider countably many parameters $M = \infty$ in the affine expansion of the diffusion coefficient (2). This would pose both theoretical and algorithmic challenges: on the theoretical side, our proof would need to be revisited since some constants are not bounded when $M \to \infty$ (in particular, the constant C in Lemma 15, cf. equation (26)). From the algorithmic point of view, having $M = \infty$ would make the size of the margin be infinite, which is of course unfeasible. Under the assumption that $\|a_m\|_{L^\infty}$ in (2) are monotone decreasing (this assumption could be weakened), then a possible approach would be to implement a so-called "buffering" procedure, as discussed in [31] (see also [44, 14, 40, 25]): the

algorithm would start considering only the first $M_0 < \infty$ parameters, and any time a parameter is "activated" (i.e. a collocation point is added along that parameter for the first time), the total number of considered parameters would increase by one, in such a way that there are always M_0 "non-activated" parameters.

Another interesting follow-up work would be to perform an extensive numerical campaign on a number of different PDEs for which Finite-Element error estimators are available, and test numerically whether the algorithm proposed here gives consistently good performances (i.e., similar to the GG algorithm) for all the PDE considered. Both these numerical investigations exceed the scope of this work and are left for future research.

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