

# A MULTILEVEL STOCHASTIC COLLOCATION ALGORITHM FOR OPTIMIZATION OF PDES WITH UNCERTAIN COEFFICIENTS

D. P. KOURI\*

**Abstract.** In this work, we apply the MG/OPT framework to a multilevel-in-sample-space discretization of optimization problems governed by PDEs with uncertain coefficients. The MG/OPT algorithm is a template for the application of multigrid to deterministic PDE optimization problems. We employ MG/OPT to exploit the hierarchical structure of sparse grids in order to formulate a multilevel stochastic collocation algorithm. The algorithm is provably first-order convergent under standard assumptions on the hierarchy of discretized objective functions as well as on the optimization routines used as pre- and post-smoothers. We present explicit bounds on the total number of PDE solves and an upper bound on the error for one V-cycle of the MG/OPT algorithm applied to a linear quadratic control problem. We provide numerical results that confirm the theoretical bound on the number of PDE solves and show a dramatic reduction in the total number of PDE solves required to solve these optimization problems when compared with standard optimization routines applied to the same problem.

**Key words.** PDE Optimization, Multilevel, Uncertainty Quantification, Sparse Grids

**AMS subject classifications.** 49M15, 65K05, 65N35, 90C15

**1. Introduction.** The numerical solution of partial differential equation (PDE) constrained optimization problems with uncertain coefficients is computationally expensive because of typically high-dimensional stochastic representations of the PDE solution. This work applies the MG/OPT algorithm [33] to solve the optimization problem

$$\underset{z \in \mathcal{Z}}{\text{Minimize}} \quad \widehat{J}(z) = J(u(z), z),$$

where  $\mathcal{Z}$  is a reflexive Hilbert space,  $\mathcal{U}$  is a Banach space, and  $u = u(z) \in \mathcal{U}$  is the solution of a PDE with uncertain coefficients. We discretize  $\widehat{J}(z)$  in the sample space using a hierarchical sparse grid collocation discretization [27]. We demonstrate that applying MG/OPT to this hierarchy of semi-discretized optimization problems may reduce the number of PDE solves required to obtain a minimizer of  $\widehat{J}(z)$  when compared with other standard optimization algorithms.

The MG/OPT algorithm is an optimization-theoretic multigrid approach to solving PDE-constrained optimization problems [33, 30]. MG/OPT is a template which allows for user-defined optimization routines, discretizations, and intergrid transfer operators [33, 30]. Moreover, MG/OPT generalizes the full approximation scheme (FAS) [25] to optimization and has traditionally been applied to a hierarchy of spatial discretizations for the state and design variables. In this work, we apply the ideas of MG/OPT to a hierarchy of stochastic discretizations.

Globalized with a line search, MG/OPT is provably convergent [33, 34]. At each level, MG/OPT is analogous to a V-cycle (or more general cycles) of multigrid. As in traditional multigrid, each level of MG/OPT requires pre- and post-smoothing. These smoothing steps correspond to performing a finite number of iterations of an optimization algorithm [33]. Recently, the authors of [21, 22, 23, 24] have developed a

---

\*Mathematics & Computer Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Building 240, Argonne, IL 60439-4844. E-mail: dpkouri@mcs.anl.gov. This author was supported by the U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research, under Contract DE-AC02-06CH11357.

recursive trust-region algorithm that accelerates the trust-region step using multigrid correction. Similarly, [47] has developed a line-search approach to multigrid optimization. Both of the multilevel trust-region and line-search algorithms are provably convergent and do not require pre- and post-smoothing.

Aside from MG/OPT and its adaptations, spatial multigrid has been applied to optimization problems governed by deterministic PDEs in [44, 8, 7, 10, 11, 12] by using multigrid solvers on the optimality system. We note that simply applying multigrid to the optimality system need not result in a minimizer since multigrid seeks only a stationary point of the optimality system [30]. This pitfall is circumvented by including target functions in the multigrid formulation. These ideas are extended to problems governed by PDEs with uncertain coefficients in [13, 14, 15]. Those works focus on multigrid in space, however, and do not consider multilevel sampling schemes. Unlike these multigrid algorithms for PDE-optimization with uncertain coefficients, the algorithm presented in this paper provides a multilevel-in-sample-space optimization routine. Moreover, one can incorporate existing spatial multigrid algorithms within the MG/OPT framework to solve the sparse-grid subproblems.

In Section 2, we present the problem formulation for the example problems considered in this paper. The problem formulation resembles standard quadratic control or least-squares type PDE-optimization. In Section 3, we review stochastic collocation and discuss hierarchical sparse-grid techniques. In Section 4 we extend MG/OPT to handle optimization of uncertain PDEs, and in Section 5 we prove the first-order convergence of MG/OPT. In Section 6, we present explicit upper bounds on V-cycle error and computational work. In Section 7, we demonstrate the power and efficiency of MG/OPT for stochastic collocation through numerical examples. In Section 8, we present conclusions and future work.

The following notation and conventions are employed throughout this paper.  $K$  denotes the finest level of sparse grid, and 1 always refers to the coarsest level of sparse grid. The index  $k$  denotes the intermediate levels of sparse grid (i.e.,  $k = 1, 2, \dots, K$ ).

**2. Problem Formulation.** Let  $D \subset \mathbb{R}^d$ ,  $d = 1, 2, 3$ , denote the physical domain and  $\Gamma \subseteq \mathbb{R}^M$  denote the finite sample space. The sample space  $\Gamma$  is endowed with the probability density  $\rho : \Gamma \rightarrow [0, \infty)$  and satisfies

$$\Gamma = \prod_{m=1}^M [a_m, b_m] \quad \text{and} \quad \rho(y) = \prod_{m=1}^M \rho_m(y_m)$$

with  $a_m < b_m$  and  $\rho_m : [a_m, b_m] \rightarrow [0, \infty)$  for  $m = 1, \dots, M$ . Such finite-dimensional probability spaces satisfy the finite-dimensional noise assumption [1] and typically result from Karhunen-Loève or polynomial chaos expansions. Let  $\mathcal{V} = \mathcal{V}(D)$  denote a Banach space of deterministic functions with domain  $D$ , and let  $\mathcal{Z} = \mathcal{Z}(D)$  denote a reflexive Hilbert space of deterministic functions with domain  $D$ .  $\mathcal{V}$  is the deterministic state space and  $\mathcal{Z}$  is the control space. The control space is deterministic; this models the situation when one must determine a control prior to observing the state of the physical system. The governing PDEs in this work have the form

$$\mathbf{A}(y)u(y) + \mathbf{N}(u(y), y) = \mathbf{F}(z, y) \quad \forall y \in \Gamma, \quad (2.1)$$

where  $\mathbf{A} : \Gamma \rightarrow \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ ,  $\mathbf{N} : \mathcal{V} \times \Gamma \rightarrow \mathcal{V}^*$ , and  $\mathbf{F} : \mathcal{Z} \times \Gamma \rightarrow \mathcal{V}^*$ . Now, let the Hilbert space  $\mathcal{W}$ ,  $\mathbf{C} \in \mathcal{L}(\mathcal{V}, \mathcal{W})$ , and  $\bar{w} \in \mathcal{W}$  be given. The prototypical example for PDE-constrained optimization is the quadratic control problem

$$\min_{z \in \mathcal{Z}} \hat{J}(z) = \frac{1}{2} \int_{\Gamma} \rho(y) \|\mathbf{C}u(z; y) - \bar{w}\|_{\mathcal{W}}^2 dy + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2, \quad (2.2)$$

where  $u(z; y) = u(y) \in \mathcal{V}$  solves (2.1) almost surely in  $\Gamma$ . The solution of this optimization problem can be approximated by sampling schemes such as Monte Carlo [31] and stochastic collocation [1, 37, 36, 48] or by projection schemes such as stochastic Galerkin [2, 3] and polynomial chaos [49, 17].

To simplify the analysis in this section, we focus on the quadratic control problem (2.2). The algorithm presented in this paper also applies to more general objective functions, although the analysis is typically more complicated [27].

The solution of (2.1) is a mapping  $y \mapsto u(y) : \Gamma \rightarrow \mathcal{V}$  and is assumed to have finite  $p^{\text{th}}$  moment for some fixed  $p \in [1, \infty)$ ; that is,  $u \in L^p_\rho(\Gamma; \mathcal{V})$ , where

$$L^p_\rho(\Gamma; \mathcal{V}) = \{v : \Gamma \rightarrow \mathcal{V} : v \text{ strongly measurable, } \int_\Gamma \rho(y) \|v(y)\|_{\mathcal{V}}^p dy < \infty\}.$$

To sample  $y \mapsto u(y)$ , we further assume that  $u \in \mathcal{U} = C^0_\rho(\Gamma; \mathcal{V})$ , where

$$C^0_\rho(\Gamma; \mathcal{V}) = \{v : \Gamma \rightarrow \mathcal{V} : v \text{ continuous, } \sup_{y \in \Gamma} \rho(y) \|v(y)\|_{\mathcal{V}} < \infty\}$$

which ensures that point evaluations of  $y \mapsto u(y)$  are possible. Furthermore, for the objective function to be well-defined, we require that  $C^0_\rho(\Gamma; \mathcal{V})$  be continuously embedded in  $L^2_\rho(\Gamma; \mathcal{V})$ .

**ASSUMPTION 2.1.** *The inclusion  $C^0_\rho(\Gamma; \mathcal{V}) \subset L^2_\rho(\Gamma; \mathcal{V})$  holds. Moreover, for each  $z \in \mathcal{Z}$  the state equation (2.1) has a unique solution  $u(z; \cdot) \in C^0_\rho(\Gamma; \mathcal{V})$  satisfying  $\|u(z; \cdot)\|_{L^2_\rho(\Gamma; \mathcal{V})} \leq c \|u(z; \cdot)\|_{C^0_\rho(\Gamma; \mathcal{V})}$  for some  $c > 0$ .*

The algorithm described in this paper requires gradient information. We use adjoints to derive the gradient,  $\nabla \hat{J}(z)$ . To ensure differentiability, we require the following assumption.

**ASSUMPTION 2.2.** *For every  $y \in \Gamma$ , the functions  $v \mapsto \mathbf{N}(v, y) : \mathcal{V} \rightarrow \mathcal{V}^*$  and  $z \mapsto \mathbf{F}(z, y) : \mathcal{Z} \rightarrow \mathcal{V}^*$  are Fréchet differentiable with Fréchet derivatives  $\mathbf{N}'(u, y)$  and  $\mathbf{F}'(z, y)$ , respectively. Moreover, the mapping  $z \mapsto u(z; \cdot) : \mathcal{Z} \rightarrow C^0_\rho(\Gamma; \mathcal{V})$  is Fréchet differentiable, and the derivative  $v = u'(z; \cdot) \delta z$  satisfies*

$$\mathbf{A}(y)v(y) + \mathbf{N}'(u(y), y)v(y) = \mathbf{F}'(z, y)\delta z \quad \forall y \in \Gamma.$$

Additionally, the adjoint equation

$$\mathbf{A}(y)^*p(y) + \mathbf{N}'(u(y), y)^*p(y) = -\mathbf{C}^*(\mathbf{C}u(z; y) - \bar{w}) \quad \forall y \in \Gamma \quad (2.3)$$

has a unique solution  $p \in C^0_\rho(\Gamma; \mathcal{V})$ .

If Assumptions 2.1 and 2.2 hold, then the gradient of the objective function  $\hat{J}(z)$  is

$$\nabla \hat{J}(z) = \alpha z - \int_\Gamma \rho(y) \mathbf{F}'(z, y)^* p(y) dy.$$

**3. Hierarchical Sampling Approaches: Sparse Grid Collocation.** Multi-level and adaptive Monte Carlo methods for the solution of the unconstrained stochastic programming problems are presented in [5, 16]. Furthermore, adaptive sparse-grid collocation methods are developed in [27, 28]. In this section, we review sparse grids [19, 4, 20, 42] with the goal of exposing their hierarchical nature.

We approximate the expected value in (2.2) using sparse-grid quadrature. Sparse-grid quadrature exhibits rapid convergence when  $y \mapsto \|\mathbf{C}u(y) - \bar{w}\|_{\mathcal{W}}^2$  is sufficiently

smooth. Tensor products of 1D quadrature operators are the foundation for sparse-grid quadrature. Let  $\{E_{j,m}\}_{j=1}^{\infty}$  denote a sequence of 1D quadrature operators defined for continuous functions on  $[a_m, b_m]$ . We assume that the degree of polynomial exactness for  $E_{j,m}$  is  $d_m^j - 1$ , where  $\{d_m^j\}_{j=1}^{\infty} \subset \mathbb{N}$  is monotonically increasing. Associated with each  $E_{j,m}$  is a finite set of knots  $N_{j,m} \subset \Gamma_m$ . For example,  $E_{j,m}$  can be Gaussian, Hermite, or Newton-Cotes quadrature operators.

To construct the sparse grid operator, we define the one-dimensional differences

$$\Delta_{1,m} = E_{1,m} \quad \text{and} \quad \Delta_{j,m} = E_{j,m} - E_{j-1,m} \quad j \geq 2.$$

Then  $E_{j,m} = \sum_{i=1}^j \Delta_{i,m}$ . Let  $\mathcal{I} \subset \mathbb{N}_+^M$  where  $\mathbb{N}_+ = \{1, 2, \dots\}$ . The general sparse-grid quadrature operator is

$$E_{\mathcal{I}} = \sum_{\mathbf{i} \in \mathcal{I}} \Delta_{i_1,1} \otimes \cdots \otimes \Delta_{i_M,M}. \quad (3.1)$$

In order to maintain the telescoping sum property described above, the multi-index set,  $\mathcal{I}$ , must satisfy the following property: If  $\mathbf{i} = (i_1, \dots, i_M) \in \mathcal{I}$  and  $\mathbf{j} = (j_1, \dots, j_M)$  is such that  $j_m \leq i_m$  for all  $m = 1, \dots, M$ , then  $\mathbf{j} \in \mathcal{I}$ . A multi-index set satisfying this property is called *admissible* [20]. Each admissible multi-index set  $\mathcal{I}$  produces a set of points  $N_{\mathcal{I}} \subset \Gamma$  called a *sparse grid*.

The general sparse-grid operator (3.1) can be written as a linear combination of tensor products of 1D quadrature operators by using the combination technique [19]:

$$E_{\mathcal{I}} = \sum_{\mathbf{i} \in \mathcal{I}} \left( \sum_{\mathbf{j} \in \{0,1\}^M} (-1)^{|\mathbf{j}|_1} \chi_{\mathcal{I}}(\mathbf{i} + \mathbf{j}) \right) (E_{i_1,1} \otimes \cdots \otimes E_{i_M,M}), \quad (3.2)$$

where  $|\mathbf{j}|_1 = j_1 + \dots + j_M$  and  $\chi_{\mathcal{I}}(\mathbf{j}) = 1$  if  $\mathbf{j} \in \mathcal{I}$  and zero otherwise. From (3.2), one can determine the particular form of the sparse grid,  $N_{\mathcal{I}}$ . Define

$$\vartheta(\mathbf{i}) = \sum_{\mathbf{j} \in \{0,1\}^M} (-1)^{|\mathbf{j}|_1} \chi_{\mathcal{I}}(\mathbf{i} + \mathbf{j}).$$

Then the sparse grid associated with  $\mathcal{I}$  is

$$N_{\mathcal{I}} = \bigcup_{\{\mathbf{i} \in \mathcal{I} : \vartheta(\mathbf{i}) \neq 0\}} (N_{i_1,1} \times \cdots \times N_{i_M,M}). \quad (3.3)$$

Now, suppose  $\{\mathcal{I}_k\}_{k=1}^{\infty}$  is a family of admissible multi-index sets satisfying

$$\{(1, \dots, 1)\} \subseteq \mathcal{I}_1 \subset \mathcal{I}_2 \subset \cdots \subset \mathbb{N}_+^M$$

and the one-dimensional nodes  $N_{j,m}$  are nested (i.e.,  $N_{j-1,m} \subset N_{j,m} \quad \forall j$ ). Then, the resulting sparse grids are nested (i.e.  $N_k = N_{\mathcal{I}_k} \subset N_{k+1} = N_{\mathcal{I}_{k+1}}$  for  $k = 1, 2, \dots$ ). Nested sparse grids are desirable for computation because they allow for the reuse of many computations in the hierarchy of sparse grids.

**3.1. Exposing the Hierarchical Sampling Structure.** Hierarchies of multi-index sets  $\mathcal{I}_k \subset \mathcal{I}_{k+1}$  can be generated in a multitude of ways. Some common methods are full tensor-product and isotropic/anisotropic Smolyak algorithms [42, 36, 1]. The multi-index sets constructed from the full tensor-product algorithm are defined as

$$\mathcal{I}_k = \{\mathbf{i} \in \mathbb{N}_+^M : \max_{\ell=1, \dots, M} |i_{\ell} - 1| \leq (k - 1)\}.$$

On the other hand, the anisotropic Smolyak algorithm employs the multi-index set

$$\mathcal{I}_k = \{\mathbf{i} \in \mathbb{N}_+^M : \sum_{\ell=1}^M \gamma_\ell |i_\ell - 1| \leq \gamma_*(k-1)\},$$

where  $\gamma = (\gamma_1, \dots, \gamma_M)$  is an  $M$ -tuple of positive real numbers and  $\gamma_* = \min_\ell \gamma_\ell$ . Each component of  $\gamma$  determines the relative importance of the associated direction; and, in the case that  $\gamma = (1, \dots, 1)$ , we recover the isotropic Smolyak sparse-grid index set. For both the full tensor-product and Smolyak algorithms, the multi-index sets create the hierarchy required above. In general, the resulting point sets  $N_k$  produced from the Smolyak algorithm are sparser than those created from the full tensor-product algorithm. Hence, the Smolyak multi-index sets require fewer solves of (2.1) to evaluate the discretized objective functions,  $\widehat{J}_k = \widehat{J}_{\mathcal{I}_k}$ .

Now, consider isotropic Smolyak sparse grids, and suppose that the one-dimensional quadrature points satisfy  $|N_{k,j}| = \mathcal{O}(2^k)$  for  $j = 1, \dots, M$ . Then, the authors of [19] show that the resulting sparse grids satisfy

$$Q_k = |N_k| = \mathcal{O}(2^k k^{M-1}).$$

The growth rate between levels  $k$  and  $k-1$  is given by

$$q_k = Q_k/Q_{k-1} \approx 2 \left( \frac{k}{k-1} \right)^{M-1}$$

for  $k$  sufficiently large. Asymptotically, as  $k \rightarrow \infty$ , the growth rate is 2, and the largest growth occurs between levels  $k=1$  and  $k=2$ , namely,  $q_2 = Q_2/Q_1 \approx 2^M$ . In fact, for  $k=1$ ,  $Q_1 = 1$  independent of the number of dimensions  $M$ . Therefore,  $q_2 = Q_2$  for all  $M$ . The growth rate  $\{q_k\}_{k=1}^\infty$  is a monotonically decreasing sequence in the interval  $[2, Q_2]$ .

A popular choice of 1D quadrature points on  $[-1, 1]$  are Clenshaw-Curtis points

$$N_{m,j} = \left\{ -\cos \left( \frac{\pi(i-1)}{d_j-1} \right) : i = 1, \dots, d_i \right\}$$

with  $d_1 = 1$  and  $d_i = 2^{j-1} + 1$  for  $j > 1$ . The Clenshaw-Curtis points are nested. Furthermore, these points satisfy the assumptions on growth rate discussed in the previous paragraph. Therefore, the sequence of growth rates for the sparse grids built on Clenshaw-Curtis nodes is decreasing on  $[2, Q_2]$ .

**3.2. Sparse-Grid Collocation.** Given an admissible multi-index set  $\mathcal{I} \subset \mathbb{N}^M$  and the associated quadrature rule  $E_{\mathcal{I}}$ , the collocation discretization of (2.2) is

$$\min_{z \in \mathcal{Z}} \widehat{J}_{\mathcal{I}}(z) = \frac{1}{2} E_{\mathcal{I}} [\|\mathbf{C}u(z) - \bar{w}\|_{\mathcal{W}}^2] + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2 \quad (3.4)$$

Note that the evaluation of the quadrature rule  $E_{\mathcal{I}}$  requires the solution of only the  $Q_{\mathcal{I}} = |N_{\mathcal{I}}|$  deterministic, decoupled PDEs

$$\mathbf{A}(y_\ell^{\mathcal{I}})u_\ell + \mathbf{N}(u_\ell, y_\ell^{\mathcal{I}}) = \mathbf{F}(z, y_\ell^{\mathcal{I}}) \quad \forall \ell = 1, \dots, Q_{\mathcal{I}},$$

where  $N_{\mathcal{I}} = \{y_1^{\mathcal{I}}, \dots, y_{Q_{\mathcal{I}}}^{\mathcal{I}}\}$  [27, 28]. This is equivalent to a stochastic collocation discretization of (2.1) [27]. The semi-discretized objective function can be written in the standard quadrature form as

$$\widehat{J}_{\mathcal{I}}(z) = \frac{1}{2} \sum_{\ell=1}^{Q_{\mathcal{I}}} \omega_\ell^{\mathcal{I}} \|\mathbf{C}u_\ell(z) - \bar{w}\|_{\mathcal{W}}^2 + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2,$$

where  $\omega_\ell^{\mathcal{I}}$  are appropriate sparse-grid quadrature weights. Moreover, if Assumptions 2.1 and 2.2 hold, then  $\widehat{J}_{\mathcal{I}}(z)$  is Fréchet differentiable with gradient

$$\nabla \widehat{J}_{\mathcal{I}}(z) = \alpha z - \sum_{\ell=1}^{Q_{\mathcal{I}}} \omega_\ell^{\mathcal{I}} \mathbf{F}'(z, y_\ell^{\mathcal{I}})^* p_\ell.$$

In the gradient,  $p_\ell \in \mathcal{V}$  solves the decoupled deterministic adjoint equations

$$\mathbf{A}(y_\ell^{\mathcal{I}})^* p_\ell + \mathbf{N}(u_\ell, y_\ell^{\mathcal{I}})^* p_\ell = -\mathbf{C}^*(\mathbf{C}u_\ell - \bar{w}) \quad \forall \ell = 1, \dots, Q_{\mathcal{I}}.$$

These decoupled adjoint equations are equivalent to a stochastic collocation discretization of the infinite-dimensional adjoint equation (2.3) [27].

We note that sparse grids typically produce both positive and negative quadrature weights [19]. The presence of negative weights may affect optimization because  $\widehat{J}_{\mathcal{I}}(z)$  may not be convex or weakly lower semi-continuous even if  $\widehat{J}(z)$  is [27, 26].

**3.3. Collocation Error Bounds.** The convergence of stochastic collocation has been extensively studied for elliptic, parabolic, and hyperbolic PDEs. See, for example, [37, 36, 35, 1, 32]. The standard result applies for both bounded and unbounded  $\Gamma$ . For simplicity, we assume  $\Gamma$  is bounded. Furthermore, we require the following assumption on the regularity of the solution  $u$  of (2.1) with respect to the parameters  $y \in \Gamma$ . For these assumptions, we use the following notation: for  $y = (y_1, \dots, y_M) \in \Gamma$ ,  $y_j^* = (y_1, \dots, y_{j-1}, y_{j+1}, \dots, y_M) \in \Gamma_j^* = \prod_{\ell \neq j} \Gamma_\ell$ . Furthermore, given  $u \in C_\rho^0(\Gamma; \mathcal{V})$ , we consider the function  $u_j^* : \Gamma_j \rightarrow C_{\rho_j^*}^0(\Gamma_j^*; \mathcal{V})$  to be defined by  $(u_j^*(\xi))(y_j^*) = u(y_1, \dots, y_{j-1}, \xi, y_{j+1}, \dots, y_M)$ , where  $\rho_j^* = \prod_{\ell \neq j} \rho_\ell$ .

**ASSUMPTION 3.1.** *Let Assumptions 2.1 and 2.2 hold. Suppose  $\Gamma$  is bounded, and let  $u \in C_\rho^0(\Gamma; \mathcal{V})$  be the solution to (2.1) for fixed  $z \in \mathcal{Z}$ . Then there exists  $\tau_j > 0$  such that  $u_j^* : \Gamma_j \rightarrow C_{\rho_j^*}^0(\Gamma_j^*; \mathcal{V})$  has an analytic extension on the set*

$$\Sigma(\Gamma_j; \tau_j) = \{\xi \in \mathbb{C} : \text{dist}(\xi, \Gamma_j) \leq \tau_j\}.$$

*Furthermore, let  $p \in C_\rho^0(\Gamma; \mathcal{V})$  be the solution to (2.3). Then there exists  $\gamma_j > 0$  such that  $p_j^* : \Gamma_j \rightarrow C_{\rho_j^*}^0(\Gamma_j^*; \mathcal{V})$  has an analytic extension on the set  $\Sigma(\Gamma_j; \gamma_j)$ .*

Similar assumptions to those in Assumption 3.1 can be found in [1, Lem. 3.2], [37, Lem. 3.2], and [36, Lem. 2.3]. For examples of the state equation (2.1) that satisfy Assumption 3.1, see [37, 36, 35, 1, 32]. For examples of optimization problems (2.2) for which (2.1) and (2.3) satisfy Assumption 3.1, see [28, 27]. If Assumption 3.1 holds, then stochastic collocation provides a convergent approximation scheme. The convergence of stochastic collocation depends on the quadrature rules used. In the case of elliptic PDEs, convergence is proven for isotropic and anisotropic tensor product quadrature built on 1D Gaussian abscissae, as well as isotropic and anisotropic sparse-grid quadrature built on Gaussian and Clenshaw-Curtis abscissae. These results are stated in [1, Thm. 4.1] for tensor products of Gaussian abscissae, in [37, Thm. 3.10, 3.11, 3.18, 3.19] for isotropic sparse grids built on Clenshaw-Curtis and Gaussian abscissae, and in [36, Thm. 3.8, 3.13] for anisotropic sparse grids built on Clenshaw-Curtis and Gaussian abscissae. The standard error bound has a specific form that we assume throughout.

**ASSUMPTION 3.2.** *Let Assumption 3.1 hold, and let  $\boldsymbol{\tau} = (\tau_1, \dots, \tau_M)$  and  $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_M)$ . Furthermore, suppose  $\mathcal{I} \subset \mathbb{N}_+^M$  is an admissible index set with*

corresponding sparse grid  $N_{\mathcal{I}}$ ,  $Q = |N_{\mathcal{I}}|$ . Then,  $u \in C_{\rho}^0(\Gamma; \mathcal{V})$  solving (2.1) and  $p \in C_{\rho}^0(\Gamma; \mathcal{V})$  solving (2.3) satisfy

$$\|E[u] - E_{\mathcal{I}}[u]\|_{L_{\rho}^{\infty}(\Gamma; \mathcal{V})} \leq C(r(\boldsymbol{\tau}), M)Q^{-\nu(\boldsymbol{\tau}, M)} \quad (3.5)$$

and

$$\|E[p] - E_{\mathcal{I}}[p]\|_{L_{\rho}^{\infty}(\Gamma; \mathcal{V})} \leq C(r(\boldsymbol{\gamma}), M)Q^{-\nu(\boldsymbol{\gamma}, M)}, \quad (3.6)$$

respectively. The function  $r : \mathbb{R}^M \rightarrow \mathbb{R}^M$  is defined componentwise for  $j = 1, \dots, M$  by  $r_j(\tau) = \log\left(\frac{2\tau}{|\Gamma_j|} + \sqrt{1 + \frac{4\tau^2}{|\Gamma_j|^2}}\right)$ .

These results are extended to the optimization context for uniformly convex linear-quadratic optimal control problems in [27]. In this case, if  $z_Q \in \mathcal{Z}$  is a first-order necessary point of (3.4) and  $z_* \in \mathcal{Z}$  is a first-order necessary point of (2.2), then the error between  $z_Q$  and  $z_*$  satisfies the upper bound

$$\|z_Q - z_*\|_{\mathcal{Z}} \leq C(r(\boldsymbol{\gamma}), M)Q^{-\nu(r(\boldsymbol{\gamma}), M)},$$

where  $\nu$  is defined in (3.6).

**4. MG/OPT as a Multilevel-in-Sample-Space Optimization Solver.** Similar to classic spatial multigrid, the hierarchy of sparse-grid operators described above induces a hierarchy of (semi-)discretized optimization problems (2.2):

$$\min_{z \in \mathcal{Z}} \widehat{\mathcal{J}}_k(z) = \frac{1}{2} \sum_{i=1}^{Q_k} \omega_i^k \|\mathbf{C}u_i(z) - \bar{w}\|_{\mathcal{W}}^2 + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2, \quad k = 1, \dots, K.$$

Recall that the evaluation of  $\widehat{\mathcal{J}}_k(z)$  requires the solution of (2.1) at all points in the sparse grid  $N_k$  (i.e.,  $Q_k = |N_k|$  PDE solves). MG/OPT applies to this hierarchy of optimization problems. In addition, the variants of MG/OPT such as recursive trust-regions [21, 22, 23, 24] and the multilevel line-search approach of [47] also apply to this hierarchy of sparse-grid discretizations, but we restrict our attention to MG/OPT.

Unlike spatial multigrid, the hierarchy of sparse-grid collocation discretization spaces appears implicitly in the definition of the semi-discretized objective function. That is, the control space is fixed, and  $\nabla \widehat{\mathcal{J}}_k(z) \in \mathcal{Z}$  for all  $k$ . Therefore, the intergrid transfer operators (prolongation and interpolation) of spatial multigrid are trivially the identity operator. Moreover, for the application of MG/OPT, it is convenient to define the *coarse-grid corrected objective functions*

$$\mathcal{J}_k(z) = \mathcal{J}_k(z | v_k) = \widehat{\mathcal{J}}_k(z) - \langle v_k, z \rangle_{\mathcal{Z}} \quad \text{for } v_k \in \mathcal{Z}.$$

The MG/OPT algorithm defines  $v_k$  at each level, but it is always the case that  $v_K = 0$ . The multilevel sparse grid optimization algorithm is stated in Algorithm 1.

We offer a few comments on the implementation of Algorithm 1. First, Algorithm 1 defines one V-cycle of MG/OPT; and, with little modification, one can define more general cycles such as W-cycles, F-cycles, or cascadic multigrid. Second, the pre- and post-smoothing steps at each level, (4.2) and (4.4), can be computed by applying a fixed number of iterations of an optimization routine as suggested in [33]. Alternatively, Borzi [9, 6] suggests applying the pre- and post-smoothing optimization routines until the following sufficient decrease conditions are satisfied:

$$\begin{aligned} \mathcal{J}_k(z_{k,1}) &< \mathcal{J}_k(z_k^-) - \eta_{k,1} \|\nabla \mathcal{J}(z_k^-)\|_{\mathcal{Z}} & \eta_{k,1} &\in (0, 1) \\ \mathcal{J}_k(z_k^+) &< \mathcal{J}_k(z_{k,3}) - \eta_{k,2} \|\nabla \mathcal{J}(z_{k,3})\|_{\mathcal{Z}} & \eta_{k,2} &\in (0, 1). \end{aligned}$$

**MG/OPT:**  $z_k^+ = \text{MG/OPT}(k, z_k^-, v_k)$

**if**  $k = 1$  **then**

Return  $z_1^+ = z_1^- + s_1$  where  $s_1$  satisfies

$$s_1 = \arg \min_{s \in \mathcal{Z}} \mathcal{J}_1(z_1^- + s) = \widehat{\mathcal{J}}_1(z_1^- + s) - \langle v_1, (z_1^- + s) \rangle_{\mathcal{Z}}. \quad (4.1)$$

**else**

**Pre-Smoothing:** Perform  $T_{1,k}$  iterations of a convergent optimization algorithm to obtain

$$s_{k,1} \approx \arg \min_{s \in \mathcal{Z}} \mathcal{J}_k(z_k^- + s) = \widehat{\mathcal{J}}_k(z_k^- + s) - \langle v_k, (z_k^- + s) \rangle_{\mathcal{Z}} \quad (4.2)$$

and update  $z_{k,1} = z_k^- + s_{k,1}$ .

**Coarse Grid Correction:** Set  $v_{k-1} = v_k + (\nabla \widehat{\mathcal{J}}_{k-1}(z_{k,1}) - \nabla \widehat{\mathcal{J}}_k(z_{k,1}))$  and approximately minimize  $\mathcal{J}_{k-1}(z) = \widehat{\mathcal{J}}_{k-1}(z) - \langle v_{k-1}, z \rangle_{\mathcal{Z}}$  using

$$z_{k,2} = \text{MG/OPT}(k-1, z_{k,1}, v_{k-1}). \quad (4.3)$$

**Line Search:** Use a line search to determine  $\lambda_k \geq 0$  which sufficiently reduces  $\mathcal{J}_k(z_{k,1} + \lambda(z_{k,2} - z_{k,1}))$  and set  $z_{k,3} = z_{k,1} + \lambda_k(z_{k,2} - z_{k,1})$ .

**Post-Smoothing:** Perform  $T_{2,k}$  iterations of a convergent optimization algorithm to obtain

$$s_{k,2} \approx \arg \min_{s \in \mathcal{Z}} \mathcal{J}_k(z_{k,3} + s) = \widehat{\mathcal{J}}_k(z_{k,3} + s) - \langle v_k, (z_{k,3} + s) \rangle_{\mathcal{Z}} \quad (4.4)$$

and return  $z_k^+ = z_{k,3} + s_{k,2}$ .

**end**

**Algorithm 1:** Recursive MG/OPT algorithm.

Third, if  $\nabla^2 \widehat{\mathcal{J}}_k(z_{k,1})$  exists and is Lipschitz continuous with Lipschitz constant  $L_k > 0$  for  $k = 1, \dots, K$  and if  $e_k = (z_{k,2} - z_{k,1})$  is a descent direction, then Borzi [9, 6] suggests the following a priori choice for the line-search parameter  $\lambda_k$ :

$$\lambda_k = \min \left\{ 2, \frac{-\langle \nabla \widehat{\mathcal{J}}_k(z_{k,1}), e_k \rangle_{\mathcal{Z}}}{\langle \nabla^2 \widehat{\mathcal{J}}_k(z_{k,1}) e_k, e_k \rangle_{\mathcal{Z}} + L_k \|e_k\|_{\mathcal{Z}}^2} \right\}.$$

This choice of  $\lambda_k$  guarantees sufficient decrease in the objective function. In general,  $L_k$  is unknown, and  $\lambda_k$  is computed by using a standard line-search rule such as backtracking. As noted in [29], the a priori choice  $\lambda_k = 1$  as commonly used in the globalization of Newton's method may not apply to MG/OPT. Furthermore, the nestedness of the sparse grids  $N_k$  implies that no additional PDE solves are required when computing  $v_{k-1}$ . For optimization problem (2.2),  $v_{k-1}$  can be written as

$$v_{k-1} = v_k + \sum_{i=1}^{Q_{k-1}} (\omega_i^{k-1} - \omega_i^k) \mathbf{F}'(z, y_i^K)^* p_i - \sum_{i=Q_{k-1}+1}^{Q_k} \omega_i^k \mathbf{F}'(z, y_i^K)^* p_i$$

where  $K$  denotes the finest level of sparse grid,  $\omega_i^k = \omega_i^{\mathcal{I}^k}$  denotes the level  $k$  sparse-grid weights,  $y_i^K = y_i^{\mathcal{I}^K}$  denotes the level  $K$  sparse-grid points ordered so that

$$N_K = \{N_1, N_2 \setminus N_1, \dots, N_K \setminus N_{K-1}\} = \{y_1^1, \dots, y_{Q_1}^1, \dots, y_{Q_{K-1}+1}^K, \dots, y_{Q_K}^K\},$$

and  $p_i \in \mathcal{V}$  solves the adjoint equation (2.3) at  $y = y_i^k$  for  $i = 1, \dots, Q_k$ .

**5. Convergence Analysis for Algorithm 1.** The analysis here follows directly from the analysis for MG/OPT in [33, 34]. The author in [9, 6] proves similar results using standard multigrid techniques. The convergence analysis for Algorithm 1 does not require restriction and prolongation operators. In fact, this analysis depends only on the sparse-grid discretization through the assumptions on the subproblems  $\widehat{J}_k(z)$ . The results in this section require the following assumptions.

ASSUMPTION 5.1. *Let  $K \in \mathbb{N}$  be the finest level of sparse-grid hierarchy and assume a minimizer of  $\widehat{J}_K(z)$  exists. Denote this minimizer by  $z_K^* \in \mathcal{Z}$ . Furthermore, let  $\mathcal{B}_r(z_K^*) = \{z \in \mathcal{Z} : \|z - z_K^*\|_{\mathcal{Z}} < r\}$  denote the open ball of radius  $r > 0$  in  $\mathcal{Z}$ .*

1.  $\widehat{J}_k(z)$  is twice continuously Fréchet differentiable and bounded below for all  $k = 1, \dots, K$ .
2. There exists  $r > 0$  independent of  $k = 1, \dots, K$  such that  $\nabla^2 \widehat{J}_k(z) \in \mathcal{L}(\mathcal{Z}, \mathcal{Z})$  is a uniformly positive-definite operator for all  $z \in \mathcal{B}_r(z_K^*)$  and  $k = 1, \dots, K$ ; that is, there exists  $\kappa_k > 0$  such that

$$\langle \nabla^2 \widehat{J}_k(z) \xi, \xi \rangle_{\mathcal{Z}} \geq \kappa_k \|\xi\|_{\mathcal{Z}}^2 \quad \forall 0 \neq \xi \in \mathcal{Z}, \forall z \in \mathcal{B}_r(z_K^*). \quad (5.1)$$

3. The smoothing iteration numbers satisfy

$$T_{1,k} \geq 0, \quad T_{2,k} \geq 0, \quad \text{and} \quad T_{1,k} + T_{2,k} > 0 \quad \text{for} \quad k = 1, \dots, K.$$

4. The optimization routines used in (4.1), (4.2), and (4.4) are first-order convergent in the sense that

$$\liminf_j \|\nabla \widehat{J}_k(z_j)\|_{\mathcal{Z}} = 0.$$

Assumption 5.1 ensures that the semi-discretized optimization problems at each level  $k$  are well-defined. Assumption 5.1.1 ensures that Newton-type methods are applicable. Assumption 5.1.2 assumes that when close to a solution (basin of attraction), the Hessian operators are positive-definite. This ensures second-order sufficient conditions hold at the minimizer. Assumptions 5.1.3-4 guarantee that Algorithm 1 makes progress toward a solution. Under these assumptions, we first prove that  $e_K = z_{K,2} - z_{K,1}$  is a descent direction.

THEOREM 5.2. *Let Assumption 5.1 hold, and let  $z_{K,1} \in \mathcal{B}_r(z_K^*)$ . Furthermore, suppose the optimization problem (4.3) is solved to the relative gradient tolerance*

$$\|\nabla \widehat{J}_{K-1}(z_{K,2}) - v_{K-1}\|_{\mathcal{Z}} \leq \gamma \kappa_{K-1} \|z_{K,1} - z_{K,2}\|_{\mathcal{Z}} \quad \text{with} \quad \gamma \in [0, 1). \quad (5.2)$$

Then  $e_K = z_{K,2} - z_{K,1}$  is a descent direction.

*Proof.* Suppose the approximate solution of (4.3) satisfies (5.2). Then there exists  $\eta \in \mathcal{Z}$  such that  $\|\eta\|_{\mathcal{Z}} \leq \gamma \kappa_{K-1} \|z_{K,2} - z_{K,1}\|_{\mathcal{Z}}$  and

$$\nabla \widehat{J}_K(z_{K,1}) = \nabla \widehat{J}_{K-1}(z_{K,1}) - \nabla \widehat{J}_{K-1}(z_{K,2}) + \eta.$$

Therefore,

$$\begin{aligned} \langle \nabla \widehat{J}_K(z_{K,1}), e_K \rangle_{\mathcal{Z}} &= \langle \nabla \widehat{J}_{K-1}(z_{K,1}) - \nabla \widehat{J}_{K-1}(z_{K,2}) + \eta, e_K \rangle_{\mathcal{Z}} \\ &= \left\langle \int_0^1 \nabla^2 \widehat{J}_{K-1}(z_{K,2} - te_K) (-e_K) dt, e_K \right\rangle_{\mathcal{Z}} + \langle \eta, e_K \rangle_{\mathcal{Z}} \\ &\leq -\kappa_{K-1} \|e_K\|_{\mathcal{Z}}^2 + \|\eta\|_{\mathcal{Z}} \|e_K\|_{\mathcal{Z}} \leq (\gamma - 1) \kappa_{K-1} \|e_K\|_{\mathcal{Z}}^2 < 0. \end{aligned}$$

Hence,  $e_K$  is a descent direction.  $\square$

The first-order convergence of Algorithm 1 is an easy consequence of Theorem 5.2.

**COROLLARY 5.3.** *Let Assumption 5.1 and inequality (5.2) hold. Furthermore, let  $K \in \mathbb{N}_+$  denote the finest level of sparse grid. Suppose  $\{z_K^{(j)}\}_{j=1}^\infty \subset \mathcal{Z}$  denotes a sequence of iterations produced by Algorithm 1 with initial guess  $z_K^{(0)} \in \mathcal{Z}$ . Then*

$$\liminf_j \|\nabla \widehat{J}_K(z_K^{(j)})\|_{\mathcal{Z}} = 0.$$

*Proof.* If for some  $j$  the iterate  $z_K^{(j)} \in \mathcal{B}_r(z_K^*)$ , then Theorem 5.2 ensures the search direction  $e_K$  is a descent direction, and Theorem 1 of [33] proves the result. On the other hand, if  $z_K^{(j)} \notin \mathcal{B}_r(z_K^*)$ , then the search direction  $e_K$  need not be a descent direction. If  $e_K$  is not a descent direction, then the line-search parameter is  $\lambda_K = 0$ . In this case, Assumption 5.1.4 (i.e., global convergence of the smoothers) ensures the global convergence of Algorithm 1.  $\square$

**REMARK 5.4.** *Corollary 5.3 also holds if we replace Assumption 5.1.2 with the assumption that the level set*

$$S = \{z \in \mathcal{Z} : \widehat{J}_K(z) \leq \widehat{J}_K(z_K^{(0)})\}$$

*is compact. Under this assumption and if the pre- and post-smoothing steps are performed by using a trust-region or line-search algorithm, then the proof of Corollary 5.3 must be modified to account for possibly no improvement from the recursive step [34, Thm. 3]. On the other hand, to ensure the descent property in Theorem 5.2 under this new assumption, the MG/OPT subproblems (4.1) and (4.3) must be replaced by*

$$\min_{s \in \mathcal{Z}} \mathcal{J}_k(s) \quad \text{subject to} \quad \|s\|_{\mathcal{Z}} \leq \Delta$$

*for some  $\Delta > 0$  sufficiently small [34, Thm. 5].*

**6. The Convex-Quadratic Case.** The main result of this section is an explicit error bound for one V-cycle of Algorithm 1 when the pre- and post-smoothing steps are performed with a finite number of conjugate gradient (CG) iterations. Before proving this result, we develop upper bounds for the total number of PDE solves required in one V-cycle.

**6.1. Problem Formulation.** Consider the hierarchy of linear-quadratic optimal control problems ( $k = 1, \dots, K$ )

$$\min_{z \in \mathcal{Z}} \widehat{J}_k(z) = \frac{1}{2} \sum_{i=1}^{Q_k} \omega_i^k \|C u_{k,i}(z) - \bar{w}\|_{\mathcal{W}}^2 + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2,$$

where  $u_{k,i}(z) = u_{k,i} \in \mathcal{V}$  solves

$$\mathbf{A}(y_i^k) u_{k,i} + \mathbf{B}(y_i^k) z = \mathbf{b}(y_i^k) \quad \text{for } i = 1, \dots, Q_k.$$

Here,  $\mathbf{A} : \Gamma \rightarrow \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$  is assumed to have a bounded inverse for all  $y \in \Gamma$ ,  $\mathbf{B} : \Gamma \rightarrow \mathcal{L}(\mathcal{Z}, \mathcal{V}^*)$ , and  $\mathbf{b} : \Gamma \rightarrow \mathcal{V}^*$ . Note that assuming  $\mathbf{A}(y)$  has a bounded inverse for all  $y \in \Gamma$  implies Assumption 2.1. Again,  $K$  denotes the finest level of sparse grid discretization, while the coarsest level is always  $k = 1$ . Furthermore, suppose

$\nabla^2 \widehat{J}_k(z) \in \mathcal{L}(\mathcal{Z}, \mathcal{Z})$  is uniformly positive-definite for  $k = 1, \dots, K$ , that is, there exists  $0 < a_k \leq A_k < \infty$  such that

$$a_k \|v\|_{\mathcal{Z}}^2 \leq \langle \nabla^2 \widehat{J}_k(z)v, v \rangle_{\mathcal{Z}} \leq A_k \|v\|_{\mathcal{Z}}^2 \quad \forall v \in \mathcal{Z}. \quad (6.1)$$

To simplify notation, denote  $\mathbf{A}_{k,i} = \mathbf{A}(y_i^k)$ ,  $\mathbf{B}_{k,i} = \mathbf{B}(y_i^k)$  and  $\mathbf{b}_{k,i} = \mathbf{b}(y_i^k)$ . By assumption,  $\mathbf{A}_{k,i}$  has a bounded inverse  $\mathbf{A}_{k,i}^{-1} \in \mathcal{L}(\mathcal{V}^*, \mathcal{V})$ , and the state variable  $u_{k,i}(z) = u_{k,i} \in \mathcal{V}$  can be written as

$$u_{k,i} = \mathbf{A}_{k,i}^{-1}(\mathbf{b}_{k,i} - \mathbf{B}_{k,i}z).$$

Substituting this expression for  $u_{k,i}$  into the objective function  $\widehat{J}_k(z)$  gives

$$\begin{aligned} \widehat{J}_k(z) &= \frac{1}{2} \sum_{i=1}^{Q_k} \omega_i^k \|\mathbf{C}\mathbf{A}_{k,i}^{-1}(\mathbf{b}_{k,i} - \mathbf{B}_{k,i}z) - \bar{w}\|_{\mathcal{W}}^2 + \frac{\alpha}{2} \|z\|_{\mathcal{Z}}^2 \\ &= \frac{1}{2} \langle \mathbf{H}_k z, z \rangle_{\mathcal{Z}} - \langle \mathbf{g}_k, z \rangle_{\mathcal{Z}} + c_k, \end{aligned}$$

where  $\mathbf{H}_k \in \mathcal{L}(\mathcal{Z}, \mathcal{Z})$  and  $\mathbf{g}_k \in \mathcal{Z}$  are defined as

$$\begin{aligned} \mathbf{H}_k &= \alpha \mathbf{I} + \sum_{i=1}^{Q_k} \omega_i^k \mathbf{B}_{k,i}^* \mathbf{A}_{k,i}^{-*} \mathbf{C}^* \mathbf{C} \mathbf{A}_{k,i}^{-1} \mathbf{B}_{k,i}, \\ \mathbf{g}_k &= \sum_{i=1}^{Q_k} \omega_i^k \mathbf{B}_{k,i}^* \mathbf{A}_{k,i}^{-*} \mathbf{C}^* (\mathbf{C} \mathbf{A}_{k,i}^{-1} \mathbf{b}_{k,i} - \bar{w}). \end{aligned}$$

Here,  $\mathbf{I} \in \mathcal{L}(\mathcal{Z}, \mathcal{Z})$  is the identity operator,  $\mathbf{H}_k = \nabla^2 \widehat{J}_k(z)$  is the the Hessian operator, and  $\nabla \widehat{J}_k(z) = \mathbf{H}_k z - \mathbf{g}_k$  is the gradient. Furthermore,  $c_k$  is the appropriately defined constant that is irrelevant in the context of optimization. Given  $z_0 \in \mathcal{Z}$ , the first-order necessary conditions are equivalent to the Newton system

$$\nabla^2 \widehat{J}_k(z_0)s = -\nabla \widehat{J}_k(z_0) \quad \iff \quad \mathbf{H}_k s = -(\mathbf{H}_k z_0 - \mathbf{g}_k). \quad (6.2)$$

**6.2. Hierarchical Sparse Grids and Inexact Conjugate Gradients.** Recall that  $\mathcal{Z}$  is a Hilbert space and that the existence of  $0 < a_k \leq A_k < \infty$  in (6.1) ensures  $\mathbf{H}_k$  is a positive-definite, bounded linear operator. Moreover, the specific form of  $\mathbf{H}_k$  implies that  $\mathbf{H}_k$  is self-adjoint. Under these conditions, we can apply the conjugate gradient algorithm (CG) to solve (6.2). The convergence of CG applied to (6.2) depends on the spectral properties of  $\mathbf{H}_k$  as shown in the following theorem. For this result, we define the  $\mathbf{H}_k$ -norm and  $\mathbf{H}_k$ -inner product,  $\|z\|_{\mathbf{H}_k} = \sqrt{\langle z, z \rangle_{\mathbf{H}_k}} = \sqrt{\langle \mathbf{H}_k z, z \rangle_{\mathcal{Z}}}$  for all  $z \in \mathcal{Z}$ .

**THEOREM 6.1.** *The sequence of iterates,  $\{z_j\} \subset \mathcal{Z}$ , generated by using CG applied to (6.2) converges to  $z_* \in \mathcal{Z}$  and*

$$\|z_* - z_j\|_{\mathbf{H}_k} \leq 2 \left( \frac{\sqrt{A_k} - \sqrt{a_k}}{\sqrt{A_k} + \sqrt{a_k}} \right)^j \|z_* - z_0\|_{\mathbf{H}_k}.$$

*Proof.* Note that  $\mathbf{H}_k$  is a self-adjoint, positive definite, bounded linear operator. Moreover, one can easily show that the  $\mathcal{Z}$ - and  $\mathbf{H}_k$ -norms are equivalent. Therefore, Theorems 7 and 11 in [39] apply and prove the convergence of CG applied to (6.2).  $\square$

Each iteration of CG requires the application of the Hessian operator to a vector. Recall that the computation of the gradient,  $\nabla \widehat{J}_k(z) = \mathbf{H}_k z - \mathbf{g}_k$  requires  $2Q_k$  PDE solves (i.e., a state solve,  $\mathbf{A}_{k,j}^{-1}$ , and an adjoint solve,  $\mathbf{A}_{k,j}^{-*}$ , for  $j = 1, \dots, Q_k$ ). Similarly, the application of the Hessian  $\mathbf{H}_k$  to a vector requires  $2Q_k$  PDE solves. Therefore, applying CG to (6.2) requires  $2Q_k(N_{\text{CG}}^k + 1)$  PDE solves, where  $N_{\text{CG}}^k$  denotes the number of CG iterations required to solve (6.2). Note that if the control space  $\mathcal{Z}$  is finite-dimensional, then  $N_{\text{CG}}^k \leq \dim(\mathcal{Z})$  in exact arithmetic.

Hessian-times-a-vector computations are computationally prohibitive for large problems even though the PDEs to be solved are linear. Fortunately we can exploit the hierarchical nature of sparse-grid discretization to possibly reduce this computational effort. Nested sparse grids allow us to build all levels of sparse-grid approximation ( $\kappa < k$ ) concurrently while computing the level  $k$  approximation. We suggest the inexact Hessian-times-a-vector algorithm listed in Algorithm 2.

**Multilevel Hessian-Times-a-Vector:** Given  $z, v \in \mathcal{Z}$  and  $\tau > 0$ .  
 Set  $Q_0 = 0$  and  $h_\kappa = \alpha v$  for  $\kappa = 1, \dots, k$ .  
**for**  $\kappa = 1, \dots, k$  **do**  
   **for**  $i = Q_{\kappa-1} + 1, \dots, Q_\kappa$  **do**  
     Solve  $\mathbf{A}_{\kappa,i} w_{\kappa,i} = \mathbf{B}_{\kappa,i} z$ .  
     Solve  $\mathbf{A}_{\kappa,i}^* p_{\kappa,i} = \mathbf{C}^* \mathbf{C} w_{\kappa,i}$ .  
     **for**  $\ell = \kappa, \dots, k$  **do**  
       Update  $h_\ell \leftarrow h_\ell + \omega_{\ell,i} \mathbf{B}_{\kappa,i}^* p_{\kappa,i}$ .  
     **end**  
**end**  
**if**  $\|h_\kappa - h_{\kappa-1}\|_{\mathcal{Z}} \leq \tau \|h_{\kappa-1}\|_{\mathcal{Z}}$  **then**  
   Set  $h_k = h_\kappa$  and exit.  
**end**  
**end**  
 Set  $\mathbf{H}_k v \approx h_k$ .

**Algorithm 2:** Inexact Hessian-times-a-vector algorithm.

In Algorithm 2 we build all quadrature estimates of  $\mathbf{H}_\kappa v$  for  $\kappa = 1, \dots, k$  concurrently by exploiting the sparse-grid hierarchy. Notice that no additional PDE solves are required in the evaluation of lower-order quadrature and that computational savings occur when Algorithm 2 terminates early with  $\kappa < k$ . In this case, Algorithm 2 performs  $2(Q_k - Q_\kappa)$  fewer PDE solves than does the standard Hessian-times-a-vector algorithm at level  $k$ . In the case of early termination, Algorithm 2 inexactly applies  $\mathbf{H}_k$  to some vector  $v$ . Fortunately Krylov methods can be adjusted to handle such inexactness. In [45, 41, 18] and the references within, the authors study the effects of inexactness on Krylov subspace methods.

Denote  $(\mathbf{H}_k + \mathbf{E}_j)v_j = h_{k,j}$  as the application of Algorithm 2 during the  $j^{\text{th}}$  iteration of the inexact Krylov method. In [41], the authors present the following bound on inexactness, which guarantees convergence of the inexact Krylov method:

$$\|\mathbf{E}_j\| \leq \frac{\ell_m \varepsilon}{\|\tilde{r}_{j-1}\|_{\mathcal{Z}}}, \quad (6.3)$$

where  $m$  is the maximum number of CG iterations,  $\varepsilon > 0$  is a user-defined tolerance,  $\tilde{r}_{j-1}$  is the inexact residual of (6.2) at the  $j^{\text{th}}$  iteration of the inexact Krylov method, and  $\ell_m > 0$  is a specific problem and algorithm constant. Under this condition, the

error between the residual from the inexact Krylov method ( $\tilde{r}_m$ ) and the exact Krylov method ( $r_m$ ) at the final iteration satisfies

$$\|r_m - \tilde{r}_m\|_{\mathcal{Z}} \leq \varepsilon. \quad (6.4)$$

See [41, Thm. 5.3, 5.4] for the specific form of  $\ell_m$  for inexact GMRES and inexact FOM. Since CG is equivalent to FOM applied to self-adjoint positive-definite operators [40], the proof of [41, Thm. 5.4] also applies to CG.

The parameter  $\ell_m$  in (6.3) is problem dependent and typically cannot be computed a priori. The authors of [41] suggest approximating  $\ell_m$  with

$$\ell_m \approx \frac{\sigma_{\min}(\mathbf{H}_k)}{m}$$

where  $\sigma_{\min}(\mathbf{H}_k)$  denotes the minimum singular value of  $\mathbf{H}_k$ . In [45], the authors set  $\ell_m = 1$  and demonstrate that in many circumstances this choice of  $\ell_m$  does not strongly affect the convergence of the algorithm [41, p. 463]. The authors in [18] propose replacing (6.3) with

$$\|\mathbf{E}_j\| \leq \frac{\sigma_{\min}(\mathbf{H}_k)}{2} \min \left\{ 1, \frac{\tilde{\ell}_{m,j}\varepsilon}{\|\tilde{r}_j\|} \right\}$$

where  $\tilde{\ell}_{m,j} > 0$  is computed by using quantities available at each Krylov iteration [18, Thm. 4.2]. This condition also ensures the residual error bound (6.4).

**REMARK 6.2.** *The relative error  $\|h_k - h_{k-1}\|_{\mathcal{Z}}/\|h_{k-1}\|_{\mathcal{Z}}$  used to terminate Algorithm 2 is not an error estimate. Therefore, early termination must be monitored, and convergence of inexact CG may not be guaranteed.*

**6.3. Exact Line Search.** For this convex-quadratic example, the  $k^{\text{th}}$ -level line-search parameter,  $\lambda_k$ , can be computed exactly. Given  $z_k \in \mathcal{Z}$ , if  $e_k \in \mathcal{Z}$  is a descent direction of  $\mathcal{J}_k(z_k + s) = \hat{\mathcal{J}}_k(z_k + s) - \langle v_k, (z_k + s) \rangle_{\mathcal{Z}}$ , then minimizing  $\mathcal{J}_k(z_k + \lambda e_k)$  with respect to  $\lambda$  yields the explicit value

$$\lambda_k = -\frac{\langle \nabla \hat{\mathcal{J}}_k(z_k) - v_k, e_k \rangle_{\mathcal{Z}}}{\langle \nabla^2 \hat{\mathcal{J}}_k(z_k) e_k, e_k \rangle_{\mathcal{Z}}} = -\frac{\langle \mathbf{H}_k z_k - \mathbf{g}_k - v_k, e_k \rangle_{\mathcal{Z}}}{\langle \mathbf{H}_k e_k, e_k \rangle_{\mathcal{Z}}}. \quad (6.5)$$

Since  $e_k$  is a descent direction, Assumption 5.1 ensures that  $\lambda_k$  is positive. The computation of the gradient requires  $2Q_k$  PDE solves, and the application of  $\mathbf{H}_k$  to the search direction  $e_k$  requires  $2Q_k$  PDE solves. Therefore, computation of  $\lambda_k$  requires  $4Q_k$  PDE solves.

**6.4. Computational Work.** We are now prepared to derive bounds on the total number of PDE solves required for one V-cycle of MG/OPT using exact CG smoothing. Let  $W_k$  denote the number of PDE solves per cycle of Algorithm 1 at level  $k$ , and let  $W_{k+1}^k$  denote the number of PDE solves required for one cycle of Algorithm 1 excluding the number of PDE solves required to solve (4.3). That is,  $W_{k+1}^k$  is the number of PDE solves required for pre- and post-smoothing, computing the coarse grid correction  $v_k$ , and computing the line-search step length  $\lambda_k$ . The structure of Algorithm 1 leads to the recursive definition of  $W_k$ :

$$W_2 = W_2^1 + W_1 \quad \text{and} \quad W_{k+1} = W_{k+1}^k + W_k \quad \implies \quad W_K = \sum_{k=2}^K W_k^{k-1} + W_1, \quad (6.6)$$

where  $W_1$  is the number of PDE solves required to exactly solve (4.1). See [43] for more details on spatial multigrid work estimates. If we use CG to solve (4.1), then  $W_1 = 2(N_{\text{CG}}^1 + 1)Q_1$ , where  $N_{\text{CG}}^1$  denotes the total number of CG iterations.

For the following results, we assume the sparse-grid growth rate satisfies

$$q_k = Q_k/Q_{k-1} = 2 \left( \frac{k}{k-1} \right)^{M-1} \quad \text{for } k = 1, 2, \dots, \quad (6.7)$$

which is satisfied for many instances of isotropic Smolyak sparse grids (recall Section 3 and [19]). We prove two results: the first result concerns pre- and post-smoothing with a constant number of iterations, while the second results deals with level-dependent pre- and post-smoothing.

**PROPOSITION 6.3.** *Let (6.7) hold. Consider Algorithm 1 with  $T_{1,k} = \tau_1 \geq 0$  iterations of CG for pre-smoothing and  $T_{2,k} = \tau_2 \geq 0$  iterations of CG for post-smoothing for  $k = 1, \dots, K$ . Then, the total number of PDE solves for a single V-cycle of Algorithm 1 satisfies*

$$W_K \leq 4(3 + \tau_1 + \tau_2)Q_K + W_1.$$

*Proof.* We require  $2Q_k$  PDE solves to compute the gradient,  $2\tau_1 Q_k$  PDE solves for pre-smoothing,  $2\tau_2 Q_k$  PDE solves for post-smoothing, and  $4Q_k$  PDE solves to compute the line-search step length. Therefore, the growth rate (6.7) implies

$$W_k^{k-1} = (4 + 2(1 + \tau_1 + \tau_2))Q_k = (6 + 2(\tau_1 + \tau_2))Q_K \prod_{j=k+1}^K q_j^{-1}.$$

Notice that

$$\begin{aligned} \prod_{j=k+1}^K q_j^{-1} &= \left( \frac{1}{2} \right)^{K-(k+1)+1} \left( \frac{k}{k+1} \cdots \frac{K-1}{K} \right)^{M-1} \\ &= \left( \frac{1}{2} \right)^{K-k} \left( \frac{k}{K} \right)^{M-1} \leq \left( \frac{1}{2} \right)^{K-k}. \end{aligned} \quad (6.8)$$

Combining these facts with (6.6) and then invoking geometric series convergence yields the desired bound.  $\square$

For our second example, we vary the number of CG iterations,  $T_{1,k}$  and  $T_{2,k}$ , at each level. This approach allows us to more accurately solve the smoothing problems (4.2) and (4.4) on the coarse levels and less accurately on the fine levels.

**PROPOSITION 6.4.** *Let (6.7) hold and let  $\tau_1, \tau_2$  be fixed non-negative integers. Moreover, suppose pre- and post-smoothing are performed with*

$$T_{j,K} = \tau_j, T_{j,K-1} = 2\tau_j, \dots, T_{j,2} = (K-1)\tau_j \quad \text{for } j = 1, 2$$

*CG iterations, respectively. Then the total number of PDE solves for a single V-cycle of Algorithm 1 satisfies*

$$W_K \leq 4(3 + 2(\tau_1 + \tau_2))Q_K + W_1.$$

*Proof.* Note that  $2 = \sum_{n=0}^{\infty} 2^{-n}$  and  $2 = \sum_{n=1}^{\infty} n2^{-n}$ . Using these facts, we obtain from the bound (6.8) and the recursive estimate (6.6),

$$\begin{aligned} W_K &\leq Q_K \sum_{k=2}^K (6 + 2(\tau_1 + \tau_2)(K - (k - 1))) \left(\frac{1}{2}\right)^{K-k} + W_1 \\ &\leq Q_K \left(12 + 2(\tau_1 + \tau_2) \sum_{k=2}^K (K - k) \left(\frac{1}{2}\right)^{K-k} + 4(\tau_1 + \tau_2)\right) + W_1 \\ &\leq 4(3 + 2(\tau_1 + \tau_2))Q_K + W_1. \end{aligned}$$

□

**6.5. Error Estimation.** We now derive an error bound for a single V-cycle of Algorithm 1 where pre- and post-smoothers are computed by using  $T_{1,k}$  and  $T_{2,k}$  iterations of CG, respectively. The error estimate in this subsection is based on the CG error estimate given in Theorem 6.1. This subsection is organized as follows. First we present a compact operator representation for a single V-cycle of Algorithm 1. Using this operator formulation, we then apply the CG error estimate in Theorem 6.1 to determine an initial upper bound for the V-cycle error. Subsequently, we prove an optimality result concerning the line-search parameter. Combining this line-search result with the CG error estimate gives the final error bound. To conclude, we present explicit bounds for the 2-level case (i.e.,  $K = 2$ ).

We seek a representation of the iterate  $z_k^+$  of Algorithm 1 as an operator equation depending on the coarse grid information  $z_\ell^-, v_\ell, \mathbf{g}_\ell, \mathbf{H}_\ell$ , and  $\lambda_\ell$  for  $\ell = 1, \dots, k$ . First, recall that  $T_{k,i}$  iterations of CG applied to (4.2) and (4.4) produce

$$z_{k,1} = (\mathbf{I} - \mathbf{P}_{k,1}\mathbf{H}_k)z_k^- + \mathbf{P}_{k,1}(\mathbf{g}_k + v_k) \quad (6.9a)$$

$$z_k^+ = (\mathbf{I} - \mathbf{P}_{k,2}\mathbf{H}_k)z_{k,3} + \mathbf{P}_{k,2}(\mathbf{g}_k + v_k), \quad (6.9b)$$

where  $\mathbf{P}_{k,i} = p_{k,i}(\mathbf{H}_k)$  and  $p_{k,i}$  is a polynomial of degree  $T_{k,i} - 1$  for  $i = 1, 2$  [40, L. 6.28]. Now, beginning on level  $k = 1$ , define  $\mathbf{S}_1 = \mathbf{H}_1^{-1}$ . Then the result of the level 1 optimization problem (4.1) can be expressed as

$$z_1^+ = (\mathbf{I} - \mathbf{S}_1\mathbf{H}_1)z_1^- + \mathbf{S}_1(\mathbf{g}_1 + v_1).$$

Employing this expression for  $z_1^+$  and the compact representations of the smoothing operators (6.9), we arrive at the following compact operator form for the  $k^{\text{th}}$ -level MG/OPT iteration:

$$z_k^+ = (\mathbf{I} - \mathbf{S}_k\mathbf{H}_k)z_k^- + \mathbf{S}_k(\mathbf{g}_k + v_k), \quad (6.10)$$

where  $\mathbf{S}_k$  is defined recursively through Algorithm 1 and satisfies

$$(\mathbf{I} - \mathbf{S}_k\mathbf{H}_k) = (\mathbf{I} - \mathbf{P}_{k,2}\mathbf{H}_k)(\mathbf{I} - \lambda_k\mathbf{S}_{k-1}\mathbf{H}_k)(\mathbf{I} - \mathbf{P}_{k,1}\mathbf{H}_k) \quad (6.11)$$

for  $k = 2, \dots, K$ .

We use the operator form (6.10) of the MG/OPT iteration to derive error bounds. First, we apply Theorem 6.1 to prove the following partial bound.

LEMMA 6.5. *Let  $k \in \{1, \dots, K\}$ ,  $\lambda_k \in \mathbb{R}$  be fixed, and  $z_k^* \in \mathcal{Z}$  satisfy*

$$\mathbf{H}_k z_k^* = (\mathbf{g}_k + v_k).$$

Furthermore, let the assumptions of Theorem 6.1 hold, and consider one V-cycle of Algorithm 1 where pre- and post-smoothing are performed by using  $T_{1,k}$  and  $T_{2,k}$  iterations of CG, respectively. Then,

$$\|z_k^* - z_k^\dagger\|_{\mathbf{H}_k} \leq 2 \left( \frac{\sqrt{A_k} - \sqrt{a_k}}{\sqrt{A_k} + \sqrt{a_k}} \right)^{T_{2,k}} \|z_k^* - z_{k,3}\|_{\mathbf{H}_k}.$$

*Proof.* This is a straightforward application of Theorem 6.1.  $\square$

The goal now is to bound the quantity  $\|z_k^* - z_{k,3}\|_{\mathbf{H}_k}$ . To this end, recall that  $e_k = (z_{k,2} - z_{k,1}) \in \mathcal{Z}$ , and note that  $e_k$  satisfies

$$e_k = \mathbf{S}_{k-1}(\mathbf{g}_k + v_k - \mathbf{H}_k z_{k,1}), = \mathbf{S}_{k-1} \mathbf{H}_k (z_k^* - z_{k,1}) \quad (6.12)$$

where  $z_k^*$  is defined in the statement of Lemma 6.5. Substituting this expression into the right-hand side of the error bound given in Lemma 6.5 gives

$$\|z_k^* - z_{k,3}\|_{\mathbf{H}_k} = \|(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)(z_k^* - z_{k,1})\|_{\mathbf{H}_k}.$$

Using this error representation, we prove the following optimality result for the exact line-search parameter computed using equation (6.5).

LEMMA 6.6. *Let  $\lambda_k$  be the exact line-search parameter computed in equation (6.5), and define  $v = (z_k^* - z_{k,1})$ . Then*

$$\lambda_k = \arg \min_{\mu \in \mathbb{R}} \frac{1}{2} \|(\mathbf{I} - \mu \mathbf{S}_{k-1} \mathbf{H}_k)v\|_{\mathbf{H}_k}^2, \quad (6.13)$$

and

$$\|(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)v\|_{\mathbf{H}_k}^2 = \langle (\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)v, v \rangle_{\mathbf{H}_k}. \quad (6.14)$$

*Proof.* Define  $j(\mu) = \frac{1}{2} \|(\mathbf{I} - \mu \mathbf{S}_{k-1} \mathbf{H}_k)v\|_{\mathbf{H}_k}^2$ . The objective function  $j : \mathbb{R} \rightarrow \mathbb{R}$  is differentiable, convex, and quadratic. Expanding  $j$  gives

$$\begin{aligned} j(\mu) &= \frac{1}{2} \|(\mathbf{I} - \mu \mathbf{S}_{k-1} \mathbf{H}_k)v\|_{\mathbf{H}_k}^2 \\ &= \frac{1}{2} \langle \mathbf{H}_k (\mathbf{I} - \mu \mathbf{S}_{k-1} \mathbf{H}_k)v, (\mathbf{I} - \mu \mathbf{S}_{k-1} \mathbf{H}_k)v \rangle_{\mathcal{Z}} \\ &= \frac{\mu^2}{2} \langle \mathbf{H}_k \mathbf{S}_{k-1} \mathbf{H}_k v, \mathbf{S}_{k-1} \mathbf{H}_k v \rangle_{\mathcal{Z}} - \mu \langle \mathbf{S}_{k-1} \mathbf{H}_k v, \mathbf{H}_k v \rangle_{\mathcal{Z}} + \frac{1}{2} \langle \mathbf{H}_k v, v \rangle_{\mathcal{Z}}. \end{aligned}$$

Setting the derivative,  $j'(\mu)$ , to zero and solving for  $\mu$  gives the optimal solution

$$\mu_* = \frac{\langle \mathbf{S}_{k-1} \mathbf{H}_k v, \mathbf{H}_k v \rangle_{\mathcal{Z}}}{\langle \mathbf{H}_k \mathbf{S}_{k-1} \mathbf{H}_k v, \mathbf{S}_{k-1} \mathbf{H}_k v \rangle_{\mathcal{Z}}}.$$

Now, since  $e_k = (z_{k,2} - z_{k,1})$  satisfies (6.12), the optimal value of  $\mu$  satisfies

$$\mu_* = \frac{\langle e_k, \mathbf{g}_k + v_k - \mathbf{H}_k z_{k,1} \rangle_{\mathcal{Z}}}{\langle \mathbf{H}_k e_k, e_k \rangle_{\mathcal{Z}}} = \lambda_k.$$

This proves (6.13), and evaluating  $2j(\lambda_k)$  proves (6.14).  $\square$

The optimality of the line-search parameter,  $\lambda_k$ , proved in Lemma 6.6 and Lemma 6.5 combined with Theorem 6.1 implies the following error bound:

$$\|z_k^* - z_k^+\|_{\mathbf{H}_k} \leq 4 \left( \frac{\sqrt{A_k} - \sqrt{a_k}}{\sqrt{A_k} + \sqrt{a_k}} \right)^{T_{1,k} + T_{2,k}} \|z_k^* - z_k^-\|_{\mathbf{H}_k}.$$

This result is comparable to the error bound for performing  $T_{1,k} + T_{2,k}$  iterations of CG with restart after  $T_{1,k}$  iterations and is overly pessimistic because it disregards the coarse-grid information. In the following, we show that the coarse-grid correction is, in fact, beneficial.

LEMMA 6.7. *Let the assumptions of Lemma 6.5 hold, and let  $\varrho(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)$  denote the spectral radius of  $(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)$ . Then*

$$\|z_k^* - z_k^+\|_{\mathbf{H}_k} \leq 4 \sqrt{\varrho(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)} \left( \frac{\sqrt{A_k} - \sqrt{a_k}}{\sqrt{A_k} + \sqrt{a_k}} \right)^{T_{1,k} + T_{2,k}} \|z_k^* - z_k^-\|_{\mathbf{H}_k}. \quad (6.15)$$

*Proof.* Lemma 6.6, in particular equality (6.14), implies

$$\|(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)(z_k^* - z_{k,1})\|_{\mathbf{H}_k} \leq \sqrt{\varrho(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)} \|z_k^* - z_{k,1}\|_{\mathbf{H}_k}.$$

Therefore, Lemma 6.5 and Theorem 6.1 imply (6.15).  $\square$

The goal now is to derive explicit bounds on the spectral radius of  $(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k)$ . In particular, we wish to prove that  $\varrho(\mathbf{I} - \lambda_k \mathbf{S}_{k-1} \mathbf{H}_k) < 1$ . This is equivalent to proving  $(1 - \lambda_k \mu) < 1$  for all eigenvalues,  $\mu$ , of  $\mathbf{S}_{k-1} \mathbf{H}_k$ . In the case of  $K = 2$ , we can prove such bounds. Note that if  $(v, \mu) \in \mathcal{Z} \times \mathbb{C}$  is an eigenpair of  $\mathbf{S}_1 \mathbf{H}_2 = \mathbf{H}_1^{-1} \mathbf{H}_2$ , then  $\mathbf{H}_2 v = \mu \mathbf{H}_1 v$ ; in other words,  $\mu$  is a generalized eigenvalue of the operator pencil  $(\mathbf{H}_2, \mathbf{H}_1)$ . Let  $\sigma(\mathbf{H}_2, \mathbf{H}_1)$  denote the spectrum of the pencil  $(\mathbf{H}_2, \mathbf{H}_1)$ . Then the spectral radius is  $\varrho(\mathbf{I} - \lambda_2 \mathbf{H}_1^{-1} \mathbf{H}_2) = 1 - \lambda_2 \min\{\mu : \mu \in \sigma(\mathbf{H}_2, \mathbf{H}_1)\}$ .

LEMMA 6.8. *Suppose there exists  $\varepsilon > 0$  such that*

$$\|\mathbf{H}_2 v - \mathbf{H}_1 v\|_{\mathcal{Z}} \leq \varepsilon \quad \forall v \in \{s \in \mathcal{Z} : \|s\|_{\mathcal{Z}} \leq 1\}. \quad (6.16)$$

*Then, the spectrum  $\sigma(\mathbf{H}_2, \mathbf{H}_1)$  satisfies*

$$\sigma(\mathbf{H}_2, \mathbf{H}_1) \subset [(1 + a_2^{-1} \varepsilon)^{-1}, 1 + a_1^{-1} \varepsilon].$$

*Proof.* Let  $\mu \in \sigma(\mathbf{H}_2, \mathbf{H}_1)$  and  $v \in \mathcal{Z}$  be a normalized eigenfunction corresponding to  $\mu$  (i.e.,  $\|v\|_{\mathcal{Z}} = 1$ ). First note that  $\mu > 0$ ; that is,

$$\mathbf{H}_2 v = \mu \mathbf{H}_1 v \quad \Rightarrow \quad \langle \mathbf{H}_2 v, v \rangle_{\mathcal{Z}} = \mu \langle \mathbf{H}_1 v, v \rangle_{\mathcal{Z}} \quad \Rightarrow \quad \mu = \frac{\langle \mathbf{H}_1 v, v \rangle_{\mathcal{Z}}}{\langle \mathbf{H}_2 v, v \rangle_{\mathcal{Z}}} > 0$$

since  $\mathbf{H}_2$  and  $\mathbf{H}_1$  are assumed to be uniformly positive-definite operators.

Write  $\mathbf{H}_1 = \mathbf{H}_2 + \delta \mathbf{H}$ , where  $\delta \mathbf{H} = \mathbf{H}_1 - \mathbf{H}_2$ . Then, substituting  $\mathbf{H}_2 + \delta \mathbf{H}$  for  $\mathbf{H}_1$  gives

$$\mathbf{H}_2 v = \mu \mathbf{H}_2 v + \mu \delta \mathbf{H} v \quad \Rightarrow \quad \delta \mathbf{H} v = \frac{1 - \mu}{\mu} \mathbf{H}_2 v \quad \Rightarrow \quad \mu^{-1} - 1 = \frac{\langle \delta \mathbf{H} v, v \rangle_{\mathcal{Z}}}{\langle \mathbf{H}_2 v, v \rangle_{\mathcal{Z}}} \leq a_2^{-1} \varepsilon.$$

Since  $\mu > 0$ , we have  $\mu \geq (1 + a_2^{-1} \varepsilon)^{-1}$ .

On the other hand,  $\mathbf{H}_2 = \mathbf{H}_1 - \delta\mathbf{H}$ , and

$$\mu\mathbf{H}_1v = \mathbf{H}_1v - \delta\mathbf{H}v \quad \Rightarrow \quad (\mu-1)\mathbf{H}_1v = -\delta\mathbf{H}v \quad \Rightarrow \quad \mu-1 = \frac{-\langle\delta\mathbf{H}v, v\rangle_{\mathcal{Z}}}{\langle\mathbf{H}_1v, v\rangle_{\mathcal{Z}}} \leq a_1^{-1}\varepsilon.$$

Therefore, we have  $\mu \leq 1 + a_1^{-1}\varepsilon$ . This proves the lemma.  $\square$

Lemma 6.8 implies the following bound on the spectral radius  $\varrho(\mathbf{I} - \lambda_2\mathbf{H}_1^{-1}\mathbf{H}_2)$ :

$$\varrho(\mathbf{I} - \lambda_2\mathbf{H}_1^{-1}\mathbf{H}_2) \leq 1 - \lambda_2(1 + a_2^{-1}\varepsilon)^{-1}.$$

In the same vein as Lemma 6.8, we can bound the line-search parameter.

LEMMA 6.9. *Suppose (6.16) holds. Then, the line-search parameter,  $\lambda$ , computed by using (6.5) satisfies*

$$\lambda_2 \in [(1 + a_1^{-1}\varepsilon)^{-1}, 1 + a_2^{-1}\varepsilon].$$

*Proof.* First, note that

$$\langle\mathbf{g}_2 + v_2 - \mathbf{H}_2z_{2,1}, e_2\rangle_{\mathcal{Z}} = \langle\mathbf{H}_1\mathbf{H}_1^{-1}(\mathbf{g}_2 + v_2 - \mathbf{H}_2z_{2,1}), e_2\rangle_{\mathcal{Z}} = \langle\mathbf{H}_1e_2, e_2\rangle_{\mathcal{Z}}.$$

Therefore,  $\lambda_2 = \frac{\langle\mathbf{H}_1e_2, e_2\rangle_{\mathcal{Z}}}{\langle\mathbf{H}_2e_2, e_2\rangle_{\mathcal{Z}}}$ . Substituting  $\mathbf{H}_1 = \mathbf{H}_2 + \delta\mathbf{H}$  gives

$$\lambda_2 = 1 + \frac{\langle\delta\mathbf{H}e_2, e_2\rangle_{\mathcal{Z}}}{\langle\mathbf{H}_2e_2, e_2\rangle_{\mathcal{Z}}} \leq 1 + a_K^{-1}\varepsilon.$$

On the other hand, substituting  $\mathbf{H}_1 = \mathbf{H}_2 - \delta\mathbf{H}$  gives

$$\lambda_2 = \left(1 + \frac{\langle\delta\mathbf{H}e_2, e_2\rangle_{\mathcal{Z}}}{\langle\mathbf{H}_1e_2, e_2\rangle_{\mathcal{Z}}}\right)^{-1} \geq (1 + a_1^{-1}\varepsilon)^{-1}.$$

This proves the desired result.  $\square$

Lemmas 6.8 and 6.9 imply the final upper bound on the spectral radius

$$\varrho(\mathbf{I} - \lambda\mathbf{H}_1^{-1}\mathbf{H}_2) \leq 1 - (1 + a_1^{-1}\varepsilon)^{-1}(1 + a_2^{-1}\varepsilon)^{-1} < 1.$$

This result shows that the spectral radius is approximately zero for small  $\varepsilon$ .

THEOREM 6.10. *Suppose (6.16) holds, and let  $K = 2$ . Then, one V-cycle of Algorithm 1 with pre- and post-smoothers performed by  $T_{1,2}$  and  $T_{2,2}$  iterations of CG, respectively, produces the iterate,  $z_2^+$ , satisfying*

$$\|z_2^* - z_2^+\|_{\mathbf{H}_2} \leq 4\sqrt{1 - (1 + a_1^{-1}\varepsilon)^{-1}(1 + a_2^{-1}\varepsilon)^{-1}} \left(\frac{\sqrt{A_2} - \sqrt{a_2}}{\sqrt{A_2} + \sqrt{a_2}}\right)^{T_{1,2}+T_{2,2}} \|z_2^* - z_2^-\|_{\mathbf{H}_2}.$$

*Proof.* This follows from Lemmas 6.7, 6.8, and 6.9.  $\square$

REMARK 6.11. *The assumptions in Lemma 6.8 are reasonable for sparse grid approximation. In the context of Assumption 3.2,  $\varepsilon \leq C(Q_1^{-\nu} + Q_2^{-\nu})$ . It is thus important to choose an initial multi-index set  $\mathcal{I}_1$  that results in a sparse grid  $N_1$  with more than one point (i.e.,  $|N_1| = Q_1 > 1$ ).*



Fig. 7.1: Depiction of the classic V-cycle and FMG cycle structures used in multigrid.

**7. Numerical Examples.** The numerical examples presented in this section demonstrate the dramatic reduction in the total number of PDE solves required by Algorithm 1 when compared with other optimization routines. These examples are presented and analyzed in detail in [28]. Furthermore, all examples are implemented in MATLAB.

For each example, we compare the number of PDE solves required when solving the fixed high-fidelity discretized optimization problem using Newton-conjugate gradients (Newton-CG) with the number of PDE solves required by Algorithm 1. Furthermore, we compare two instances of Algorithm 1, V-cycles and F-cycles (FMG). The FMG algorithm first solves the problem on the coarsest grid, then increases the grid level after each V-cycle. FMG gives an efficient method for obtaining a good initial guess for the V-cycle. Figure 7.1 demonstrates both a single V-cycle and the FMG cycle.

**7.1. Optimal Control of a 1D Elliptic PDE with Discontinuous Coefficients.** In this example, the governing PDE is a steady 1D diffusion equation with discontinuous diffusion parameter for which the location of discontinuity is uncertain [27, 28]. The motivation for this problem is the control of subsurface flow in fractured media.

**7.1.1. Infinite-Dimensional Formulation.** Let  $D = (-1, 1)$ , and let  $\rho(y)$  denote the uniform density on  $\Gamma = [-0.1, 0.1] \times [-0.5, 0.5]$ . Consider the governing PDE

$$-\partial_x (\epsilon(y, x) \partial_x u(y, x)) = f(y, x) + z(x) \quad (y, x) \in \Gamma \times D, \quad (7.1a)$$

$$u(y, -1) = u(y, 1) = 0 \quad y \in \Gamma, \quad (7.1b)$$

with random field coefficients

$$\epsilon(y, x) = \begin{cases} 0.1 & \text{if } x \leq y_1 \\ 10 & \text{if } x > y_1 \end{cases} \quad \text{and} \quad f(y, x) = \exp\left(- (x - y_2)^2\right).$$

The optimization problem is

$$\min_{z \in L^2(-1,1)} \hat{J}(z) = \frac{1}{2} \int_{\Gamma} \rho(y) \int_{-1}^1 (u(z; y, x) - 1)^2 dx dy + \frac{\alpha}{2} \int_{-1}^1 z(x)^2 dx, \quad (7.2)$$

where  $u(y, x) = u(z; y, x)$  solves (7.1) and the penalty parameter is  $\alpha = 10^{-4}$ . Relating (7.2) to (2.2),  $\mathcal{V} = H_0^1(D)$ ,  $\mathcal{W} = L^2(D)$ , and  $\mathcal{Z} = L^2(D)$ . Furthermore, the operators in (2.1) are defined as

$$\langle \mathbf{A}(y)u, v \rangle_{\mathcal{V}^*, \mathcal{V}} = 0.1 \int_{-1}^{y_1} u'(x)v'(x) dx + 10 \int_{y_1}^1 u'(x)v'(x) dx,$$

$\mathbf{N}(u, y) \equiv 0$ , and  $\mathbf{F}(z, y) = \mathbf{b}(y) - \mathbf{B}(y)z$ , where

$$\langle \mathbf{b}(y), v \rangle_{\mathcal{V}^*, \mathcal{V}} = \int_{-1}^1 f(y, x)v(x) \, dx \quad \text{and} \quad \langle \mathbf{B}(y)z, v \rangle_{\mathcal{V}^*, \mathcal{V}} = - \int_{-1}^1 z(x)v(x) \, dx.$$

Additionally,  $\mathbf{C}$  is the canonical injection from  $H_0^1(D)$  into  $L^2(D)$  and  $\bar{w} \equiv 1$ . The solution to (7.1) is continuous with respect to  $y \in \Gamma$  but need not be differentiable. To circumvent this complication, we use the domain decomposition formulation described in [28].

**7.1.2. Discretization.** We discretize the PDE (7.1) in  $D$  using piecewise linear finite elements. The finite-element mesh varies for each collocation point and is uniform on each subinterval  $[-1, y_1]$  and  $[y_1, 1]$ . The control variable is also discretized by using continuous piecewise linear finite elements on a uniform mesh of  $N = 128$  intervals. Furthermore, we construct the sparse-grid hierarchy using isotropic Smolyak sparse grids built on 1D Gauss-Patterson points with maximum level fixed to  $K = 8$ . The largest sparse grid has  $Q_8 = 1, 793$  points.

**7.1.3. Spectral Analysis of the Discretized Hessians.** Since  $\widehat{J}(z)$  is quadratic, the estimates derived in Section 6 apply when CG is used as smoothers in Algorithm 1. After discretization, the Hessian matrix at each sparse-grid level is bounded and positive-definite. The maximum and minimum eigenvalues of the Hessian matrices are relatively constant between levels. At each level, the maximum eigenvalue is approximately  $1.64 \times 10^{-2}$ , and the minimum is approximately  $3.85 \times 10^{-7}$ . Since the Hessians are positive definite, Theorem 6.1 and the work bounds derived in Section 6 apply. The V-cycle error bound in Theorem 6.1 depends on the generalized eigenvalues of the matrix pencils  $(\nabla^2 \widehat{J}_k(z), \nabla^2 \widehat{J}_{k-1}(z))$ . The maximum and minimum generalized eigenvalues for each level for this hierarchy of matrix pencils are approximately one, as proven in Section 6. Figure 7.2 depicts the absolute difference between one and the maximum (solid red) and minimum (solid black) generalized eigenvalues. As expected from the analysis in Section 6, the decay of the errors is approximately linear with respect to  $\log_{10} Q_k$ . The red dashed line was fit by using the maximum eigenvalues and decays at a rate of  $\nu = 1.63$ . The black dashed line was fit by using the minimum eigenvalues and decays at a rate of  $\nu = 2.08$ .

**7.1.4. Optimization Results.** We solve the high fidelity problem ( $K = 8$ ) using CG, which we terminate according to the relative residual stopping criterion

$$\|\nabla^2 \widehat{J}_K(z)s + \nabla \widehat{J}_K(z)\|_{\mathcal{Z}} \leq 10^{-6} \|\nabla \widehat{J}_K(z)\|_{\mathcal{Z}}. \quad (7.3)$$

The multilevel collocation algorithm uses CG as pre- and post-smoothers at each level. Algorithm 1 also uses CG to solve (4.1) on the coarsest grid ( $k = 1$ ) using the relative residual condition (7.3). The smoothers are computed as in Theorem 6.4 with  $T_{1,k} = K - k + 1 = T_{2,k}$  iterations of CG at each level. The smoother exits early if the relative residual condition (7.3) is satisfied. Disregarding early exit of the smoothers results in the theoretical upper bound on the number of PDE solves for one V-cycle

$$W_K \lesssim 28Q_K + 2(N_{\text{CG}}^1 + 1) = 50,280 \quad \text{PDE solves,}$$

where the total number of CG iterations on the coarse grid was  $N_{\text{CG}}^1 = 37$ .

The results for this example are tabulated in Table 7.1. Solving the high-fidelity optimization problem with CG resulted in 100,408 PDE solves. For Algorithm 1, one

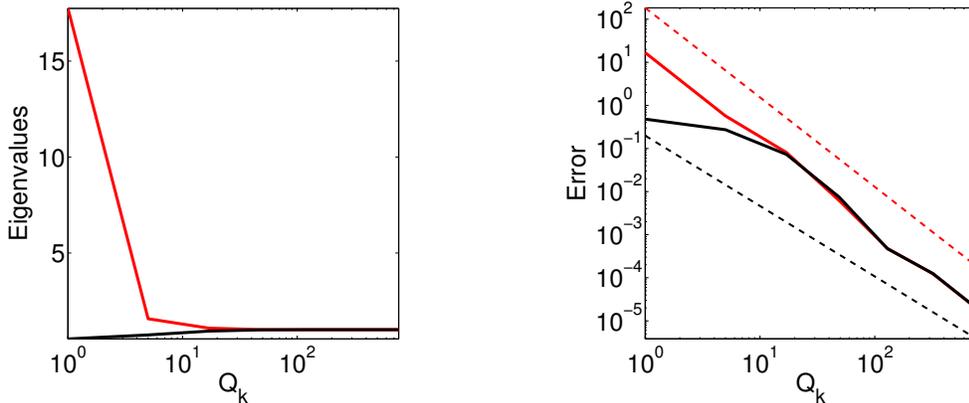


Fig. 7.2: Error between one and the minimum/maximum generalized eigenvalues of the matrix pencil  $(\nabla^2 \hat{J}_k(z), \nabla^2 \hat{J}_{k-1}(z))$ . The horizontal axis is the number of collocation points. The error for the minimum (black lines) and maximum (red lines) eigenvalues decays linearly with respect to  $\log_{10} Q_k$ . The decay rate is  $\nu = 1.63$  for the minimum eigenvalues and  $\nu = 2.08$  for the maximum eigenvalues.

	$\hat{J}_K(z)$	PDE Solves	Ratio	Theoretical	Ratio
CG	0.12638509	100,408	1.00	-	-
iCG	0.12638509	67,880	1.48	-	-
V-Cycle(1)	0.12638715	20,586	4.88	50,280	2.00
V-Cycle(2)	0.12638510	37,758	2.66	100,560	1.00
FMG	0.12638509	18,114	5.54	-	-

Table 7.1: Final objective value, number of PDE solves, ratio of PDE solves compared with CG, and theoretical upper bound on the number of PDE solves for each algorithm: CG for the high-fidelity problem (CG), inexact CG (iCG), one and two V-cycles (V-Cycle(i),  $i=1,2$ ), and one F-cycle of Algorithm 1 (FMG).

V-cycle required 36,760 PDE solves and reduced the norm of the gradient on the finest level  $K = 8$  to approximately  $10^{-5}$ . Two V-cycles required 64,940 PDE solves and satisfied the relative residual condition (7.3). FMG required 24,558 PDE solves and also satisfied the relative residual condition (7.3). All instances of Algorithm 1 resulted in a reduction in PDE solves when compared with CG on the fixed high-fidelity grid, but FMG was the clear winner with a savings of over 4 times fewer PDE solves.

**7.2. Optimal Control of Steady Burger's Equation.** We now consider the optimal control of the steady Burger's equation. Optimal control of the deterministic Burger's equation is analyzed in [46].

**7.2.1. Infinite-Dimensional Formulation.** Let  $D = (0, 1)$ , and let  $\rho(y)$  denote the uniform density on  $\Gamma = [-1, 1]^4$ . Consider the governing PDE

$$-\nu(y)\partial_{xx}u(y, x) + u(y, x)\partial_x u(y, x) = f(y, x) + z(x) \quad (y, x) \in \Gamma \times D, \quad (7.4a)$$

$$u(y, 0) = d_0(y), \quad u(y, 1) = d_1(y) \quad y \in \Gamma, \quad (7.4b)$$

where the random field coefficients are

$$\nu(y) = 10^{y_1-2}, \quad f(y, x) = \frac{y_2}{100}, \quad d_0(y) = 1 + \frac{y_3}{1000}, \quad \text{and} \quad d_1(y) = \frac{y_4}{1000}.$$

The optimization problem is

$$\min_{z \in L^2(-1, 1)} \widehat{\mathcal{J}}(z) = \frac{1}{2} \int_{\Gamma} \rho(y) \int_{-1}^1 (u(z; y, x) - 1)^2 dx dy + \frac{\alpha}{2} \int_{-1}^1 z(x)^2 dx, \quad (7.5)$$

where  $u(y, x) = u(z; y, x)$  solves (7.4) and the penalty parameter is  $\alpha = 10^{-3}$ . Relating (7.5) to (2.2), the function spaces are  $\mathcal{V} = H_0^1(D)$ ,  $\mathcal{W} = L^2(D)$ , and  $\mathcal{Z} = L^2(D)$ . For each  $y \in \Gamma$ , the control operator,  $\mathbf{F}(\cdot, y) : \mathcal{Z} \rightarrow \mathcal{V}^*$ , can be written as

$$\mathbf{F}(z, y) = -\mathbf{b}(y) - \mathbf{B}z.$$

The operators  $\mathbf{A} : \Gamma \rightarrow \mathcal{L}(\mathcal{V}, \mathcal{V}^*)$ ,  $\mathbf{B} : \Gamma \rightarrow \mathcal{L}(\mathcal{Z}, \mathcal{V}^*)$ ,  $\mathbf{N} : \mathcal{V} \rightarrow \mathcal{V}^*$  and  $\mathbf{b} : \Gamma \rightarrow \mathcal{V}^*$  are defined in [28]. Moreover, the observation operator  $\mathbf{C}$  is the canonical injection of  $H_0^1(D)$  into  $L^2(D)$  and  $\bar{w} \equiv 1$ .

**7.2.2. Discretization.** We discretize the state and control variables using continuous piecewise linear finite elements on a uniform partition of  $D = (0, 1)$ . To sufficiently resolve the possible stiff behavior of (7.4), we use a mesh of  $N = 512$  uniform intervals. To solve the resulting system of finite-dimensional nonlinear equations, we use Newton's method with a backtracking line search. Furthermore, we construct the sparse-grid hierarchy using isotropic Smolyak sparse grids built on 1D Clenshaw-Curtis points with maximum level fixed to  $K = 8$ . The largest sparse grid has  $Q_8 = 7,537$  points.

**7.2.3. Optimization Results.** We solve the high-fidelity optimization problem ( $K = 8$ ) and the coarse-grid problem (4.1) using Newton-CG. We terminate CG using the relative residual stopping condition,

$$\|\nabla^2 \mathcal{J}_k(z)s + \nabla \mathcal{J}_k(z)\|_{\mathcal{Z}} \leq \eta_k(z) \|\nabla \mathcal{J}_k(z)\|_{\mathcal{Z}}, \quad (7.6)$$

where the forcing function,  $\eta_k : \mathcal{Z} \rightarrow (0, 1)$ , is defined as

$$\eta_k(z) = \min\{10^{-2}, \|\nabla \widehat{\mathcal{J}}_k(z)\|_{\mathcal{Z}}\}. \quad (7.7)$$

This choice of  $\eta_k$  ensures q-quadratic convergence of Newton-CG whenever the initial guess  $z_0 \in \mathcal{Z}$  is sufficiently close to the optimal solution  $z_* \in \mathcal{Z}$  [38, Thm. 7.2]. To globalize Newton-CG, we employ a backtracking line search. Furthermore, we exit Newton-CG if the norm of the gradient of the objective function is less than the gradient tolerance  $\text{gtol}$ . For the high-fidelity problem  $\text{gtol} = 10^{-6}$  whereas for the coarse-grid problem  $\text{gtol} = 10^{-8}$ .

Similarly, we use a finite number of iterations of inexact Newton with inexact CG (Newton-iCG) for pre- and post-smoothing. We require inexact CG because we use Algorithm 2 for Hessian-times-vector computations. To apply the smoothers, we

	Nonlinear	Ratio	Linear	Ratio
Newton-CG	30,148	1.00	678,330	1.00
Newton-iCG	30,148	1.00	45,556	14.89
V-Cycle(1)	34,198	0.88	37,708	17.99
FMG	12,473	2.42	14,903	45.52

Table 7.2: Number of nonlinear and linear PDE solves required by the four different algorithms: Newton-CG with a backtracking line search, Newton with inexact CG and backtracking line search (Newton-iCG), one V-cycle of Algorithm 1 (V-Cycle(1)), and one F-cycle of Algorithm 1 (FMG). “Ratio” refers to the ratio of the number of solves for Newton-CG with the number of solves for the other algorithms.

perform  $T_{1,k} = T_{2,k} = 1$  outer iterations of Newton-iCG. That is, we apply inexact CG to approximately solve the Newton system (6.2) at each level,  $k$ . Inexact CG is terminated according to the relative residual condition (7.6) where, for fixed  $z \in \mathcal{Z}$ , the forcing function is set to

$$\eta_k(z) = \min\{2^{-(K-k+1)}, \|\nabla \mathcal{J}_k(z)\|_{\mathcal{Z}}^{1/2}\}$$

for each level  $k$ . This specific choice of  $\eta_k$  ensures q-superlinear convergence of Newton-CG [38, Thm. 7.2] and permits less work on the finer grids.

The primary computational work for general nonlinear PDE constrained optimization problems is PDE solves. To evaluate the objective function, we must solve  $Q_k$  deterministic instances of the state equation (7.4). To compute the gradient, we require  $Q_k$  nonlinear and  $Q_k$  linear PDE solves corresponding to the state and adjoint equations, respectively. To apply the Hessian to a vector, we require the solution to the state equation, the adjoint equation, and the state and adjoint sensitivity equations which, is a total of  $Q_k$  nonlinear PDE solves and  $3Q_k$  linear PDE solves. The total number of PDE solves can be reduced by storing state and adjoint variables, although recomputation may be essential depending on memory limitations. We store state and adjoint variables in our implementation.

As in the previous example, we compare the cost of the high-fidelity solution with Newton-iCG, one V-cycle of Algorithm 1, and one F-cycle of Algorithm 1 (FMG). For the high-fidelity problem, Newton-CG required 30,148 nonlinear and 678,330 linear PDE solves to meet the gradient tolerance. By using inexact CG to solve the Newton system, we reduce the number of linear PDE solves to 45,556 while maintaining the number of nonlinear solves. After one V-cycle, Algorithm 1 successfully met the gradient tolerance. Although this V-cycle required more nonlinear PDE solves, it reduced the number of linear PDE solves by a factor of 17.99 when compared with Newton-CG. On the other hand, FMG successfully met the gradient tolerance and only required 27,376 nonlinear and linear PDE solves, 14,903 of which were nonlinear PDE solves. FMG reduced the total number of nonlinear PDE solves by a factor of 2.42 and linear PDE solves by a factor of 45.52 when compared with Newton-CG. These results are tabulated in Table 7.2.

**8. Conclusions.** In this work, we present a hierarchical sparse-grid discretization for optimization problems governed by PDEs with uncertain coefficients, and we apply the MG/OPT framework [33, 30] to exploit this multilevel-in-sample-space discretization. The MG/OPT algorithm, Algorithm 1, is provably first-order con-

vergent under standard assumptions. The hierarchical sparse-grid discretized optimization problems can similarly be handled with other globally convergent variants of MG/OPT such as recursive trust-regions [21, 22, 23, 24] and the multilevel line-search approach [47].

In the case of quadratic optimal control of linear PDEs, we derived explicit upper bounds on the number of PDE solves required for a single V-cycle of Algorithm 1. We also proved error bounds for one V-cycle when CG is used as a pre- and post-smoother. We present numerical examples that confirm these upper bounds, and we demonstrate the immense reduction in the number of PDE solves required by Algorithm 1 when compared with Newton-CG applied to a fixed high-fidelity discretized problem.

The number of PDE solves can further be reduced by using the adaptive collocation approach in [27, 28] as a pre- and post-smoother. Alternatively, with slight modification, one can apply the MG/OPT algorithm to solve the trust-region sub-problems that arise in the adaptive collocation framework of [27, 28]. The framework in [27, 28] adaptively builds a hierarchy of sparse-grid index sets that can be used in the multilevel framework presented here. This coupling of the multilevel and adaptive approach is ideal as both methods perform a majority of their work on coarse sparse grids, resulting in significantly fewer PDE solves. In addition, the adaptive approach exploits any anisotropic features of the sample space to further reduce the number of collocation points. This coupling is left as future work.

## REFERENCES

- [1] I. BABUŠKA, F. NOBILE, AND R. TEMPONE, *A stochastic collocation method for elliptic partial differential equations with random input data*, SIAM Rev., 52 (2010), pp. 317–355.
- [2] I. BABUŠKA, R. TEMPONE, AND G. E. ZOURARIS, *Galerkin finite element approximations of stochastic elliptic partial differential equations*, SIAM J. Numer. Anal., 42 (2004), pp. 800–825 (electronic).
- [3] ———, *Solving elliptic boundary value problems with uncertain coefficients by the finite element method: the stochastic formulation*, Comput. Methods Appl. Mech. Engrg., 194 (2005), pp. 1251–1294.
- [4] V. BARTHELMANN, E. NOVAK, AND K. RITTER, *High dimensional polynomial interpolation on sparse grids*, Adv. Comput. Math., 12 (2000), pp. 273–288. Multivariate polynomial interpolation.
- [5] F. BASTIN, C. CIRILLO, AND PH. L. TOINT, *An adaptive Monte Carlo algorithm for computing mixed logit estimators*, Comput. Manag. Sci., 3 (2006), pp. 55–79.
- [6] A. BORZI, *Multilevel methods in optimization with partial differential equations*. Lecture notes, Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens-Universität Graz, Graz, Austria.
- [7] A. BORZI, *Multigrid methods for optimality systems*, tech. report, Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens Universität Graz, 2003. Habilitationsschrift.
- [8] ———, *Multigrid methods for parabolic distributed optimal control problems*, J. Comput. Appl. Math., 157 (2003), pp. 365–382.
- [9] A. BORZI, *On the convergence of the MG/OPT method*, Proc. Appl. Math. Mech., 5 (2005), pp. 735–736.
- [10] A. BORZI AND G. BORZI, *An efficient algebraic multigrid method for solving optimality systems*, Comput. Vis. Sci., 7 (2004), pp. 183–188.
- [11] A. BORZI, K. ITO, AND K. KUNISCH, *Optimal control formulation for determining optical flow*, SIAM J. Sci. Comput., 24 (2002), pp. 818–847 (electronic).
- [12] A. BORZI AND V. SCHULZ, *Multigrid methods for PDE optimization*, SIAM Review, 51 (2009), pp. 361–395.
- [13] ———, *Computational Optimization of Systems Governed by Partial Differential Equations*, Computational Science and Engineering, Vol. 8, SIAM, Philadelphia, 2012.
- [14] A. BORZI, V. SCHULZ, C. SCHILLINGS, AND G. VON WINCKEL, *On the treatment of distributed uncertainties in PDE constrained optimization*, GAMM Mitteilungen, 33 (2010), pp. 230–246.

- [15] A. BORZÌ AND G. VON WINCKEL, *Multigrid methods and sparse-grid collocation techniques for parabolic optimal control problems with random coefficients*, SIAM J. Sci. Comput., 31 (2009), pp. 2172–2192.
- [16] R. H. BYRD, G. M. CHIN, W. NEVEITT, AND J. NOCEDAL, *On the use of stochastic hessian information in optimization methods for machine learning*, SIAM Journal on Optimization, 21 (2011), pp. 977–995.
- [17] B. J. DEBUSSCHERE, H. N. NAJM, P. P. PÉBAY, O. M. KNIO, R. G. GHANEM, AND O. P. LE MAÎTRE, *Numerical challenges in the use of polynomial chaos representations for stochastic processes*, SIAM J. Sci. Comput., 26 (2004), pp. 698–719 (electronic).
- [18] X. DU, E. HABER, M. KARAMPATAKI, AND D. B. SZYLD, *Varying iteration accuracy using inexact conjugate gradients in control problems governed by pdes*, Tech. Report 08-06-27, Department of Mathematics, Temple University, 2008.
- [19] T. GERSTNER AND M. GRIEBEL, *Numerical integration using sparse grids*, Numer. Algorithms, 18 (1998), pp. 209–232.
- [20] ———, *Dimension-adaptive tensor-product quadrature*, Computing, 71 (2003), pp. 65–87.
- [21] S. GRATTON, A. SARTENAER, AND PH. L. TOINT, *On recursive multiscale trust-region algorithms for unconstrained minimization*, in Oberwolfach Reports: Optimization and Applications, C. Lemarechal F. Jarre and J. Zowe, eds., 2005.
- [22] ———, *Second-order convergence properties of trust-region methods using incomplete curvature information, with an application to multigrid optimization*, J. Comput. Math., 24 (2006), pp. 676–692.
- [23] ———, *Recursive trust-region methods for multiscale nonlinear optimization*, SIAM J. Optim., 19 (2008), pp. 414–444.
- [24] C. GROSS AND R. KRAUSE, *On the convergence of recursive trust-region methods for multiscale non-linear optimization and applications to non-linear mechanics*, SIAM J. Numer. Anal., 47 (2009), pp. 3004–3069.
- [25] W. HACKBUSCH, *Multigrid Methods and Applications*, Computational Mathematics, Vol. 4, Springer-Verlag, Berlin, 1985.
- [26] D. P. KOURI, *Optimization governed by stochastic partial differential equations*, master’s thesis, Department of Computational and Applied Mathematics, Rice University, Houston, TX, 2010. Available as CAAM TR10-20.
- [27] ———, *An Approach for the Adaptive Solution of Optimization Problems Governed by Partial Differential Equations with Uncertain Coefficients*, PhD thesis, Department of Computational and Applied Mathematics, Rice University, Houston, TX, May 2012. Available as CAAM TR12-10.
- [28] D. P. KOURI, M. HEINKENSCHLOSS, D. RIDZAL, AND B. G. VAN BLOEMEN WAANDERS, *A trust-region algorithm with adaptive stochastic collocation for pde optimization under uncertainty*, Tech. Report ANL/MCS-P3035-0912, Department of Mathematics and Computer Science, Argonne National Laboratory, 2012.
- [29] R. M. LEWIS AND S. G. NASH, *A multigrid approach for the optimization of systems governed by differential equations*, tech. report, American INstitute of Aeronautics and Astronautics, 2000.
- [30] ———, *Model problems for the multigrid optimization of systems governed by differential equations*, SIAM J. Sci. Comput., 26 (2005), pp. 1811–1837 (electronic).
- [31] J. S. LIU, *Monte Carlo strategies in scientific computing*, Springer Series in Statistics, Springer, New York, 2008.
- [32] M. MOTAMED, F. NOBILE, AND R. TEMPONE, *A stochastic collocation method for the second order wave equation with a discontinuous random speed*, Tech. Report MOX Report 36/2011, MOX Modeling and Scientific Computing, Politecnico di Milano, Italy, 2011.
- [33] S. G. NASH, *A multigrid approach to discretized optimization problems*, Optim. Methods Softw., 14 (2000), pp. 99–116. International Conference on Nonlinear Programming and Variational Inequalities (Hong Kong, 1998).
- [34] ———, *Convergence and descent properties for a class of multilevel optimization algorithms*, tech. report, Systems Engineering and Operators Research Department, George Mason University, 2010.
- [35] F. NOBILE AND R. TEMPONE, *Analysis and implementation issues for the numerical approximation of parabolic equations with random coefficients*, Int. J. Numer. Methods Engrg., 80 (2009), pp. 979–1006.
- [36] F. NOBILE, R. TEMPONE, AND C. G. WEBSTER, *An anisotropic sparse grid stochastic collocation method for partial differential equations with random input data*, SIAM J. Numer. Anal., 46 (2008), pp. 2411–2442.
- [37] ———, *A sparse grid stochastic collocation method for partial differential equations with ran-*

- dom input data*, SIAM Journal on Numerical Analysis, 46 (2008), pp. 2309–2345.
- [38] J. NOCEDAL AND S. J. WRIGHT, *Numerical Optimization*, second ed., Springer Verlag, Berlin, 2006.
  - [39] W.M. PATTERSON, *Iterative methods for the solution of a linear operator equation in Hilbert space - a survey*, Lecture Notes in Mathematics, Springer-Verlag, 1974.
  - [40] Y. SAAD, *Iterative Methods for Sparse Linear Systems*, PWS Publishing Company, Boston, 1996.
  - [41] V. SIMONCINI AND D. B. SZYLD, *Flexible inner-outer Krylov subspace methods*, SIAM J. Numer. Anal., 40 (2002), pp. 2219–2239 (electronic) (2003).
  - [42] S. A. SMOLJAK, *Quadrature and interpolation formulae on tensor products of certain function classes*, Soviet Math. Dokl., 4 (1963), pp. 240–243.
  - [43] U. TROTTEBERG, C. W. OOSTERLEE, AND A. SCHÜLLER, *Multigrid*, Academic Press, San Diego, CA, 2001. With contributions by A. Brandt, P. Oswald and K. Stüben.
  - [44] M. VALLEJOS AND A. BORZÌ, *Multigrid optimization methods for linear and bilinear elliptic optimal control problems*, Computing, 82 (2008), pp. 31–52.
  - [45] J. VAN DEN ESHOF AND G. L. G. SLEIJPEN, *Inexact Krylov subspace methods for linear systems*, SIAM J. Matrix Anal. Appl., 26 (2004), pp. 125–153 (electronic).
  - [46] S. VOLKWEIN, *Mesh-independence for an augmented Lagrangian–SQP method in Hilbert space*, SIAM J. Control and Optimization, 38 (2000), pp. 767–785.
  - [47] Z. WEN AND D. GOLDFARB, *A line search multigrid method for large-scale nonlinear optimization*, SIAM J. Optim., 20 (2009), pp. 1478–1503.
  - [48] D. XIU AND J. S. HESTHAVEN, *High-order collocation methods for differential equations with random inputs*, SIAM J. Sci. Comput., 27 (2005), pp. 1118–1139 (electronic).
  - [49] D. XIU AND G. E. KARNIADAKIS, *Modeling uncertainty in flow simulations via generalized polynomial chaos*, J. Comput. Phys., 187 (2003), pp. 137–167.

The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory (“Argonne”). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.