OPTIMAL INTERPOLATION AND COMPATIBLE RELAXATION IN CLASSICAL ALGEBRAIC MULTIGRID

JAMES BRANNICK, FEI CAO, KARSTEN KAHL, ROB FALGOUT AND XIAOZHE HU

ABSTRACT. In this paper, we consider a classical form of optimal algebraic multigrid (AMG) interpolation that directly minimizes the two-grid convergence rate and compare it with the so-called ideal form that minimizes a certain weak approximation property of the coarse space. We study compatible relaxation type estimates for the quality of the coarse grid and derive a new sharp measure using optimal interpolation that provides a guaranteed lower bound on the convergence rate of the resulting two-grid method for a given grid. In addition, we design a generalized bootstrap algebraic multigrid setup algorithm that computes a sparse approximation to the optimal interpolation matrix. We demonstrate numerically that the BAMG method with sparse interpolation matrix (and spanning multiple levels) outperforms the two-grid method with the standard ideal interpolation (a dense matrix) for various scalar diffusion problems with highly varying diffusion coefficient.

1. INTRODUCTION

We analyze algebraic multigrid (AMG) coarsening algorithms for linear systems of algebraic equations

\begin{equation}
Au = f,
\end{equation}

coming from cell-centered finite volume discretizations of the scalar elliptic diffusion problem

\begin{equation}
\begin{cases}
-\nabla \cdot (a(x)\nabla u) = f & \text{in } \Omega \\
u = 0 & \text{on } \partial \Omega
\end{cases}
\end{equation}

where \( \Omega = [0,1] \times [0,1] \). The discrete solution and right-hand side satisfy \( u, f \in \mathbb{R}^n \) and \( A \in \mathbb{R}^{n\times n} \) is a symmetric and positive definite matrix. We consider the case where the diffusion coefficient \( a(x) \) is highly oscillatory, which is a problem that motivated the design of the original classical AMG setup algorithm [5, 6].

Multigrid solvers for solving (1.2) involve a smoother, \( M \), with error propagator given by \( I - M^{-1}A \) and a coarse-level correction with error propagator given by \( I - \Pi_A = I - P A_c^{-1} P^T A \), where \( P \in \mathbb{R}^{n\times n_c} \) denotes the interpolation matrix and \( A_c = P^T A P \) is the Galerkin variational coarse-level matrix. The error propagation matrix of the resulting two-level method reads

\begin{equation}
E_{TG} = (I - M^{-1}A)(I - \Pi_A).
\end{equation}

In AMG, the smoother \( M \) is typically fixed and then interpolation \( P \) is constructed in an automated setup algorithm that takes as input the system matrix \( A \) and computes \( P \) and \( A_c \). The main task in the AMG setup algorithm is thus to construct a stable interpolation matrix \( P \) such that a certain approximation property holds and both \( P \) and \( A_c \) are sparse matrices. The latter sparsity requirement implies that the procedure can be applied recursively in order to construct an optimal multilevel solver.
Numerous setup algorithms have been developed for constructing matrix-dependent interpolation, going back to the original classical AMG algorithm \[5, 6\]. Generally speaking, the setup algorithm for constructing $P$ can be separated into three tasks:

1. Choosing the set of coarse variables, $C$, with cardinality $n_c = |C|$.
2. Determining the nonzero sparsity structure of $P$.
3. Computing the values of the nonzero entries in $P$.

Oftentimes, steps (1) and (2) of the setup algorithm are combined into a single step, as in smoothed aggregation AMG (SA) \[22\] where the choice of aggregates also determines the sparsity structure of the columns of $P$. The coefficients of the columns of $P$ are then chosen to approximate certain error components that the smoother cannot treat efficiently, assumed in most cases to be error that is dominated by the eigenvectors of the system matrix with small eigenvalues. In other approaches, e.g., classical AMG, steps (1)-(3) are implemented in different stages within the setup algorithm \[5\]. Specifically, the notion of strength of coupling between neighboring unknowns is used in a maximal independent set algorithm to choose the coarse variable set $C$. Next, the strongly and weakly coupled neighbors of each of the fine degrees of freedom are determined and, finally, the coefficients of the corresponding row of interpolation are computed in a way that ensures that certain components of the error (e.g., the constant vector) are well approximated locally. We note that in both approaches, once the coarse degrees of freedom $C$ and the entries of the interpolation matrix $P$ are selected they are fixed and the setup algorithm proceeds to construct the next coarser level. In this way, the algorithm is applied recursively without any measure of the quality of the resulting coarse space in approximating the error in the current solution for the fine-level equations.

Compatible relaxation (CR) \[1, 7, 16\] and adaptive \[12, 13\] and bootstrap AMG \[2, 4, 8, 9, 10\] were introduced as techniques to modify and adjust the coarse variable set and interpolation, respectively. The basic idea in these approaches is to develop local measures to assess the suitability of the computed coarse space for a given problem. Although these approaches have been successfully developed and extended to handle numerous applications, certain theoretical issues remain unresolved. For example, although the convergence rates of the CR algorithms that are typically used in practice give a qualitative measure of the suitability of the coarse set, they do not accurately predict the convergence rate of the resulting two-grid solver for ideal interpolation in general (see \[3, 7\]), which is the aim of the approach. Moreover, the so-called ideal interpolation matrix used as the basis of CR does not in general give the fastest possible convergence rate of the two-level method over all possible choices of $P$ and, hence, it may not provide a reliable measure of the quality of the coarse variable set for certain problems.

In this paper, we study these issues further with the aim of gaining a deeper understanding of AMG from theoretical and practical points of view. In Section \[2\], we derive the optimal classical AMG interpolation matrix and then contrast it with the so-called ideal form that minimizes a certain weak approximation property of the coarse space. Section \[3\] introduces measures of the quality of the coarse grid based on the notions of compatible relaxation \[11, 17\] and ideal interpolation as well as this new optimal form of classical AMG interpolation. We show that the reliability and robustness of CR depends critically on the choice of the coarse variable type and that when the simplified (and computable) $F$-relaxation form of CR is used, the resulting estimates of the two-grid solver with ideal interpolation and full smoothing are not sharp in general. Then, we derive an iteration for accurately approximating the convergence of the two-grid method with ideal $P$ and show that it can be efficiently computed
in practice. We note, however, that even this more accurate CR-type estimate is not reliable in general since for certain scalar diffusion test problems that we consider the optimal P results in significantly faster convergence. To address this limitation, we derive a sharp variant of CR based on the optimal classical AMG interpolation matrix. On the other hand, we derive an equivalence between the optimal form of classical AMG interpolation and the so-called ideal interpolation matrix in the case that F-smoothing is used in the resulting two-grid solver. In addition, we derive a generalization of the ideal interpolation operator and show that for proper choices of the coarse variables this generalized ideal interpolation is equivalent to the optimal form. Section 4 contains numerical results that illustrate these findings for scalar diffusion test problems. In addition, this section contains the derivation of a generalized bootstrap AMG (BAMG) setup algorithm that aims to approximate the optimal interpolation matrix with a sparse approximation. The main new feature of the algorithm is that it computes approximations to eigenvectors with small eigenvalues of the generalized eigenvalue problem for \( (A, \tilde{M}) \), where \( A \) denotes the system matrix and \( \tilde{M} \) the symmetrized smoother. Numerically, we show that the BAMG method (spanning multiple levels) with sparse \( P \) outperforms the two-grid method with the ideal \( P \) (which is a dense matrix) for our test problems.

2. TWO-LEVEL THEORY AND OPTIMAL CLASSICAL AMG INTERPOLATION

In [15], the following identity for convergence rate of the two-level method is introduced

\[
\|E_{TG}(P)\|_A^2 = 1 - \frac{1}{\text{sup}_v \kappa(P, v)}, \quad \kappa(P, v) = \frac{\|I - \Pi_{\tilde{M}}(P))v\|_{\tilde{M}}^2}{\|v\|_A^2},
\]

where \( \Pi_{\tilde{M}}(P) \) is the \( (\cdot, \cdot)_{\tilde{M}} \) orthogonal projection on \( \text{range}(P) \), with \( \tilde{M}^{-1} = M^{-1} + M^{-T} - M^{-T}AM^{-1} \) denoting the symmetrized smoother, so that \( \tilde{M} = M(M + M^T - A)^{-1}M^T \). Note that, assuming \( M + M^T - A \) is symmetric and positive definite (SPD) is equivalent to assuming the convergence of the chosen smoother defined by \( M \).

Using (2.1) it is straightforward to derive the optimal two-grid convergence rate \( \|E_{TG}(P)\|_A^2 \) with respect to \( P \), for a given smoother \( M \). We note that this result is found in [15] (see Corollary 4.1) and more recently in the review paper [25]. From this general form of optimal \( P \) we then derive the classical AMG form of optimal \( P \) via a post-scaling, which is the result of primary interest in this paper. In particular, we focus on studying this optimal classical AMG interpolation and comparing it in a practical setting with the so-called ideal classical AMG interpolation matrix.

**Lemma 1.** Let \( P : \mathbb{R}^{n_c} \rightarrow \mathbb{R}^n \) be full rank and let \( \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \) and \( v_1, v_2, \ldots, v_n \) denote the eigenvalues and orthonormal (w.r.t \((\cdot, \cdot)_{\tilde{M}}\) for convenience of representation) eigenvectors of the generalized eigenvalue problem

\[
Ax = \lambda Mx.
\]

Then the minimal convergence rate of the two-grid method is given by

\[
\|E_{TG}(P)\|_A^2 = 1 - \kappa_2, \quad \kappa_2 := \inf_{\dim(\text{range}(P)) = n_c} \frac{1}{\text{sup}_v \kappa(P, v)} = \lambda_{n_c+1},
\]

where the optimal interpolation operator \( P_2 \) satisfies

\[
\text{range}(P_2) = \text{range}(\{v_1 \ v_2 \ \cdots \ v_{n_c}\}).
\]
For sake of definiteness we set \( P_\sharp = (v_1 \ v_2 \ \cdots \ v_n) \) throughout the paper.

Proof. Starting with the equality in (2.1) first observe that if we denote \( P = \text{range}(P) \) and its \( \tilde{M} \)-orthogonal complement by \( S \) we find that for any \( P \)

\[
\frac{1}{\sup_v \kappa(P,v)} = \inf_v \frac{\|v\|_A^2}{\|(I - \pi_{\tilde{M}}(P))v\|_M^2} \leq \inf_{v \in S} \frac{\|v\|_A^2}{\|v\|_M^2}.
\]

Thus, we obtain for any \( P \) that

\[
\|E_{TG}(P)\|_A^2 \geq 1 - \inf_{v \in S} \frac{\|v\|_A^2}{\|v\|_M^2}.
\]

Finally due to \( \dim(S) + \dim(P) = n \) we get

\[
\inf_{\dim(P) = n_c} \|E_{TG}(P)\|_A^2 \geq 1 - \sup_{\dim(S) = n-n_c} \inf_{v \in S \setminus \{0\}} \frac{\|v\|_A^2}{\|v\|_M^2}.
\]

Based on Courant-Fischer Min-max representation, we obtain:

\[
\inf_{\dim(P) = n_c} \|E_{TG}(P)\|_A^2 \geq 1 - \lambda_{n_c+1}.
\]

The equality in this bound is obtained by setting \( S = S_\sharp = \text{range}(v_{n_c+1} \ v_{n_c+2} \ \cdots \ v_n) \).

Now, since \( P \) is the \( \tilde{M} \)-orthogonal complement of \( S \), it follows that \( P = P_\sharp \) and

\[
\|E_{TG}(P_\sharp)\|_A^2 = 1 - \lambda_{n_c+1}.
\]

Finally, the optimal convergence rate for the two-grid method is obtained by choosing any interpolation that has the same range as \( P_\sharp \), namely, by setting

\[
P = P_\sharp Z, \quad \text{where we assume } Z^{-1} \text{ exists}.
\]

In this way, one obtains the same convergence rate since by direct computation

\[
E_{TG}(P_\sharp Z) = (I - M^{-1}A)(I - P_\sharp Z((P_\sharp Z)^T A P_\sharp Z)^{-1}(P_\sharp Z)^T A)
\]

\[
= (I - M^{-1}A)(I - P_\sharp ((P_\sharp)^T A P_\sharp)^{-1}(P_\sharp)^T A) =: E_{TG}(P_\sharp).
\]

□

We note that the above identity for the projection on \( P_\sharp \) holds for \( \Pi_X(P_\sharp) \) as well, where \( X \) is assumed to be any SPD matrix. This is summarized in the following corollary.

**Corollary 1.** Any projection \( \Pi_X(P) = P(P^T X P)^{-1} P^T X \) is invariant with respect to post-multiplication of interpolation \( P \) by an invertible matrix \( Z, \ P \leftarrow PZ \). Here \( X \) is assumed to be any SPD matrix.

Proof. The proof is identical to the derivation for \( E_{TG}(P_\sharp Z) \), where the system matrix \( A \) is replaced by \( X \) and the smoother is omitted. □

In order to derive the standard classical AMG form of the optimal interpolation \( P_\sharp \), we use the fact that the spectral radius of \( E_{TG} \) remains unchanged if we replace \( P_\sharp \) by \( P_\sharp Z \) for any nonsingular (invertible) matrix \( Z \).
Remark 1. The classical AMG form of interpolation, assuming a splitting of the fine-level degrees of freedom into $C$ and $F$, is given by

\[(2.5)\]
\[P = \begin{bmatrix} W \\ I \end{bmatrix} \{ F \} \setminus \{ C \},\]

where $C \subset \{1, \ldots, n\}$ and $F = \{1, \ldots, n\} \setminus C$, and $W \in \mathbb{R}^{||F|| \times ||C||}$ defines the interpolation weights. Thus, if we reorder the optimal interpolation matrix so that it has the form

\[(2.6)\]
\[P_\sharp = \begin{bmatrix} P_f & P_c \end{bmatrix},\]

and such that $P_c$ is non-singular, then it follows that the interpolation matrix

\[(2.7)\]
\[\bar{P}_\sharp = P_\sharp P_c^{-1} = \begin{bmatrix} \bar{W} \\ I \end{bmatrix}, \quad \bar{W} = P_f P_c^{-1}\]

also minimizes $\sup_{v \neq 0} \kappa(v)$.

The optimal $P$ given in Lemma [ ] and the resulting classical AMG form, $P_\sharp$, are in general not of direct use in practice since they require the computation of $n_c$ eigenvectors of the generalized eigenproblem, given by (2.2), and they yield a dense interpolation matrix. In the remainder of this section, we make various connections between the optimal classical AMG interpolation matrix and existing two-grid theory used in deriving classical AMG forms of interpolation.

2.1. An approximation property and ideal interpolation. AMG approaches for constructing interpolation $P$ are based on an approximation property of the coarse space, which is formulated as

\[(2.8)\]
\[\mu_X(PR) := \sup_v \frac{\|(I - PR)v\|_X^2}{\|v\|_A^2} \leq \eta \forall v \in \mathbb{R}^n,\]

where $R : \mathbb{R}^n \to \mathbb{R}^{n_c}$ defines the coarse variable type, i.e., $u_c = Ru$, and must be chosen such that $RP = I$ and the matrix $X \in \mathbb{R}^{n_c \times n}$ is symmetric positive definite.

Remark 2. Note that the left side in (2.8) will precisely determine the convergence rate if $X = \tilde{M}$ and $R = (PT\tilde{M}P)^{-1}PT\tilde{M}$. If $X$ is not equal to $\tilde{M}$, but instead bounded from above such that

\[(2.9)\]
\[(\tilde{M}v, v) = \|v\|_\star^2 \leq \sigma(Xv, v),\]

then

\[\|(I - \Pi_{\tilde{M}}v\|_M^2 \leq \|(I - PR)v\|_M^2 \leq \sigma\|(I - PR)v\|_X^2.\]

As a consequence, the two-level method is a uniform contraction in $\| \cdot \|_A$-norm if $\eta$ is uniformly bounded for some $X$ such that (2.9) holds. A typical choice for $X$, which motivates the classical AMG approach, is $X = D$ (the diagonal of $A$).

As noted above, in the classical AMG setting that is the focus of this paper, interpolation has the form given in (2.5). The choice of restriction $R$ used in defining the coarse variable type in this setting is not unique in that it only needs to satisfy $RP = I$. For example, an
the optimal one. Next, we derive a result relating this form of ideal interpolation to
minimizer in this lemma gives a generalization of the so-called ideal interpolation matrix
optimal forms of interpolation are one in the same, given proper choices of
more general choice of \( Z \) arises in classical AMG. Moreover, if we consider the condition
we consider the definition of \( P \) that was used in [16] for the construction of
Moreover, if we consider the condition
\( \bar{R}_Z \) defined in Lemma 3 below. The derivation of the result uses the
following generalization of a lemma from [16] that gives the optimal choice for \( P \) given some
\( R \) such that \( RP = I \) and any SPD matrix \( X \). The choice here is more general in the use of
\( Z_\ast \) which is any full rank matrix of dimension \( n_c \), where for the specific choice \( Z_\ast = R^T \) we
arrive at the formulation given in [16].

**Lemma 2.** Let \( R \) be given and satisfy \( RP = I \). Define \( S : \mathbb{R}^{n_f} \to \mathbb{R}^n \), where \( n_f = n - n_c \) such that \( RS = 0 \). Then, ideal interpolation is the solution to the min-max problem
\( \mu_X^\ast = \min_{P} \mu_X(PR) \) and is given by

\[
P_\ast := (I - \Pi_A(S))Z_\ast = (I - S(S^TAS)^{-1}S^T A)Z_\ast
\]

where \( P_\ast \) satisfies (by definition) \( P_\ast^T AS = 0 \) and \( Z_\ast : \mathbb{R}^{n_c} \to \mathbb{R}^n \) is full rank. Further, the
the corresponding minimum has the closed form

\[
\mu_X^\ast = \frac{1}{\lambda_{\min}((S^T XS)^{-1}(S^T AS))}.
\]

In order to minimize the measure \( \mu_X \) with respect to \( P \), the only requirement that ideal
interpolation \( P_\ast \) needs to satisfy, apart from the usual requirements that \( RP_\ast = I \) and
\( RS = 0 \), is the condition that \( P_\ast^T AS = 0 \) (see Equation (3.9) in [16]). This condition in
turn is satisfied for the choice above involving the \( A \)-orthogonal projection on range(\( S \)).
Moreover, if we consider the condition \( RP_\ast = I \), we find that

\[
RP_\ast = R(I - \Pi_A(S))Z_\ast = RZ_\ast,
\]

(since \( RS = 0 \)) and, thus, assuming that \( RP_\ast = I \) is equivalent to the assumption that
\( RZ_\ast = I \).

Now, if we choose \( Z_\ast = R^T \), then it must hold that \( RR^T = I \), which is the result that
was used in [16] for the construction of \( P_\ast \) with \( Z_\ast = R^T \). However, in our construction
we consider the definition of \( P_\ast \) for \( Z_\ast \) which allows for more general choices of \( R \), as well as
the relation between \( P_\ast \) and \( P_\ast \) that we derive next, which does not hold when we assume
\( Z_\ast = R^T \).

The next lemma, Lemma 3, concerns the choice of \( Z_\ast = R^T \) and shows that our format
is indeed more general in terms of the choice of \( Z_\ast \). Specifically, we show that with this
more general choice of \( Z_\ast \) (one that is not directly related to the choice of \( R \)) the ideal and
optimal forms of interpolation are one in the same, given proper choices of \( R \), \( S \) and \( Z_\ast \). The
minimizer in this lemma gives a generalization of the so-called ideal interpolation matrix
arising in classical AMG. Next, we derive a result relating this form of ideal interpolation to
the optimal one.
Remark 3. For the upper ideal $P_\star$ we can also see it can also has following format:

\begin{equation}
(2.14) \quad P_\star = \begin{bmatrix} S & Z_\star \end{bmatrix} \begin{bmatrix} -(S^T A S)^{-1} (S^T A Z_\star) \end{bmatrix}.
\end{equation}

which clearly show that when your choice of $\begin{bmatrix} S & Z_\star \end{bmatrix} = I$, then the ideal $P_\star$ will have classical AMG format (2.5). In [16] there is a specific case when choosing $Z_\star = R^T$.

Lemma 3. For the optimal classical AMG form of interpolation $P = \tilde{P}_t$ and for $X = \tilde{M}$ one obtains, in light of Lemmas 2 and 3, that

\begin{equation}
(2.15) \quad \tilde{R}_t = (\tilde{P}_t^T P_c P_c^T)^T \tilde{M}, \quad S^t_\star = (v_{n+1} \cdots v_n)
\end{equation}

and

\begin{equation}
(2.16) \quad \mu^\star_{\tilde{M}} := \frac{1}{\lambda_{\min}((S^T_\star \tilde{M} S^T_\star)^{-1} (S^T_\star A S^T_\star))} = \frac{1}{\lambda_{n+1}}.
\end{equation}

For these choices of $R = \tilde{R}_t$, $S = S^t_\star$ and $P = \tilde{P}_t$, we have that $\tilde{R}_t \tilde{P}_t = I$, $\tilde{R}_t S^t_\star = 0$ and $\tilde{P}_t \tilde{R}_t = \Pi_{\tilde{M}}(P_t) = \Pi_A(P_t)$, so that the assumptions of Lemma 2 hold. Moreover, the resulting ideal $P$ obtained from minimizing the measure in (2.8) has the same form as the optimal one, namely

\begin{equation}
(2.17) \quad P_\star = (I - S^t_\star (S^T_\star A S^T_\star)^{-1} S^T_\star A) Z_\star = \Pi_{\tilde{M}}(\tilde{P}_t) Z_\star = \tilde{P}_t (\tilde{R}_t Z_\star) = \tilde{P}_t,
\end{equation}

where $P_\star$ is defined in Lemma 2 and from (2.13) we require $\tilde{R}_t Z_\star = I$. We postpone further discussion on the choice of $Z_\star$ to the remark below that follows the proof of this lemma.

Proof. The result in (2.17) is established by noting that $(v_i, v_j�_{\tilde{M}} = \delta_{ij}$ and, thus, $S^T_\star \tilde{M} S^T_\star = I$ and

\[ S^T_\star A S^T_\star = \text{diag}(\lambda_1, \ldots, \lambda_n) = \Lambda_{S^T_\star}, \]

implying

\[ S^T_\star \tilde{M} = (\tilde{M} S^T_\star)^T = (AS^T_\star \Lambda_{S^T_\star}^{-1})^T = (S^T_\star A S^T_\star)^{-1} S^T_\star A. \]

Hence,

\[ \Pi_{\tilde{M}}(S^t_\star) = S^T_\star (S^T_\star \tilde{M} S^T_\star)^{-1} S^T_\star \tilde{M} = S^T_\star S^T_\star \tilde{M} = S^T_\star (S^T_\star A S^T_\star)^{-1} S^T_\star A = \Pi_A(S^T_\star). \]

Likewise, one can show that $P_t \tilde{R}_t = \Pi_{\tilde{M}}(P_t) = \Pi_A(P_t)$. Now, since $I - \Pi_{\tilde{M}}(S^t_\star) = \Pi_{\tilde{M}}(P_t)$, which follows by definition, we have

\[ P_\star = (I - S^t_\star (S^T_\star A S^T_\star)^{-1} S^T_\star A) Z_\star = \Pi_{\tilde{M}}(\tilde{P}_t) Z_\star = \tilde{P}_t (\tilde{R}_t Z_\star) = \tilde{P}_t, \]

where $\tilde{R}_t Z_\star = I$ is by equivalence (2.13). Thus, if one chooses the optimal forms $R = \tilde{R}_t$, $S = S^t_\star$ and $X = \tilde{M}$, then the measure in (2.8) also has as its minimizer the optimal form of interpolation $P_\star$ given in Lemma 1.

\[ \Box \]

Remark 4. For the standard case where $Z_\star = \tilde{R}_t^T$, it follows that $\tilde{R}_t \tilde{R}_t^T \neq I$ and so $\tilde{R}_t P_\star \neq I$ and the results from the previous lemma do not hold. Indeed, based on definition of $\tilde{R}_t$ we have

\[ \tilde{R}_t P_\star := \tilde{R}_t (I - \Pi_A(S)) \tilde{R}_t^T = \tilde{R}_t \tilde{R}_t^T = (\tilde{P}_t^T P_c P_c^T)^T \tilde{M} \tilde{M} (\tilde{P}_t^T P_c P_c^T) = P_c P_c^T \tilde{M}^2 P_c P_c^T \neq I. \]

Hence, from this example we see that the $P_\star$ construction in [16] is not general enough for the derivation in the previous lemma since it does not apply to this optimal choice of $R = \tilde{R}_t$. 


The next result characterizes the standard so-called ideal interpolation matrix arising in the classical AMG literature.

**Remark 5.** Given the classical AMG form of matrix-dependent interpolation in (2.5) and the splitting \( C \subset \{1, \ldots, n\} \) and \( F = \{1, \ldots, n\} \setminus C \), consider reordering the matrix such that

\[
A = \begin{bmatrix}
A_{ff} & A_{fc} \\
A_{cf} & A_{cc}
\end{bmatrix}
\]

Then, practical choices of \( R \) and \( S \) are as follows

\[
R = \begin{bmatrix} 0 & I \end{bmatrix} \quad \text{and} \quad S = \begin{bmatrix} I & 0 \end{bmatrix},
\]

where for these choices \( RS = 0 \) and \( RP = I \). In this setting, we have that ideal interpolation is given by

\[
P_* = \begin{bmatrix} W_* & I \end{bmatrix}, \quad W_* = -A_{ff}^{-1}A_{fc}.
\]

Hence, for these simpler choices of \( R \) and \( S \), the optimal and ideal \( P \) are in general different and, as we show in the numerics section, this difference can lead to substantial changes in convergence rates of the resulting two-grid method in certain cases. We note though that this form of the ideal \( P \) is also optimal in terms of energetic stability in the following sense.

**Remark 6.** In [16] the following is derived: Assuming that the coarse variables have been constructed so that \( \mu_*^{\tilde{M}} \) is bounded for all \( \mathbf{v} \neq 0 \), then using a \( P \) that satisfies the following stability property also implies convergence of the resulting two-level method

\[
\langle APR\mathbf{v}, PR\mathbf{v}\rangle \leq \beta \langle A\mathbf{v}, \mathbf{v}\rangle \quad \forall \mathbf{v},
\]

where \( \beta \geq 1 \) is a constant. This more general result is interesting because it allows for various approaches of defining interpolation. Moreover, it separates the tasks of selecting the coarse variables and defining interpolation. We note that (2.21) has been used extensively in the literature [20, 23, 11] to derive various techniques for constructing an energetically stable \( P \). It is also easy to see that if we choose the optimal forms of \( R \) and \( S \) given in Lemma 3, then with the optimal form of classical AMG interpolation \( \bar{P}_z \) given in (2.7) it follows that \( \bar{P}_z \bar{R}_z = \Pi_{\bar{M}}(\bar{P}_z) = \Pi_A(\bar{P}_z) \) (see the proof in the lemma) so that \( \beta = \beta_2 = 1 \) in (2.21), which is of course the minimal value since \( \Pi_A(\bar{P}_z) := \bar{P}_z(\bar{P}_z^T A \bar{P}_z)^{-1}\bar{P}_z^T A \) is the \( A \)-orthogonal projection on range(\( \bar{P}_z \)).

### 3. Compatible Relaxation and Optimal Interpolation

In this section, we introduce the notion of compatible relaxation (CR) and show how the process can be used to obtain a bound on the convergence rate of the two-grid method with ideal interpolation, namely we present a bound on \( \mu_*^{\bar{M}} \) that uses the convergence rate of CR. The resulting bound in turn gives a measure of the quality of the coarse variable set, since it shows that, for the given set \( C \) there exists an interpolation matrix (the ideal one) such that the two-grid method convergence is acceptable. We then consider CR in terms of \( \bar{R}_z \) and \( S_z \) defined in Lemma 3 and contrast this approach to the more practical choices that have been considered in our previous studies of this topic.
Compatible relaxation, as defined by Brandt [1], is a modified relaxation scheme that keeps the coarse-level variables invariant. Generally, the compatible relaxation iteration is defined as

\[ v_{k+1} = (I - S M_S^{-1} S^T A) v_k, \]

where \( M_S = S^T M S \) and, as in Lemma 2, we assume that \( R \) and \( S \) are chosen such that \( RS = 0 \). Note that from this assumption it follows that \( R v_{k+1} = R v_k \) and thus we can consider compatible relaxation in the \( L_2 \) complementary space, leading to an iteration of the form

\[ v_{k+1} = (I - M_S^{-1} A_S) v_k, \]

where \( A_S = S^T A S \). Now, the convergence rate of this iteration is related to the measure \( \mu^*_M \) in (2.12) as follows

\[ \mu^*_M \leq \frac{\Delta^2}{1 - \rho_S}. \]

Here, \( \Delta \geq 1 \) measures the deviation of \( M \) from its symmetric part (see [16]) and

\[ \rho_S = \| (I - M_S^{-1} A_S) \|_{A_S}. \]

Note that, although we use \( \rho \) to represent the spectral radius of a matrix, the quantity \( \rho_S \) is in general only an upper bound for the spectral radius of compatible relaxation; it is equal to the spectral radius when \( M \) is symmetric. For this reason, we work with the symmetrized Gauss Seidel smoother \( \tilde{M} \) in all cases, which gives \( \Delta = 1 \) in the above bound.

If iteration (3.2) is fast to converge, then \( \mu^*_M \) is bounded, that is, fast convergence of CR implies a coarse variable set of good quality and the existence of a \( P \) such that the resulting two-level method is uniformly convergent. One can then estimate the value of \( \rho_S \) in (3.4) in practice by running the compatible relaxation iteration in (3.2) and monitoring its convergence.

**Remark 7.** In the classical AMG setting, given a choice of the coarse and fine variable sets, \( C \) and \( F \), and assuming that \( R \) and \( S \) are defined as in (2.19) we have that the iteration in (3.2) reduces to simple \( F \)-relaxation

\[ v_{k+1} = (I - M_f^{-1} A_f) v_k, \]

which is straightforward to compute. We note that though this variant of CR is user-friendly, it has been observed in practice that its spectral radius does not provide an accurate prediction of the convergence rate of the two-level method with ideal interpolation in some cases [11]. Thus, the bound in (3.3) may not be sharp for such problems.

**Remark 8.** When \( P = P_\star \) (the ideal interpolation operator) and \( R \) and \( S \) are defined as in (2.19), then it is easy to show that

\[ I - \Pi_A(P_\star) = I - P_\star (P_\star^T A P_\star)^{-1} P_\star^T A = S (S^T A S)^{-1} S^T A = \begin{pmatrix} I & -W \\ 0 & 0 \end{pmatrix}, \]

where \( W = W_\star \) is given in (2.20). This result implies that the spectral radius of the two-grid method with ideal interpolation, \( \rho(E_{TG}(P_\star)) \) with \( E_{TG}(P_\star) := (I - M^{-1} A)(I - \Pi_A(P_\star)) \), can be accurately estimated in practice if an estimate of \( A_f^{-1} \) is available. Moreover, the fast convergence of the \( F \)-relaxation form of CR in (3.5) implies that \( A_f \) is well conditioned and
(as we show later in the numerical experiments) that $A^{-1}$ can be efficiently estimated using a polynomial approximation [11]. In particular, if we consider compatible relaxation defined by (3.2) and assume that $\rho_s \leq \delta < 1$, then we have that

$$\kappa(A^{-1}) \leq \kappa(M^{-1}_f) \frac{1 + \delta}{1 - \delta},$$

where $\kappa(A)$ is the condition number of the matrix $A$. In the numerical tests, we use the diagonally scaled preconditioned Conjugate Gradient iteration to compute an approximation to $A^{-1}$.

The approximation obtained by CR can be made optimal if we use the optimal forms of $R_s$, $S$, and $P$, as defined in Lemma 3.

**Remark 9.** If, instead, we use the optimal choices of $R$ and $S$, namely, $R_\sharp$ and $S_\sharp$, and we assume that the smoother is symmetric Gauss Seidel, then instead of arriving at the $F$-relaxation form of CR given in (3.5) we have that

$$\tilde{M}_S = S_\sharp^T \tilde{M} S_\sharp = I \quad \text{and} \quad A_S = S_\sharp^T A S_\sharp = \Lambda_{S_\sharp} := \text{diag}(\lambda_{n_c+1}, \ldots, \lambda_n),$$

where $\lambda_i$ are the generalized eigenvalues of the eigenproblem involving $(A, \tilde{M})$. Thus, the spectral radius of the CR error propagation matrix is given by

$$\rho_{S_\sharp}(I - \tilde{M}_S^{-1} A_S) = 1 - \min_i (\Lambda_{S_\sharp})_{ii} = 1 - \lambda_{n_c+1}.$$

Here, unlike the simplified version of CR given above, the convergence rate of this form of CR does not depend on the actual coarse points that are chosen, but only on the cardinality of the coarse variable set $n_c = |C|$. However, if we recall the optimal form of classical AMG interpolation given in (2.7):

$$\bar{P}_\sharp = P_\sharp P_c^{-1} = \begin{bmatrix} W \\ I \end{bmatrix}, \quad \bar{W} = P_f P_c^{-1},$$

then we observe that $P_c$, used in constructing the classical AMG form of optimal interpolation does depend on the choice of coarse grid points. Hence, in this setting we can use CR to determine the number of coarse points that are required in order to achieve a certain convergence rate of the resulting two-grid method and then we choose the set $C$ so that $P_c$ is well conditioned. This assumption in turn implies $P_c^{-1}$ is computable in the approximation to $\bar{P}_\sharp$ and as we show numerically this also tends to produce a local (decaying) optimal interpolation matrix.

### 3.1. An equivalence between ideal and optimal interpolation for $F$-relaxation.

If we consider the reduction-based AMG framework and assume the forms of $R$ and $S$ given in (2.19), then we can establish an equivalence between the minimizers of $\mu^*_{\tilde{M}}$ in (2.12) and $\kappa_\sharp$ in (2.3) with respect to $P$. However, as we show in the numerical results section, in the case of full smoothing (i.e., using $M$ not $M_f$ in the solve phase) $\mu^*_{\tilde{M}}$ does not generally provide a useful estimate of $\kappa_\sharp$.

The reduction-based AMG method (or algebraic hierarchical basis scheme) is based on the following block factorization of $A$ in terms of $R$ and $S$:

$$A = \begin{bmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{bmatrix} F C = \begin{bmatrix} I & 0 \\ A_{cf} A_{ff}^{-1} & I \end{bmatrix} \begin{bmatrix} A_{ff} & 0 \\ 0 & A_{cc} - A_{cf} A_{ff}^{-1} A_{fc} \end{bmatrix} \begin{bmatrix} I & A_{ff}^{-1} A_{fc} \\ 0 & I \end{bmatrix},$$
implying
\begin{equation}
A^{-1} = \begin{bmatrix}
I & -A_{ff}^{-1}A_{fc}
\end{bmatrix}
\begin{bmatrix}
A_{ff}^{-1} & 0
\end{bmatrix}
\begin{bmatrix}
I & 0
\end{bmatrix}
\begin{bmatrix}
I & 0
0 & S_A^{-1}
\end{bmatrix}
\begin{bmatrix}
-A_{cf}A_{ff}^{-1} & 0
\end{bmatrix}
\begin{bmatrix}
I
I
\end{bmatrix},
\end{equation}
where \(S_A = A_c - A_{cf}A_{ff}^{-1}A_{fc}\). Equivalently, one can solve the system using the two-level method with ideal interpolation \(P_*\), which gives \(A_c = P_*^TAP_* = S_A\) and again results in an exact solve, assuming exact \(F\)-relaxation, i.e., \(M_{ff} = A_{ff}\) in
\begin{equation}
E_{TG} = (I - SM_{ff}^{-1}S^TA)(I - \Pi_A(P_*))(I - SM_{ff}^{-1}S^TA) = I - B^{-1}_{TG}A,
\end{equation}
where \(M_{ff} = S^TMS\) and \(\Pi_A(P_*)\) is an \(A\)-orthogonal projection on \(\text{range}(P_*)\) as defined in (2.20).

Now, consider the block factorized smoother
\begin{equation}
M_{HB} = \begin{bmatrix}
M_{ff} & 0
\end{bmatrix}
\begin{bmatrix}
I & M_{ff}^{-1}A_{fc}
\end{bmatrix}
\begin{bmatrix}
\tau I
0
I
\end{bmatrix},
\end{equation}
where for sufficiently large \(\tau\) we have that \(M_{HB}^T + M_{HB} - A\) is symmetric and positive definite. We note that
\begin{equation}
M_{HB}^{-1} = \begin{bmatrix}
M_{ff} & A_{fc}
\end{bmatrix}
\begin{bmatrix}
\tau I + A_{cf}M_{ff}^{-1}A_{fc}
\end{bmatrix}^{-1}
\begin{bmatrix}
M_{ff}^{-1} + \tau^{-1}M_{ff}^{-1}A_{fc}A_{cf}M_{ff}^{-1} - \tau^{-1}M_{ff}^{-1}A_{fc}
-\tau^{-1}A_{cf}M_{ff}^{-1} \tau^{-1}I
\end{bmatrix}
\rightarrow \begin{bmatrix}
M_{ff}^{-1}
0
0
\end{bmatrix},
\end{equation}
where in the last step we take \(\tau \rightarrow \infty\). Thus, as \(\tau\) approaches infinity the factorized smoother converges to simple \(F\)-relaxation involving \(M_{ff}^{-1}\).

Next, we set \(M_{ff} = A_{ff}\) and note that in this case the symmetrized smoother is given by:
\begin{equation}
\tilde{M}_{HB} = \begin{bmatrix}
A_{ff} & A_{fc}
\end{bmatrix}
\begin{bmatrix}
\tau I - 1
\end{bmatrix}
\begin{bmatrix}
\tau^2X^{-1} + A_{cf}A_{ff}^{-1}A_{fc}
\end{bmatrix},
\end{equation}
where \(X^{-1} = 2\tau I - S_A\). Now, considering the generalized eigen-problem involving \(A\) and \(\tilde{M}_{HB}\), it follows that
\begin{equation}
\tilde{M}_{HB}A = \begin{bmatrix}
A_{ff} & A_{fc}
\end{bmatrix}
\begin{bmatrix}
\tau I - 1
\end{bmatrix}
\begin{bmatrix}
\tau^2X^{-1} + A_{cf}A_{ff}^{-1}A_{fc}
\end{bmatrix}
\begin{bmatrix}
A_{ff}
A_{cf}
\end{bmatrix}
= \begin{bmatrix}
I & *
0 & *
\end{bmatrix},
\end{equation}
so that \(\lambda_{n_{c+1}} = \ldots = \lambda_n = 1\) for any choice of hierarchical splitting. Thus, if we consider using the optimal interpolation operator \(\tilde{P}_z\) given in (2.7), then the above result shows that the resulting two-level method with exact \(F\)-relaxation (where \(M_{ff} = A_{ff}\) in \(\tilde{M}_{HB}\)) gives an exact solve for any value of \(\tau\), since in this case
\[||E_{TG}||_A^2 = 1 - \lambda_{n_{c+1}} = 1 - 1 = 0\]
for any value of \(n_c\).

Also (3.17) also implies \(S_z = \begin{bmatrix}
I
0
\end{bmatrix}\) as in (2.19). Then
\begin{equation}
(I - \tilde{M}_{HB}^{-1}A)^TAS_z = (\tilde{M}_{HB} - A)\tilde{M}_{HB}^{-1}AS_z = \begin{bmatrix}
0 & 0
0 & *
\end{bmatrix}
\begin{bmatrix}
I & *
0 & *
\end{bmatrix}
\begin{bmatrix}
I
0
\end{bmatrix}
= 0.
\end{equation}
Thus \(\text{range}(I - \tilde{M}_{HB}^{-1}A) = \text{range}(P_z)\), since \(P_z\) and \(S_z\) are \(A\)-orthogonal. Then \(||E_{TG}||_A = 0\).

Moreover, since when \(\tau \rightarrow \infty\), it follows that \(M_{HB}\) converges to \(F\)-relaxation and assuming that \(M_{ff} = A_{ff}\), it follows that
\[\lim_{\tau \rightarrow \infty}(\tilde{P}_z)_{\tau} \rightarrow P_*,\]
that is the optimal interpolation operator converges to the ideal one. Here, we emphasize the dependence of \( \tilde{P}_\tau \) on \( \tau \), since the eigenvectors of the generalized eigen-problem involving \( \tilde{M}_{HB} \) depend on \( \tau \) and, thus, so do the columns of \( \tilde{P}_\tau \). However, when \( M_{ff} \neq A_{ff} \), but instead \( M_{ff} \approx A_{ff} \), then \( \lim_{\tau \to \infty} \tilde{P}_\tau \neq \tilde{P}_\cdot \). Similarly, as we show in the numerical results in the next section, in the case of full smoothing the two-level method that uses optimal interpolation will generally converge faster than the two-level method with ideal interpolation.

For the limiting case of \( \tau \to \infty \), we have

\[
\lim_{\tau \to \infty} M_{HB}^{-1} = \begin{bmatrix} M_{ff}^{-1} & 0 \\ 0 & 0 \end{bmatrix},
\]

We note that for this limiting case, the matrix becomes singular and so a pseudo inverse is needed. Now, if \( M_{ff}^{-1} = A_{ff}^{-1} \), then

\[
\lim_{\tau \to \infty} \tilde{M}_{HB} A = \begin{bmatrix} I & A_{ff}^{-1}A_{fc} \\ 0 & 0 \end{bmatrix},
\]

So in analogy to the case \( \tau < \infty \), the optimal \( P \) is composed of \( n_c \) eigenvectors of the above matrix on the right-hand side, namely, the eigenvectors corresponding to zero eigenvalues of

\[
\begin{bmatrix} I & A_{ff}^{-1}A_{fc} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} v_f \\ v_c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},
\]

and so

\[
v_f = -A_{ff}^{-1}A_{fc}v_c.
\]

Thus, the eigenvectors have the form

\[
v = \begin{bmatrix} -A_{ff}^{-1}A_{fc} \\ I \end{bmatrix} v_c = P_\star v_c.
\]

Hence, the range of the ideal and the optimal interpolation matrices are the same if F-relaxation is used for smoothing.

4. Numerical Experiments

Numerically, we consider four different test problems coming from discretizations of (1.2), corresponding to different distributions of the diffusion coefficient \( a(x) \). The first two Problems P1 and P3 are ones where the interfaces of the jumps do not intersect, namely,

\[
a(x) = \begin{cases} 1 & x \in \Omega_1, \\ 10^{-k_{ij}} & x \in \Omega \setminus \Omega_1, \end{cases}
\]

where the domain \( \Omega_1 \) corresponds to the one given by the white regions in the plot on the left in Figure 4.1. For problem P1, \( k_{ij} = k \in \mathbb{Z}^+ \) for all \( i, j \), and for problem P3 \( k_{ij} \in \{1, 2, \ldots, k\} \), where the values are selected randomly with uniform distribution (using built-in Matlab function \texttt{randi})

In the next two tests, Problems P2 and P4, we consider a checkerboard pattern for the distribution of the jumps, where now \( \Omega_1 \) corresponds to the white regions in the plot on the right in Figure 4.1. For problem P2, the distribution in \( \Omega \setminus \Omega_1 \) is again uniform with \( k_{ij} = k \in \mathbb{Z}^+ \) for all \( i, j \) and for problem P4 we select the value \( k_{ij} \) randomly as in problem P3.

We use a standard cell-centered finite volume method (see [14, 21]) for discretizing P1-P4 and choose a structured grid \( 0 = x_0 < x_1 < \cdots < x_{N+1}, \ x_i = \frac{i}{N+1}, \ 0 = y_0 < y_1 < \)
\[ \cdots < y_{N+1}, y_j = \frac{j}{N+1}. \]

Note that \( h = h_x = h_y = \frac{1}{N+1} \). Here, each cell \([x_{i-1}, y_{j-1}] \times [x_i, y_j]\) is used as the control volume and the unknowns are located at each cell center \((x_{i-\frac12}, y_{j-\frac12}) = (x_{i-1} + \frac{h}{2}, y_{j-1} + \frac{h}{2})\). To define \( a(x) \) on the interfaces of neighboring subdomains we use a harmonic average, e.g., for an interface \( S \) we have \( a^- \neq a^+ \) in general, where \( a^- = a(x) \) in the volume on one side of the interface \( S \) and \( a^+ = a(x) \) in the volume on the other side of \( S \). We then write the discretized system as

\[
\frac{a_r u_{i+1,j} + a_w u_{i-1,j} + a_n u_{i,j+1} + a_s u_{i,j-1} - (a_r + a_w + a_n + a_s) u_{i,j}}{V} = f_{i,j},
\]

where \( f_{i,j} = \int_V f dV \) and \( V \) is the control volume \([x_{i-1}, y_{j-1}] \times [x_i, y_j]\) and \( a_* \) are harmonic averages of \( a(x) \) on the two neighboring cells as in [19]. We assume Dirichlet boundary conditions and if an edge \( S \) is on the boundary of \( \Omega \), we set \( u_{i+\frac12,j} = 0 \).

4.1. Compatible relaxation: measuring the quality of \( C \). We begin with tests that compare the standard \( F \)-relaxation form of CR in (3.5), the estimate of \( E_{TG}(P) \) obtained by using the identity in (3.6) to apply the coarse-grid correction with ideal interpolation \((P = P_\star \text{ in (2.20))}, \) and the spectral radius of \( E_{TG}(P_\star) \), that is, the two-grid method with optimal interpolation, for Problems P1-P4. In all tests, we use forward Gauss-Seidel for pre-smoothing and backward Gauss-Seidel for post-smoothing in defining \( E_{TG} \) in (3.13) and we consider standard full-coarsening \((h \rightarrow 2h, \text{ see Figure 4.6})\) to define the coarse variable set \( C \subset \{1, ..., n\} \) for different choices of the problem size \( n = N \times N \). The results of these tests for various values of the jump discontinuity defined by parameter \( k \) are given in Table 1.1. The table at the top contains approximations of the spectral radius of \( E_{TG}(P_\star) \) together with the ideal interpolation matrix, i.e., when \( W_\star = -A_{ij}^{-1}A_k \). The second table contains estimates of the two-grid convergence rate obtained by running 5 steps of the iteration (3.6) starting with a random initial guess, where the action of \( A_{ij}^{-1} \) in (3.6) is approximated by \( L = 2 \) diagonally preconditioned Conjugate Gradient iterations. Here, we combine the iteration (3.6) with Gauss-Seidel pre- and post-smoothing, which then mimics the two-grid method with ideal \( P = P_\star \). The third table contains results of the \( F \)-relaxation form of CR for symmetric Gauss Seidel, again assuming full coarsening as the choice of \( C \). And the bottom table contains results of the two-grid method with optimal interpolation, \( P_\star \).

Overall, we see that CR convergence rates are acceptable for all problems and choices of the problem parameters except for Problem P4. Moreover, from the results obtained in the middle table it is clear that one can obtain an accurate estimate of \( E_{TG}(P) \) using (3.6) with a small number of inner PCG iterations to approximate \( A_{ij}^{-1} \), again in all cases except for...
Problem P4. This poor performance observed for Problem P4 is of course expected since in this case the convergence of $F$-relaxation with full coarsening is $\rho > .9$ and so $A_f$ may not be well conditioned in the sense of the bound given in (3.7). In general, these results suggest that full coarsening may not be a good choice for Problem P4. However, as we show in the next set of experiments, with optimal interpolation full coarsening does give acceptable results. The rapid convergence observed in these tests, especially for Problem P4, can be explained using the results provided in Figure 4.5 which contains plots of the spectra of $A$ and $(A, \tilde{M})$. Here, we see that the eigenvalues of $(A, \tilde{M})$ vary substantially from the eigenvalues of $A$, e.g. in the right plot for Problem P4, less than $\frac{n}{4}$ of the generalized eigenvalues are different from 1. Thus, for our choice of full coarsening with $n = \frac{n}{4}$, we obtain very fast convergence.

We note that if we instead consider red-black coarsening for problem P4, then $F$-relaxation becomes an exact solve, i.e., the spectral radius of the CR iteration, $\rho_s = 0$. In addition, when using the same red-black coarsening and iteration (3.6), again with 2 inner PCG iterations, we obtain an estimate of the spectral radius of $\rho$ using the same red-black coarsening and iteration (3.6), again with 2 inner PCG iterations, we obtain very fast convergence.

Finally, in Section 3, we showed that in general the two-level method with optimal interpolation will converge faster than the method with ideal interpolation. Here, we observe these results numerically for Problems P1-P4 in the bottom set of results. Overall, we observe that the reported convergence results are consistent with the theoretical result that $\rho(E_{TG}(P_\star)) \leq \rho(E_{TG}(P_c))$ and for Problems P2 and P4 a significant improvement is observed. We note that for the Poisson problem (i.e., $k = 0$), the two-grid method with optimal $P$ and full coarsening has its spectral radius bounded by .14 independent of the problem size $n$.

4.2. Compatible relaxation with optimal interpolation. As discussed in Section 3, the convergence rate of the $F$-relaxation form of compatible relaxation can be used to measure the quality of the coarse variable set in that it bounds the min -- max solution $\mu_{\tilde{M}}^*$ in (2.8). Recall that this construction assumes the so-called ideal interpolation operator in (2.11), which as we showed above does not give the best choice of the classical AMG form of interpolation due to the forms of $R$ and $S$ given in (2.19) that are assumed in this setting.

Our aim in this section is to study the use of CR together with the optimal forms of $R$ and $S$ given in Lemma 3, namely, $\tilde{R}_\star = (\tilde{P}_\star P_c P^T_\star)^T \tilde{M}$ and $S_\star = (v_{n+1} \cdots v_n)$, which leads to the optimal interpolation matrix as the minimizer of $\mu_{\tilde{M}}^*$. Here, $P_c$ defines the matrix used in deriving the classical AMG form of $P_z$ given in (2.7): $P_z = P_z P_c^{-1} = \left[ \begin{array}{c} P_f P_c^{-1} \\ I \end{array} \right]$, $P_z = \left[ \begin{array}{c} P_f \\ P_c \end{array} \right] \left[ \begin{array}{c} v_1 \\ \cdots \\ v_{n_c} \end{array} \right]$, with the set $C$ chosen such that $P_c$ is non-singular. The arrow notation is used to denote that $P_z$ with columns consisting of the smallest $n_c$ eigenvectors of the generalized eigenproblem for $(A, \tilde{M})$ is reordered according to the $C - F$ splitting of the unknowns. Note that from Lemma 2, we have that the classical AMG form of optimal interpolation $P_z$ not only


Table 4.1. Spectral radius of two-grid methods with ideal interpolation (top), using CG to approximate $A_{ff}^{-1}$ (top-middle), results for compatible relaxation (bottom-middle) and with optimal interpolation (bottom), applied to Problems P1-P4 (with symmetric GS as smoother).

| Size | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ | $P_1$ | $P_2$ | $P_3$ | $P_4$ |
|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 16   | 0.242 | 0.176 | 0.512 | 0.693 | 0.075 | 0.052 | 0.493 | 0.839 | 0.007 | 0.005 | 0.499 | 0.937 | 7e-5  | 5e-5  | 500   | 999   |
| 32   | 0.243 | 0.177 | 0.524 | 0.786 | 0.075 | 0.052 | 0.520 | 0.939 | 0.007 | 0.005 | 0.516 | 0.995 | 7e-5  | 5e-5  | 512   | 1.00  |
| 64   | 0.244 | 0.177 | 0.530 | 0.777 | 0.075 | 0.052 | 0.527 | 0.927 | 0.007 | 0.005 | 0.522 | 0.989 | 7e-5  | 5e-5  | 515   | 1.00  |
| 128  | 0.244 | 0.178 | 0.533 | 0.790 | 0.075 | 0.052 | 0.526 | 0.951 | 0.007 | 0.005 | 0.523 | 0.998 | 7e-5  | 5e-5  | 517   | 1.00  |

Table 4.1. Spectral radius of two-grid methods with ideal interpolation (top), using CG to approximate $A_{ff}^{-1}$ (top-middle), results for compatible relaxation (bottom-middle) and with optimal interpolation (bottom), applied to Problems P1-P4 (with symmetric GS as smoother).

yields the optimal two-grid convergence rate, i.e., it gives $\kappa_\sharp$ in (2.3), it also minimizes the approximation property $\mu_{\tilde{M}}$ with respect to $P$. Given the above choice of $S = S_\sharp$ we have that the spectral radius of CR is given by (see (3.9))

\begin{equation}
\rho_\sharp(I - \tilde{M}_{S_\sharp}^{-1}A_{S_\sharp}) = 1 - \lambda_{n_c+1}.
\end{equation}

Here, $\tilde{M}$ denotes the symmetric Gauss-Seidel smoother. Note that, the CR rate gives the same result as the convergence rate of the two-grid method with optimal interpolation, namely, the same rate obtained with $\kappa_\sharp$. However, unlike the simplified $F$-relaxation version of CR given in (3.5), the convergence rate of this form of CR does not depend on the actual coarse points that are chosen, instead it only depends on the cardinality of the coarse variable set $n_c = |C|$. The choice of the coarse variable set now defines the matrix $P_\sharp$ that is used in constructing the classical AMG form of optimal interpolation. Hence, in this setting we can use CR to determine the number of coarse points that are required in order to achieve a
certain convergence rate of the resulting two-grid method and then we choose the set $C$ so that $P_c$ is well conditioned.

The problem of finding a well-conditioned submatrix $P_c$ can be viewed as finding a subset of $n_c$ columns of $P^T \#$ that form a well conditioned basis of $\mathbb{R}^{n_c}$ or in looser terms a set of $n_c$ columns that are as linearly independent as possible. Besides the condition number of the basis, i.e., a measure for its orthogonality, another natural formalization of this question is the volume of the parallelepiped spanned by the bases. In the case that all columns of $P^T \#$ have comparable norm, a maximal volume (determinant) basis has a small condition number and vice versa. Unfortunately, finding the maximal volume submatrix is an NP-hard problem (cf. [26]), but there exists a greedy algorithm (cf. Algorithm 1) that is able to find a sub-matrix $P_c$ with locally maximal determinant (see [18] for details).

Even though there is no guarantee that the submatrix found in this way has a small condition number, we find in practice that the large eigenvalues tend to stay within the same order. In contrast, the nearly zero eigenvalues of $P_c$ move away from the origin significantly when the algorithm is applied to some random initial choice of coarse grid.

Figures 4.2 - 4.4 contain results of the algorithm applied to our scalar diffusion problem in (1.2) for different choices of the diffusion tensor $a(x)$, namely, the distribution for our test problems P1-P4 with $k = 4$. For all tests we use a discretization of the problem with $35 \times 35$ finite volumes. Each figure contains plots of the choice of coarse variable set $C$, denoted by the black circles as well as the volume and condition numbers of the depicted choice of $C$. We depict the initial (random) choice of the $C$ set and the set determined by the maxvol algorithm. Further, we show a plot of the convergence rate versus the cardinality of $n_c = |C|$, and plots of three (randomly chosen) columns of the resulting optimal classical AMG form of interpolation that we obtain for the given coarse grid and then computing $\bar{P}$ by multiplying $P_\#$ by $P_c^{-1}$. We observe that, in all tests, the set of coarse variables properly aligns with the choice of $a(x)$ and the given smoother. For example, in Figure 4.3 we naturally obtain standard full coarsening. For the results in Figure 4.4 for Problem P4 using a red-black ordered block smoother we see that the coarse points largely lie on the boundaries of the subdomains, as expected.

In addition, the plots of the convergence rates are given on the top right and allow one to choose $n_c = |C|$ with a guaranteed lower bound on the convergence rate of the resulting two-grid method, namely the one obtained with $\bar{P}$. Finally, we note that the columns of the resulting optimal classical AMG form of interpolation are highly localized for all test problems.

**Algorithm 1: maxvol coarse variable selection**

- **Input:** $P_\#$ and $n_c$,
- **Output:** $C$, $F$

Choose initial set $C$ such that $|C| = n_c$, set $X := (P_\#)_C$.

Calculate $\bar{P}_\# := \pi P_\# X^{-1} = \begin{pmatrix} I \\ W \end{pmatrix}$ // reordered according to $C$-$F$

while $\max_{i,j} |(\bar{P}_\#)_{i,j}| > 1$

$(i',j') = \text{argmax}\{|(\bar{P}_\#)_{i,j}|\}$ // $i > n_c$, i.e., $i \notin C$

Set $C = (C \setminus \{j'\}) \cup \{i'\}$ // swap rows $j'$ and $i'$

Update $\bar{P}_\#$ //rank one updates

**4.3. Bootstrap AMG and the generalized eigenproblem.** In this section, we consider designing a bootstrap AMG setup algorithm that aims at solving the generalized eigenproblem in (2.2) to compute test vectors used in constructing least squares interpolation.
We note that in the original BAMG setup algorithm developed in [4] the eigen-problem involving only $A$ was used to compute approximate eigenvectors that are provided as input to the least squares process that constructs the interpolation matrix. As we will point out there are only a few changes that are needed in order to adapt the least squares interpolation and bootstrap multilevel setup to the generalized eigenvalue problem.

Plots of the eigenvalues of $A$ and $(A, \tilde{M})$ for various tests with $N = 16$ are provided in Figure 4.5. These results show that for Problem P4 the spectrum of $A$ and $(A, \tilde{M})$ differ substantially, especially with respect to the number of near-null eigenvectors. This observation together with the fact that the optimal interpolation matrix has as columns eigenvectors of the generalized eigen-problem involving $A$ and $\tilde{M}$ suggest that AMG interpolation should be based on approximating these generalized eigenvectors. To test this idea we compare the BAMG setup that uses eigen-approximations of $A$ to the one that uses eigen-approximations of $\tilde{M}^{-1}A$.

4.3.1. Bootstrap AMG setup. For definiteness, we provide an outline of the version of the bootstrap AMG setup that was designed and analyzed in [4] and that we use in our tests.
We point out the modifications that are necessary to adjust the components of the method to the generalized eigenvalue problem.

The least squares interpolation matrix used in BAMG is defined to fit collectively a set of test vectors (TVs) that should characterize the eigenvectors with small eigenvectors of the system matrix (or the generalized eigenproblem). Assuming the sets of interpolatory variables, $C_i$, for each $i \in F$, and a set of test vectors, $\mathcal{V} = \{v^{(1)}, \ldots, v^{(k)}\}$, have been determined, the $i$th row of $P$, denoted by $p_i$, is defined as the minimizer of the local least squares problem:

\begin{equation}
\mathcal{L}(p_i) = \sum_{\kappa=1}^{k} \omega_k \left( v_{i}^{(\kappa)} - \sum_{j \in C_i} (p_i)_j v_{j}^{(\kappa)} \right)^2 \rightarrow \min.
\end{equation}

Here, the notation $v_{\tilde{\Omega}}$ denotes the canonical restriction of the vector $\tilde{v}$ to the set $\tilde{\Omega} \subset \Omega$, e.g., $v_{(i)}$ is simply the $i$th entry of $v$. Conditions on the uniqueness of the solution to minimization problem (4.4) and an explicit form of the minimizer have been derived in [4]. In contrast to
\[ |\det(P_c)| = 4.888 \cdot 10^{-255} \]
\[ \kappa(P_c) = 1.787128 \cdot 10^{13} \]

\[ |\det(P_c)| = 8.594 \cdot 10^{-47} \]
\[ \kappa(P_c) = 20.529 \]

**Figure 4.4.** Red-black block Gauss-Seidel for \( P^4 \), \( 5 \times 5 \) blocks (\( k = 4, 35 \times 35, n_c = 144 \)). (top left) initial random choice of \( C \); (top center) \( C \) determined by \texttt{maxvol}; (top right) CR convergence rate \( \rho_{S^2} = 1 - \lambda_{n_c+1} \) w.r.t. ratio \( \frac{n_c}{n} \); (bottom row) three columns of \( P^2 \) with \( C \) from \texttt{maxvol}.

**Figure 4.5.** Lower \( \frac{3}{4} \) of the spectra of \( (A, \widetilde{M}) \) (solid line) and \( A \) (dashed line), which is scaled by \( \lambda_{\text{max}}(A) \). (left) Lex. Gauss-Seidel for \( P^1 \) (\( k = 4, 35 \times 35 \)); (center) Lex. Gauss-Seidel for \( P^2 \) (\( k = 4, 35 \times 35 \)); (right) Red-black block Gauss-Seidel with \( 5 \times 5 \) blocks for \( P^4 \) (\( k = 4, 35 \times 35 \)).
the original least squares interpolation we choose the weights $\omega_\kappa > 0$ by

$$
\omega_\kappa = \frac{\|v^{(\kappa)}\|_X}{\|v^{(\kappa)}\|_A}.
$$

In the original formulation $X = I$ corresponds to the inverse Rayleigh-Quotient of $v^{(\kappa)}$. Choosing $X = \widetilde{M}$ the weight is the inverse generalized Rayleigh-Quotient w.r.t. the pencil $(A, \widetilde{M})$.

The test vectors used in the least squares process are computed using a bootstrap multilevel setup cycle. The algorithm begins with relaxation applied to the homogenous system,

$$
(4.5) \quad A_l x_l = 0,
$$
on each grid, $l = 0, \ldots, L - 1$; assuming that a priori knowledge of the algebraically smooth error is not available, these vectors are initialized randomly on the finest grid, whereas on all coarser grids they are defined by restricting the existing test vectors computed on the previous finer grid.

Once an initial MG hierarchy has been computed, the current sets of TVs are further enhanced on all grids using the existing multigrid structure. Specifically, the given hierarchy is used to formulate a multigrid eigensolver which is then applied to an appropriately chosen generalized eigenproblem to compute additional test vectors. This overall process is then repeated with the current AMG method applied in addition to (or replacing) relaxation as the solver for the homogenous systems in (4.5). Figure 4.7 provides an schematic outline of the bootstrap $V$- and $W$-cycle setup algorithms. In general, $V^m$ and $W^m$ denote setup algorithms that use $m$ iterations of the $V$- and $W$-cycles, respectively.

The rationale behind the multilevel generalized eigensolver (MGE) is as follows. Assume an initial multigrid hierarchy has been constructed. Given the initial Galerkin operators $A_0, A_1, \ldots, A_L$ on each level and the corresponding interpolation operators $P^l_{l+1}, l = 0, \ldots, L - 1$, define the composite interpolation operators as $P^l_l = P^l_{l+1} \cdots P^{l-1}_0$, $l = 1, \ldots, L$. Then, for any given vector $x_l \in \mathbb{R}^{n_l}$ we have $\langle x_l, x_l \rangle_{A_l} = \langle P_l x_l, P_l x_l \rangle_A$. Furthermore, defining $X_l = P^T_l X P_l$ for any $X$ symmetric and positive definite we obtain

$$
\frac{\langle x_l, x_l \rangle_{A_l}}{\langle x_l, x_l \rangle_{X_l}} = \frac{\langle P_l x_l, P_l x_l \rangle_A}{\langle P_l x_l, P_l x_l \rangle_X}.
$$
This observation in turn implies that on any level \( l \), given a vector \( x^{(l)} \in \mathbb{R}^{n_l} \) and \( \lambda^{(l)} \in \mathbb{R} \) such that \( A_l x^{(l)} = \lambda^{(l)} X_l x^{(l)} \), its Rayleigh quotient (RQ) fulfills

\[
\text{rq}(P_l x^{(l)}) := \frac{\langle P_l x^{(l)}, P_l x^{(l)} \rangle_A}{\langle P_l x^{(l)}, P_l x^{(l)} \rangle_X} = \lambda^{(l)}. \tag{4.6}
\]

This provides a relation among the eigenvectors and eigenvalues of the operators in the multigrid hierarchy on all levels with the eigenvectors and eigenvalues of the finest-grid matrix pencil \((A, X)\). Again one obtains the original formulation of the bootstrap setup cycle by choosing \( X = I \) and by choosing \( X = \tilde{M} \) one obtains a setup cycle that yields approximations to the eigenvectors of the matrix pencil \((A, \tilde{M})\). We note that the eigenvalue approximations in (4.6) are continuously updated within the algorithm so that the overall approach resembles an inverse Rayleigh-Quotient iteration found in eigenvalue computations (cf. [24]). For additional details of the algorithm and its implementation we refer to the paper [4].

To illustrate the effect of the choice of \( T_l \) in the MGE bootstrap process, we provide results in which a \( W^2 \)-cycle bootstrap setup using four forward Gauss Seidel pre- and four backward Gauss Seidel post-smoothing steps to compute the set of relaxed vectors \( V^r \) and set of bootstrap vectors \( V^e \) coming from the MGE process, with \( k_r = |V^r| = 8 \) and \( k_e = |V^e| = 8 \), respectively. The sets \( V^r \) and \( V^e \) are then combined to form the set of TVs \( V \) that is used to compute the least squares interpolation operator on each level. In these tests, only relaxation is applied to the homogenous systems in both setup cycles to update the sets \( V^r \). We use forward Gauss Seidel as a pre-smoother and backward Gauss Seidel as the post-smoother in the solve phase as well. The coarse grids and sparsity structure of interpolation are defined as in the previous tests on all levels, i.e., by full coarsening and nearest neighbor interpolation as depicted in Figure 4.3, and the problem is coarsened to a coarsest level with \( h = 1/8 \).

The results of our experiments are given in Table 4.2. Here, we observe that using the generalized eigen-problem in the BAMG setup gives uniformly better results, than just working with eigen-approximations of \( A \). In addition, if we compare the results obtained in the left table with the results given earlier (see Table 4.1), then we see that the multilevel BAMG
approach (with sparse $P$) converges faster than the two-level method that uses the ideal interpolation operator.

| Size / k | 1    | 2    | 4    | 8    |
|----------|------|------|------|------|
| 17²      | .276 | .377 | .398 | .626 |
| 33²      | .260 | .256 | .302 | .445 |
| 65²      | .261 | .256 | .299 | .427 |
| 129²     | .261 | .256 | .299 | .427 |

| Size / k | 1    | 2    | 4    | 8    |
|----------|------|------|------|------|
| 17²      | .357 | .592 | .405 | .966 |
| 33²      | .416 | .591 | .302 | .953 |
| 65²      | .261 | .256 | .303 | .573 |
| 129²     | .261 | .256 | .305 | .571 |

Table 4.2. BAMG setup results for Problem P4 with $X = \tilde{M}$ (left) and $X = I$ (right).

5. Conclusion

In this paper, we introduced an optimal form of classical AMG interpolation and a measure of the quality of the coarse variable set that gives precise estimates of the convergence rate of two-grid method with this optimal choice of interpolation, which is based on eigenvectors of the generalized eigen-problem involving the system matrix and its associated symmetrized smoother. We derived the equivalence between the ideal and optimal forms of interpolation in the case of reduction-based AMG (i.e., when $F$-relaxation is used) and we showed numerically that in the case of full smoothing the convergence rates of two-grid methods with these different choices can vary substantially. We also showed that for full smoothing and a proper choice of the coarse variable type, the optimal and ideal interpolation matrices have the same range. Finally, using these new results we designed a generalized bootstrap AMG setup algorithm that incorporates this generalized eigen-problem and illustrated the utility of the approach when applied to a scalar diffusion problem with highly varying diffusion coefficient. Numerically, we observed that the BAMG method (spanning multiple levels) with sparse $P$ outperforms the two-grid method with the ideal $P$ (which is a dense matrix). In addition, in our tests of the BAMG algorithm we did not use strength of connection in defining the sparsity structure of interpolation, instead we simply limited interpolation to nearest neighbors defined in terms of the geometry. This is another issue that we intend to study in detail in the future.

References

[1] A. Brandt. General highly accurate algebraic coarsening. ETNA, 10:1–20, 2000. Special issue on the Ninth Copper Mountain Conference on Multilevel Methods.
[2] A. Brandt. Multiscale scientific computation: review 2001. In T. J. Barth, T. F. Chan, and R. Haimes, editors, Multiscale and Multiresolution Methods: Theory and Applications, pages 1–96. Springer, Heidelberg, 2001.
[3] A. Brandt, J. Brannick, K. Kahl, and I. Livshits. Bootstrap AMG: status, open problems and outlook. Journal of Numerical Mathematics: Theory, Methods and Applications, 8(1):112–135, 2015.
[4] A. Brandt, J. Brannick, K. Kahl, and I. Livshits. Bootstrap AMG., SIAM Journal of Scientific Computing, 33:612–632, 2011.
[5] A. Brandt, S. McCormick, and J. Ruge. Algebraic multigrid (AMG) for automatic multigrid solution with application to geodetic computations. Technical report, Colorado State University, Fort Collins, Colorado, 1983.
[6] A. Brandt, S. McCormick, and J. Ruge. Algebraic multigrid (AMG) for sparse matrix equations. In Sparsity and its applications (Loughborough, 1983), pages 257–284. Cambridge Univ. Press, Cambridge, 1985.
[7] J. Brannick and R. Falgout. Compatible relaxation and coarsening in algebraic multigrid. *SIAM J. Sci. Comp.*, 32(3):1393–1416, 2010.
[8] J. Brannick and K. Kahl. Bootstrap AMG for the Wilson Dirac system. *SIAM Journal of Scientific Computing*, 36(3):321–347, 2014.
[9] J. Brannick, K. Kahl, and I. Livshits. Algebraic distances as a measure of AMG strength of connection for anisotropic diffusion problems. *Electronic Transactions in Numerical Analysis*, 44:472–496, 2015.
[10] J. Brannick, K. Kahl, and S. Sokolovic. An adaptively constructed algebraic multigrid preconditioner for irreducible markov chains. *Journal of Applied Numerical Mathematics*. Submitted January 19, 2015, arXiv:1402.4005.
[11] J. Brannick and L. Zikatanov. Algebraic multigrid methods based on compatible relaxation and energy minimization. In *Proceedings of the 16th International Conference on Domain Decomposition Methods*, volume 55 of *Lecture Notes in Computational Science and Engineering*, pages 15–26. Springer, 2007.
[12] M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge. Adaptive smoothed aggregation oSA. *SIAM J. Sci. Comput.*, 25:1896–1920, 2004.
[13] M. Brezina, R. Falgout, S. MacLachlan, T. Manteuffel, S. McCormick, and J. Ruge. Adaptive algebraic multigrid. *SIAM J. Sci. Comput.*, 27(4):1261–1286 electronic, 2006.
[14] Robert Eymard, Thierry Gallouët, and Raphaèle Herbin. Finite volume methods. *Handbook of numerical analysis*, 7:713–1018, 2000.
[15] R. Falgout, P. Vassilevski, and L. Zikatanov. On two–grid convergence estimates. *Numerical Linear Algebra with Applications*, 12(5-6):471–494, 2005.
[16] R. D. Falgout and P. S. Vassilevski. On generalizing the AMG framework. *SIAM J. Numer. Anal.*, 42(4):1669–1693, 2004. UCRL-JC-150807.
[17] S. A. Goreinov, I. V. Oseledets, D. V. Savostyanov, E. E. Tyrtyshnikov, and N. L. Zamarashkin. How to Find a Good Submatrix, pages 247–256. World Scientific, April 2010.
[18] Donald E Knuth. Semi-optimal bases for linear dependencies. *Linear and Multilinear Algebra*, 17(1):1–4, 1985.
[19] C. Liu, Z. Liu, and S. McCormick. An efficient multigrid scheme for elliptic equations with discontinuous coefficients. *Communications in Applied Numerical Methods*, 8:621–631, 1992.
[20] Jan Mandel, Marian Brezina, and Petr Vanek. Energy optimization of algebraic multigrid bases. 1998. CU Denver Technical Report.
[21] Alexander A Samarskii. *The theory of difference schemes*, volume 240. CRC Press, 2001.
[22] P. Vaněk, J. Mandel, and M. Brezina. Algebraic multigrid by smoothed aggregation for second and fourth order elliptic problems. *Computing*, 56:179–196, 1996.
[23] W. L. Wan, Tony F. Chan, and Barry Smith. An energy-minimizing interpolation for robust multigrid methods. *SIAM J. Sci. Comp.*, 21(4):16321649, 2000.
[24] J. Wilkinson. The algebraic eigenvalue problem. Clarendon Press, Oxford, 1965.
[25] J. Xu and L. Zikatanov. Algebraic multigrid methods. article: arXiv:1611.01917.
[26] Ali Ivri and Malik Magdon-Ismail. Exponential inapproximability of selecting a maximum volume submatrix. *Algorithmica*, 65(1):159, 2013.