

Closed-form multigrid smoothing factors for lexicographic Gauss–Seidel

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This paper aims to present a unified framework for deriving analytical formulas for smoothing factors in arbitrary dimensions, under certain simplifying assumptions. To derive these expressions we rely on complex analysis and geometric considerations, using the maximum modulus principle and Möbius transformations. We restrict our attention to pointwise and block lexicographic Gauss–Seidel smoothers on a d -dimensional uniform mesh, where the computational molecule of the associated discrete operator forms a $(2d + 1)$ -point star. In the pointwise case, the effect of a relaxation parameter is analysed. Our results apply to any number of spatial dimensions and are applicable to high-dimensional versions of a few common model problems with constant coefficients, including the Poisson and anisotropic diffusion equations, as well as a special case of the convection–diffusion equation. We show that in most cases our formulas, exact under the simplifying assumptions of local Fourier analysis, form tight upper bounds for the asymptotic convergence of geometric multigrid in practice. We also show that there are asymmetric cases where lexicographic Gauss–Seidel smoothing outperforms red–black Gauss–Seidel smoothing; this occurs for certain model convection–diffusion equations with high mesh Reynolds numbers.

Keywords: multigrid; smoothing factor; local Fourier analysis; elliptic partial differential equations; Gauss–Seidel.

1. Introduction

In this paper we revisit a problem that is as old as the days of geometric multigrid (Hackbusch, 1985; Wesseling, 1992; Trottenberg *et al.*, 2001): the (analytical) computation of smoothing factors on a uniform mesh. To that end, consider the d -dimensional linear elliptic partial differential equation (PDE)

$$\mathcal{L}u = f,$$

with prescribed boundary conditions, discretized on a rectangular grid with uniform mesh spacing h . This yields a linear system of the form

$$\sum_j \mathcal{L}_{\vec{I}, \vec{J}}^h u_j^h = f_{\vec{I}}^h, \quad (1.1)$$

where \vec{I} and \vec{J} vary over \mathbb{Z}^d . We will assume that the associated computational molecule forms a $(2d + 1)$ -point star or equivalently that $\mathcal{L}_{\vec{I}, \vec{J}}^h$ is of the form

$$\mathcal{L}_{\vec{i}, \vec{j}}^h = \begin{cases} a & \text{if } \vec{i} - \vec{j} = \vec{0}, \\ -b_k^+ & \text{if } \vec{i} - \vec{j} = \mathbf{e}_k, \\ -b_k^- & \text{if } \vec{i} - \vec{j} = -\mathbf{e}_k, \\ 0 & \text{otherwise.} \end{cases} \quad (1.2)$$

The connection between $\mathcal{L}_{\vec{i}, \vec{j}}^h$ and the computational molecule is illustrated in Fig. 1. We assume throughout that $\mathcal{L}_{\vec{i}, \vec{j}}^h$ satisfies

$$a \geq \sum_{k=1}^d (b_k^+ + b_k^-) \quad \text{and} \quad b_k^+, b_k^- > 0 \quad \text{for all } k \in \{1, \dots, d\}, \quad (1.3)$$

so that $[\mathcal{L}_{\vec{i}, \vec{j}}^h]$ is a diagonally dominant M-matrix (Varga, 1962, p. 85). Note that in the context of multigrid, there are cases (for example, convection–diffusion) where this property may hold on the finest grid but not on coarser grids, potentially leading to difficulties with convergence.

The eigenfunctions of certain simple relaxation schemes form a complete set of Fourier modes, and the eigenvalues can be split into high frequencies and low frequencies according to their wave numbers. The smoothing factor is then defined as the maximal absolute value of the high-frequency eigenvalues (Brandt, 1977; Trottenberg *et al.*, 2001, p. 104). In particular, the smoothing factor of lexicographic Gauss–Seidel (GS-LEX), which we focus on in this paper, falls into this category provided one makes the simplifying assumption of an infinite grid, as in local Fourier analysis (LFA).

For $d \leq 2$ the smoothing factors of GS-LEX can be computed using standard techniques from multivariate calculus, and several results are available in closed form. On the other hand, for $d > 2$ the resulting system of equations is typically intractable, and the literature is much sparser with regard to closed-form formulas. In this case the smoothing factor may be computed numerically by scanning over a dense set of high frequencies, but this may be computationally expensive, especially if one seeks to identify a trend with respect to parameters in the underlying PDE. An example here is the convection–diffusion equation, where one may wish to determine how the smoothing factor changes as a function of the mesh Reynolds numbers.

For red–black Gauss–Seidel (GS-RB), smoothing factors have been obtained for a broad class of *symmetric* operators of the form (1.2) in arbitrary dimensions and for both pointwise and block relaxations (see Yavneh, 1995). In this paper we offer complementary analysis for GS-LEX in arbitrary

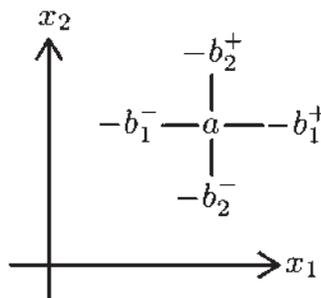


FIG. 1. The computational molecule associated with the operator \mathcal{L}^h ($d = 2$).

dimensions and include the asymmetric case, under certain simplifying assumptions. We show that in the strongly asymmetric setting, GS-LEX can be a better smoother than GS-RB. This is in contrast to the symmetric case, where the latter is superior. We also analyse the effect of a relaxation parameter.

The remainder of this paper is organized as follows. Section 2 is devoted to the derivation of our main results. In Section 3 we demonstrate the generality of our approach by applying it to a few examples and comparing against measured asymptotic convergence rates. We also present in this section a few comparisons of GS-LEX with GS-RB. Finally, in Section 4 we draw some conclusions.

2. Smoothing analysis

We will assume an ordering in which grid points are ordered according to the following rule: along dimension k , unknowns are ordered from $-e_k$ to $+e_k$ if $b_k^+ \leq b_k^-$ and from $+e_k$ to $-e_k$ otherwise. For convenience, let us define

$$c_k \equiv \max(b_k^+, b_k^-)/a,$$

$$d_k \equiv \min(b_k^+, b_k^-)/a.$$

It is straightforward to show that the smoothing factor of pointwise GS-LEX predicted by LFA is given by

$$\mu^{\text{pt}} = \max_{\tilde{\theta} \in \Theta^d} \left| \frac{\sum_{k=1}^d d_k e^{i\theta_k}}{1 - \sum_{k=1}^d c_k e^{-i\theta_k}} \right|, \tag{2.1}$$

where $\Theta^d = [-\pi, \pi]^d \setminus (-\pi/2, \pi/2)^d$ is the set of rough modes in d dimensions and $i \equiv \sqrt{-1}$.

We restrict our analysis to the case

$$d_k = \alpha c_k, \tag{2.2}$$

where $\alpha \in (0, 1]$ is a constant independent of k . This restriction includes all cases where $[\mathcal{L}_{I,j}^h]$ is symmetric but also includes other cases, for example, the case of the convection–diffusion equation with all mesh Reynolds numbers equal.

It is well known that pointwise smoothing is ineffective for highly anisotropic problems (Trottenberg *et al.*, 2001, p. 131); one way to resolve this is the use of block smoothers (Trottenberg *et al.*, 2001, p. 134). Such smoothers are defined by a partitioning of $\{1, \dots, d\}$ into disjoint subsets

$$\mathcal{I}_b \subset \{1, \dots, d\} \quad \text{and} \quad \mathcal{I}_p = \{1, \dots, d\} \setminus \mathcal{I}_b,$$

where coordinates belonging to \mathcal{I}_b are relaxed simultaneously. To avoid degenerate cases, we assume that both \mathcal{I}_p and \mathcal{I}_b are nonempty. In this case the smoothing factor is given by

$$\mu^{\text{block}} = \max_{\tilde{\theta} \in \Theta^d} \left| \frac{\sum_{k \in \mathcal{I}_p} d_k e^{i\theta_k}}{1 - \sum_{k \in \mathcal{I}_p} c_k e^{-i\theta_k} - \sum_{k \in \mathcal{I}_b} (c_k e^{-i\theta_k} + d_k e^{i\theta_k})} \right|. \tag{2.3}$$

It is worth noting that the computational cost per iteration of a block smoother is higher than that of a point smoother. However, for highly anisotropic cases this overhead is typically small compared to the gains in convergence rates.

Our analysis shows that μ^{pt} depends only on α and any two of the quantities

$$c \equiv c_1 + c_2 + \dots + c_d, \quad c_m \equiv \min(c_1, \dots, c_d), \quad c_r \equiv c - c_m, \quad (2.4)$$

regardless of the number of dimensions, d .

Similarly, in the case that \mathcal{L}^h is symmetric, our analysis shows that the block smoothing factor μ^{block} depends on any two of the quantities

$$C^p = \sum_{k \in \mathcal{I}_p} c_k, \quad C_m^p = \min_{k \in \mathcal{I}_p} c_k, \quad C_r^p = C^p - C_m^p, \quad (2.5)$$

as well as any two of C^b , C_m^b and C_r^b (which are defined analogously).

Expressions for μ^{pt} and μ^{block} are given in Theorems 2.5 and 2.6, respectively.

2.1 Pointwise relaxation

Starting from (2.1), we complex-conjugate the denominator and apply (2.2) to obtain

$$\mu^{\text{pt}} = \max_{\vec{\theta} \in \Theta^d} \left| \frac{\sum_{k=1}^d d_k e^{i\theta_k}}{1 - \sum_{k=1}^d c_k e^{-i\theta_k}} \right| = \max_{\vec{\theta} \in \Theta^d} \left| \frac{\alpha \sum_{k=1}^d c_k e^{i\theta_k}}{1 - \sum_{k=1}^d c_k e^{i\theta_k}} \right| \equiv \max_{\vec{\theta} \in \Theta^d} \left| \frac{\alpha g(\vec{\theta})}{1 - g(\vec{\theta})} \right|,$$

where $g(\vec{\theta}) \equiv \sum_{k=1}^d c_k e^{i\theta_k}$.

The key to our analysis lies in the observation that this may be rewritten as

$$\mu^{\text{pt}} = \max_{z \in g(\Theta^d)} |f(z)|,$$

where

$$f(z) \equiv \frac{\alpha z}{1 - z}$$

is analytic in the punctured plane $\mathbb{C} \setminus \{1\}$.

If the set $g(\Theta^d)$ is sufficiently well behaved (a connected open set or the closure of one) and does not contain the point $z = 1$, the maximum principle (Gamelin, 2001, p. 88) applies and we can write

$$\mu^{\text{pt}} = \max_{z \in \partial g(\Theta^d)} |f(z)|,$$

where $\partial g(\Theta^d)$ denotes the boundary of $g(\Theta^d)$.

However, computing $g(\Theta^d)$ explicitly is challenging because for certain values of $\{c_k\}$ it contains a hole in the vicinity of the origin—see Example 2.3. Keeping track of this hole is difficult—we avoid the issue by proving that we can replace $g(\Theta^d)$ with a simply connected set D equivalent to it in the following sense.

DEFINITION 2.1 Let $A, B \subset \mathbb{C}$. We say $A \sim B$ if

$$\sup_A |f| = \sup_B |f|$$

for all functions f analytic in a neighborhood of $A \cup B$.

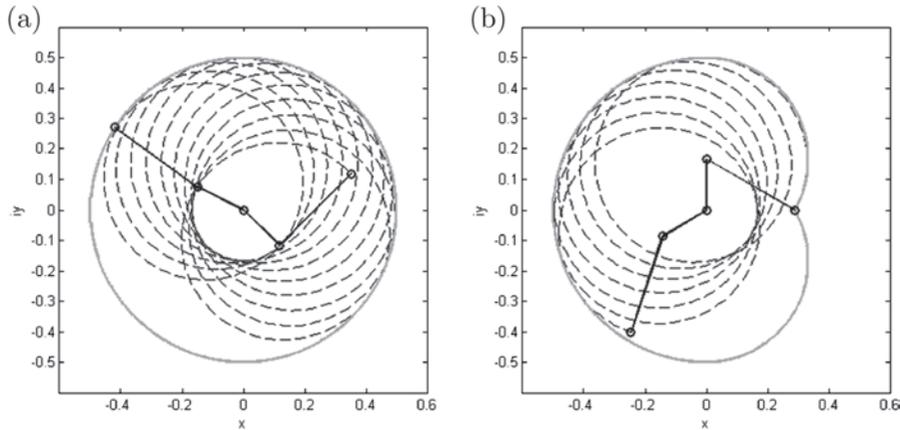


FIG. 2. An illustration of Example 2.3: (a) If a double pendulum with arms of length $\frac{1}{6}$ and $\frac{1}{3}$ is allowed to swing freely, it remains inside a disk of radius 0.5. (b) If one arm is constrained to lie in the left half plane, the pendulum swings in the heart-shaped region shown. In both cases the pendulum is unable to reach a set of points surrounding the origin.

The following observation establishes an important sufficient condition for two sets to be equivalent.

OBSERVATION 2.2 Let $A, B \subset \mathbb{C}$, and suppose B is a connected open set, or the closure thereof. If $\partial B \subseteq A \subseteq \bar{B}$, then $A \sim B$.

To see this, let f be any function analytic in a neighborhood of $A \cup B = B$. We clearly have $\sup_{\partial B} |f| \leq \sup_A |f| \leq \sup_B |f|$, but the maximum modulus principle implies the equality of the leftmost and rightmost terms.

In light of Observation 2.2, our goal is to find a simply connected set D such that $\partial D \subseteq g(\Theta^d) \subseteq \bar{D}$. This is done in Lemma 2.4, but first we build some intuition with a simple example.

EXAMPLE 2.3 Suppose $d = 2$ and \mathcal{L}^h arises from a centred-difference discretization of the Laplacian-like operator $\mathcal{L} = 0.5\partial_{xx} + \partial_{yy}$, giving $a = 3$, $b_1^+ = b_1^- = 0.5$ and $b_2^+ = b_2^- = 1$. Then $c_1 = 1/6$, $c_2 = 1/3$ and

$$g(\theta_1, \theta_2) = \frac{1}{6}e^{i\theta_1} + \frac{1}{3}e^{i\theta_2}.$$

Geometrically, $g(\theta_1, \theta_2)$ may be viewed as a double pendulum with arms of length $1/6$ and $1/3$, making angles θ_k ($k = 1, 2$) with the x -axis. As (θ_1, θ_2) varies over $[-\pi, \pi]^2$, this pendulum (and therefore the range of g) remains confined to the disk of radius 0.5 shown in Fig. 2(a). Furthermore, the boundary of the disk is swept out as the double pendulum completes a full revolution with a constant angle of 180° between the arms. By Observation 2.2, $g([-\pi, \pi]^2)$ is equivalent to this disk in the sense of Definition 2.1.

However, if (θ_1, θ_2) is constrained to lie in Θ^2 , then $|\theta_k| \geq \pi/2$ for at least one $k \in \{1, 2\}$. In other words, at least one arm is constrained to lie in the left half plane. With this constraint, $g(\theta_1, \theta_2)$ now lives in the set shown in Fig. 2(b)—the union of two disks and a half disk, as demonstrated in Fig. 3. It is simple to show that the boundary of this set is once again in the range of g , so this heart-shaped set provides us with the D we are looking for.

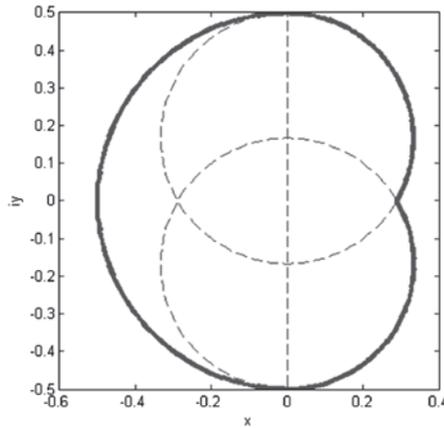


FIG. 3. The heart-shaped set D is the union of two disks and a half disk.

Note that while $g(\Theta^2) \sim D$, it is not true that $g(\Theta^2) = D$ since $0 \in D$ but $|g| \geq \frac{1}{3} - \frac{1}{6} > 0$.

LEMMA 2.4 Let $B(r, z)$ denote the closed ball of radius $r \geq 0$ centred at $z \in \mathbb{C}$. Let \mathbb{C}^- denote the set of all complex numbers with negative real part, and let \sim be the relation in Definition 2.1. Then

$$g(\Theta^d) \sim [B(c, 0) \cap \mathbb{C}^-] \cup B(c_r, ic_m) \cup B(c_r, -ic_m) \equiv D,$$

$$g([-\pi, \pi]^d) \sim B(c, 0),$$

where c, c_m and c_r are defined in (2.4).

Proof. By Observation 2.2 we clearly have $g([-\pi, \pi]^d) \sim B(c, 0)$ since $|g(\theta_1, \dots, \theta_d)| \leq c$ and $g(\theta, \dots, \theta) = c e^{i\theta}$. On the other hand, if $\vec{\theta} \in \Theta^d$, then there is a j such that $|\theta_j| \geq \pi/2$. Assuming that we have made some fixed choice of j and set θ_j to a fixed value α , the remaining variables $\{\theta_k\}_{k \neq j}$ range over $[-\pi, \pi]^{d-1}$. It follows that g is confined to $B(c - c_j, c_j e^{i\alpha})$, and therefore

$$g(\Theta^d) \subseteq \bigcup_{|\alpha| \geq \frac{\pi}{2}} \bigcup_{j=1}^d B(c - c_j, c_j e^{i\alpha}).$$

But $B(c - c_j, c_j e^{i\alpha}) \subseteq B(c_r, c_m e^{i\alpha})$ for all j since $|z - c_j e^{i\alpha}| \leq c - c_j$ implies that

$$|z - c_m e^{i\alpha}| \leq |z - c_j e^{i\alpha}| + |c_j e^{i\alpha} - c_m e^{i\alpha}| \leq (c - c_j) + (c_j - c_m) = c_r.$$

Therefore,

$$g(\Theta^d) \subseteq \bigcup_{|\alpha| \geq \frac{\pi}{2}} B(c_r, c_m e^{i\alpha}).$$

It can be shown that any $z \in B(c_r, c_m e^{i\alpha})$ obeying $\text{Re}(z) \geq 0$ lies in $B(c_r, ic_m)$ if $\text{Im}(z) \geq 0$ and $B(c_r, -ic_m)$ if $\text{Im}(z) \leq 0$. Similarly, since $|z| \leq c$ we have $z \in B(c, 0) \cap \mathbb{C}^-$ if $\text{Re}(z) < 0$. It follows that

$$g(\Theta^d) \subseteq D.$$

It is trivial to show that $\partial D \subseteq g(\Theta^d)$, which completes the proof. □

Lemma 2.4 and Definition 2.1 allow us to conclude that

$$\mu^{\text{pt}} = \max_{\partial D} |f|, \tag{2.6}$$

provided f is analytic in a neighborhood of D , that is, provided we can show that $1 \notin D$. To that end, we note that the diagonal dominance of \mathcal{L}^h implies that

$$\begin{aligned} c &= \frac{\sum_{k=1}^d \max(b_k^+, b_k^-)}{a} \\ &\leq \frac{\sum_{k=1}^d \max(b_k^+, b_k^-)}{\sum_{k=1}^d (b_k^+ + b_k^-)} < 1. \end{aligned}$$

The desired result follows from the observation

$$D \cap \mathbb{R} = \left[-c, \sqrt{c_r^2 - c_m^2} \right] \subseteq [-c, c).$$

THEOREM 2.5 The smoothing factor of pointwise GS-LEX applied to discrete operators of the form (1.2) obeying the constraints (1.3) and (2.2) is given by

$$\mu^{\text{pt}}(c_m, c_r, \alpha) = \frac{\alpha c_r + \alpha \sqrt{c_m^2 + (c_m^2 - c_r^2)^2}}{1 + c_m^2 - c_r^2}, \tag{2.7}$$

where c_m and c_r are defined in (2.4) and α is defined in (2.2).

Proof. ∂D is the union of the three semicircular arcs

$$\begin{aligned} S_1 &= \left\{ c e^{i\theta} : \theta \in \left[\frac{\pi}{2}, \frac{3\pi}{2} \right] \right\}, & S_2 &= \left\{ ic_m + c_r e^{i\theta} : \theta \in \left[-\sin^{-1} \left(\frac{c_m}{c_r} \right), \frac{\pi}{2} \right] \right\}, \\ S_3 &= \{ z \in \mathbb{C} : \bar{z} \in S_2 \}. \end{aligned}$$

By (2.6), it suffices to compute the maximum of the maxima of $|f|$ over S_1 , S_2 and S_3 . However, since $|f(\bar{z})| = |f(z)|$, the maxima over S_2 and S_3 are the same and hence we omit S_3 from consideration. Furthermore, it is trivial to show that the maximum of $|f|$ over S_1 is achieved at ic , the point of intersection of S_1 and S_2 . Therefore, the maximum of $|f|$ over S_2 is at least as large as the maximum over S_1 —hence we may omit S_1 as well.

It follows that the maximum of $|f|$ over D is attained on the semicircle S_2 . However, it is also true that the maximum is attained on the full circle $|z - ic_m| = c_r$, as this circle contains S_2 and is contained in D . It is more convenient to work with the full circle, so we conclude that

$$\mu^{\text{pt}} = \max_{|z - ic_m| = c_r} |f(z)|. \tag{2.8}$$

Now, $f(z) = \frac{\alpha z}{1-z}$ is a Möbius transform, and hence the image of a circle is either a circle or a line (Gamelin, 2001, p. 65). Since the circle $|z - ic_m| = c_r$ does not contain any poles of f , it follows that $f(\{|z - ic_m| = c_r\})$ is a circle.

If we let $z_c \in \mathbb{C}$ and $r \geq 0$ denote the centre and radius, respectively, of this circle, then from (2.8) we have

$$\mu^{pt} = \max_{w \in f(\{|z - ic_m| = c_r\})} |w| = |z_c| + r. \quad (2.9)$$

To find the parameters z_c and r , we first decompose f into a sequence of elementary Möbius transformations: $f = f_4 \circ f_3 \circ f_2 \circ f_1$, where $f_1(z) = z - 1$, $f_2(z) = z^{-1}$, $f_3(z) = -\alpha z$ and $f_4(z) = z - \alpha$. Then, starting with the circle $|z - ic_m| = c_r$, we track the changes in its centre and radius as we compute its image under f_1 , then compute the image of the result under f_2 , and so on.

Since f_1 , f_3 and f_4 are all either translations or dilations, the steps involving them are straightforward. For f_2 we make the observation that the image of a circle with radius R and centre z_0 under inversion is the circle with radius R' and centre z'_0 given by

$$z'_0 = \frac{\bar{z}_0}{|z_0|^2 - R^2} \quad \text{and} \quad R' = \frac{R}{||z_0|^2 - R^2|};$$

this fact can easily be derived from the argument found in Gamelin (2001, p. 66). In the end we find that

$$r = \frac{\alpha c_r}{1 + c_m^2 - c_r^2}$$

and

$$z_c = \alpha \frac{c_r^2 - c_m^2}{1 + c_m^2 - c_r^2} + i\alpha \frac{c_m}{1 + c_m^2 - c_r^2},$$

which completes the proof. \square

Note that the smoothing factor μ^{pt} is proportional to α . Since the latter is small when the operator \mathcal{L}^h is strongly asymmetric, this suggests that GS-LEX may be particularly effective in this regime. In particular, as $\alpha \rightarrow 0$ the part of \mathcal{L}^h above its diagonal is converging to the zero matrix, and for $\alpha = 0$ we have that \mathcal{L}^h is lower triangular and GS-LEX becomes a (direct) solver. See also Section 3 for further illustrations of this behaviour.

2.2 SOR smoothing

It is well known that the smoothing factors of GS-RB, Jacobi-RB¹ and Jacobi can be greatly improved by incorporating a relaxation parameter (Yavneh, 1996; Trottenberg *et al.*, 2001; Zubair *et al.*, 2007). For example, for the standard seven-point centred-difference discretization of the three-dimensional Poisson problem, overrelaxation with $\omega = 1.15$ improves the smoothing factor of GS-RB (equivalent to Jacobi-RB in this specific case) from $\mu \approx 0.44$ to $\mu \approx 0.23$ (Yavneh, 1996). For the same problem, the smoothing factor of Jacobi is improved from $\mu = 1$ (no convergence) to $\mu = 5/7$ by underrelaxation with $\omega = 6/7$ (Trottenberg *et al.*, 2001, p. 73).

We can analyse the effect of a relaxation parameter ω in GS-LEX smoothing by repeating the steps of Theorem 2.5 with the Möbius transformation

$$f_\omega(z) = \frac{\alpha z + \frac{1}{\omega} - 1}{\frac{1}{\omega} - z}$$

¹Jacobi-RB consists of a Jacobi sweep over the red points, followed by a Jacobi sweep over the black points using the updated values at red points; see, for example, Trottenberg *et al.* (2001, p. 173).

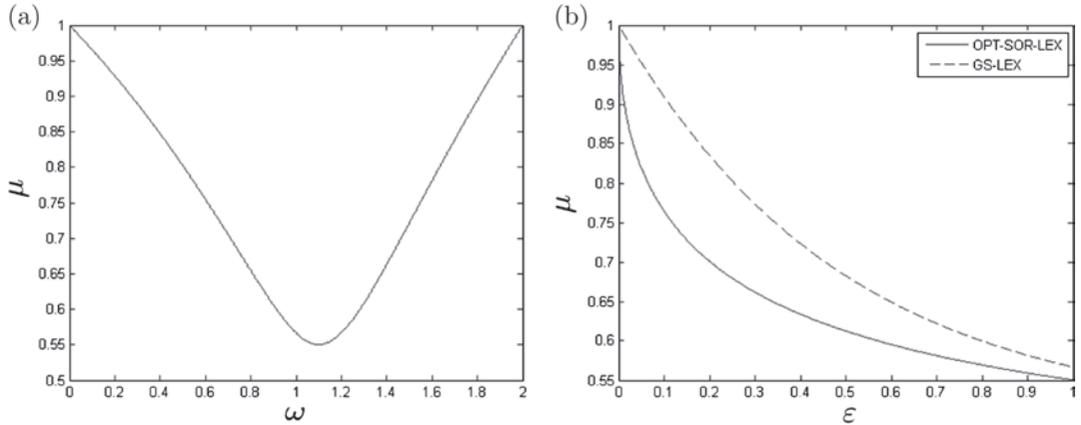


FIG. 4. Left: Smoothing factor of SOR-LEX with relaxation parameter ω , as a function of ω , for the standard seven-point centred-difference discretization of the three-dimensional Poisson problem. Right: Smoothing factors of GS-LEX and optimal SOR-LEX applied to the anisotropic diffusion problem $-\varepsilon u_{xx} - u_{yy} - u_{zz} = f$, as a function of ε , assuming seven-point centred-difference discretization.

used in place of f . Note that we must assume that $\omega < \frac{1}{\sqrt{c_r^2 - c_m^2}}$ in order to ensure that f_ω has no poles in D .

Making use of the factorization $f_\omega = f_4 \circ f_3 \circ f_2 \circ f_1$, where $f_1(z) = z - \frac{1}{\omega}$, $f_2(z) = z^{-1}$, $f_3(z) = (1 - \frac{1+\alpha}{\omega})z$ and $f_4(z) = z - \alpha$, we obtain

$$\mu_{\text{SOR}}^{\text{pt}}(\omega) = \frac{c_r \left| 1 - \frac{1+\alpha}{\omega} \right| + \sqrt{c_m^2 \left(1 - \frac{1+\alpha}{\omega} \right)^2 + \left(\frac{1}{\omega} \left(1 - \frac{1}{\omega} \right) + \alpha(c_m^2 - c_r^2) \right)^2}}{\frac{1}{\omega^2} + c_m^2 - c_r^2}. \tag{2.10}$$

Figure 4(a) shows a plot of $\mu_{\text{SOR}}^{\text{pt}}$ as a function of $\omega \in [0, 2]$ for the three-dimensional Poisson problem mentioned above ($c_m = 1/6$, $c_r = 1/3$, $\alpha = 1$). The optimal smoothing factor $\mu \approx 0.551$ is attained at $\omega \approx 1.1$, a modest improvement over the smoothing factor $\mu \approx 0.567$ obtained when $\omega = 1$. This finding supports the conclusion (Trottenberg *et al.*, 2001, p. 105) that for GS-LEX, the inclusion of a relaxation parameter is not necessarily worth the extra work per iteration (two operations per point per relaxation sweep).

In Fig. 4(b), the anisotropic problem $-\varepsilon u_{xx} - u_{yy} - u_{zz} = f$ is discretized using standard seven-point centred differences, and the theoretical smoothing factors of both GS-LEX and optimal SOR-LEX (obtained by numerical minimization of (2.10)) are plotted against ε .

2.3 Block relaxation

In this section we analyse the smoothing properties of block GS-LEX relaxation. To keep the algebra manageable, we restrict the scope of our analysis to the case that $[\mathcal{L}_{i,j}^h]$ is symmetric ($\alpha = 1$). Our main result is Theorem 2.6, that establishes a connection between block and pointwise smoothing factors.

Since $\alpha = 1$, we have $c_k = d_k$ for all k —substituting this into equation (2.3), complex-conjugating the denominator and then simplifying, we obtain

$$\begin{aligned} \mu^{\text{block}} &= \max_{\vec{\theta} \in \Theta^d} \left| \frac{\sum_{k \in \mathcal{I}_p} c_k e^{i\theta_k}}{1 - 2 \sum_{k \in \mathcal{I}_b} c_k \cos \theta_k - \sum_{k \in \mathcal{I}_p} c_k e^{i\theta_k}} \right| \\ &= \max_{(z,x) \in G(\Theta^d)} \left| \frac{z}{1-x-z} \right|, \end{aligned}$$

where $G: \Theta^d \rightarrow \mathbb{C} \times \mathbb{R}$ is given by $G(\vec{\theta}) = (G_1(\vec{\theta}), G_2(\vec{\theta}))$ with

$$\begin{aligned} G_1(\vec{\theta}) &= \sum_{k \in \mathcal{I}_p} c_k e^{i\theta_k} \quad \text{and} \\ G_2(\vec{\theta}) &= 2 \sum_{k \in \mathcal{I}_b} c_k \cos \theta_k. \end{aligned}$$

Defining $z' = z/(1-x)$, this becomes

$$\mu^{\text{block}} = \max_{z' \in \mathcal{A}} \left| \frac{z'}{1-z'} \right| = \max_{z' \in \mathcal{A}} |f(z')|, \tag{2.11}$$

where f is defined in Section 2.1 and

$$\mathcal{A} \equiv \left\{ z/(1-x) : (z,x) \in G(\Theta^d) \right\}.$$

We will show that \mathcal{A} is \sim (in the sense of Definition 2.1) to the union of a scaled copy of the set D from Lemma 2.4 and a particular ball centred at the origin. This fact will allow us to express μ^{block} in terms of μ^{pt} .

If $\vec{\theta} \in \Theta^d$, then there is a j such that $|\theta_j| \geq \pi/2$. If $j \in \mathcal{I}_p$, it follows that

$$\{\theta_k\}_{k \in \mathcal{I}_p} \in \Theta^{|\mathcal{I}_p|} \quad \text{and} \quad \{\theta_k\}_{k \in \mathcal{I}_b} \in [-\pi, \pi]^{|\mathcal{I}_b|},$$

while if $j \in \mathcal{I}_b$, then

$$\{\theta_k\}_{k \in \mathcal{I}_p} \in [-\pi, \pi]^{|\mathcal{I}_p|} \quad \text{and} \quad \{\theta_k\}_{k \in \mathcal{I}_b} \in \Theta^{|\mathcal{I}_b|}.$$

The function G_1 has the same form as g of Section 2.1 with the variables $\{\theta_k\}_{k=1}^d$ replaced by $\{\theta_k\}_{k \in \mathcal{I}_p}$. Thus, Lemma 2.4 applies with C^p, C_m^p and C_r^p playing the roles of c, c_m, c_r :

$$G_1(\Theta^d) \sim \begin{cases} D(C_m^p, C_r^p) & \text{if } k \in \mathcal{I}_p, \\ B(C^p, 0) & \text{otherwise.} \end{cases}$$

At the same time we have

$$G_2(\Theta^d) = \begin{cases} [-2C^b, 2C^b] & \text{if } k \in \mathcal{I}_p, \\ [-2C^b, 2C_r^b] & \text{otherwise.} \end{cases}$$

Assuming $j \in \mathcal{I}_p$, since G_1 and G_2 depend on disjoint variables we have

$$A \Big|_{j \in \mathcal{I}_p} = \bigcup_{x \in G_2(\Theta^d)} \Big|_{j \in \mathcal{I}_p} \frac{1}{1-x} G_1(\Theta^d) \Big|_{j \in \mathcal{I}_p} \sim \bigcup_{x \in [-2C^b, 2C^b]} \frac{1}{1-x} D(C_m^p, C_r^p).$$

Note that if $2C^b < 1$, then for all $x \in [-2C^b, 2C^b]$ we have

$$\frac{1}{1-x} D(C_m^p, C_r^p) \subseteq \frac{1}{1-2C^b} D(C_m^p, C_r^p).$$

It follows from the diagonal dominance of \mathcal{L}^h and the condition $\alpha = 1$ that $c \leq 0.5$. Since $C^b < c$, we have $2C^b < 1$ as desired, and therefore,

$$A \Big|_{j \in \mathcal{I}_p} \sim \frac{1}{1-2C^b} D(C_m^p, C_r^p) = D\left(\frac{C_m^p}{1-2C^b}, \frac{C_r^p}{1-2C^b}\right). \tag{2.12}$$

A similar analysis with $j \in \mathcal{I}_b$ shows that

$$A \Big|_{j \in \mathcal{I}_b} \sim B\left(\frac{C^p}{1-2C_r^b}, 0\right).$$

THEOREM 2.6 The smoothing factor of block GS-LEX applied to *symmetric* discrete operators of the form (1.2) obeying the constraints (1.3) and (2.2) is given by

$$\mu^{\text{block}} = \max\left(\mu^{\text{pt}}(\tilde{c}_m, \tilde{c}_r, \alpha = 1), \frac{C^p}{1-C^p-2C_r^b}\right), \tag{2.13}$$

where

$$\tilde{c}_m = \frac{C_m^p}{1-2C^b}, \quad \tilde{c}_r = \frac{C_r^p}{1-2C^b},$$

and $C^p, C_m^p, C_r^p, C^b, C_r^b$ are defined in (2.5).

Proof. Clearly the maximum of $|f|$ over A is the maximum of the separate maxima over $A \Big|_{j \in \mathcal{I}_p}$ and $A \Big|_{j \in \mathcal{I}_b}$. By (2.12) and Theorem 2.5 we have

$$\max_{z \in A \Big|_{j \in \mathcal{I}_p}} |f(z)| = \mu^{\text{pt}}(\tilde{c}_m, \tilde{c}_r, 1),$$

provided f is analytic in a neighborhood of $D(\tilde{c}_m, \tilde{c}_r)$. From the inequalities $C^p, C^b < c \leq 1/2$, it is easy to show $\tilde{c} \equiv \tilde{c}_m + \tilde{c}_r \leq 1$, and the desired result follows in the same way as in Section 2.1.

Similarly, since $C_r^b, C^p < 1/2$ we have

$$1 \notin B\left(\frac{C^p}{1-2C_r^b}, 0\right) \sim A \Big|_{j \in \mathcal{I}_b}.$$

It follows from the maximum modulus principle that $f(z)$ attains its maximum modulus over $A \Big|_{j \in \mathcal{I}_b}$ at $z = C^p / (1 - 2C_r^b)$, and therefore,

$$\max_{z \in A \Big|_{j \in \mathcal{I}_b}} |f(z)| = \frac{C^p}{1 - C^p - 2C_r^b},$$

which completes the proof. \square

Theorem 2.6 shows that applying a block smoother can be equivalent to applying a point smoother to a related problem.

3. Examples

In this section we apply Theorems 2.5 and 2.6 to a few examples, obtaining formulas for the smoothing factors of standard discretizations of several common PDEs; these are then compared with the measured asymptotic convergence rate of multigrid with GS-LEX smoothing. We also include measured convergence rates with GS-RB smoothing and show that while the latter has better smoothing properties for the symmetric case (Yavneh, 1995), lexicographic smoothing is more effective in the strongly asymmetric setting of the convection-dominated convection–diffusion equation. All experiments are done on a rectangular domain with homogeneous Dirichlet boundary conditions. Unless stated otherwise, we use the Galerkin coarse grid operator $\mathcal{L}^{2h} = I_h^{2h} \mathcal{L}^h I_{2h}^h$ in our experiments, where I_{2h}^h is the prolongation operator with linear interpolation and $I_h^{2h} = 2^d (I_{2h}^h)^T$ is the restriction operator with full weighting. The asymptotic convergence rate ρ is estimated from the sequence of residuals $\{r^{(k)}\}_{k=0}^m$ using the identity

$$\rho = \lim_{m \rightarrow \infty} \sqrt[m]{\frac{\|r^{(m)}\|_2}{\|r^{(0)}\|_2}}$$

and approximating the limit with a sufficiently large value of m (see Trottenberg *et al.*, 2001, p. 54, for justification).

EXAMPLE 3.1 Suppose the d -dimensional Poisson problem

$$-\Delta u = f$$

is discretized using centred differences on a uniform grid. Theorem 2.5 gives a general formula for the smoothing factor of pointwise GS-LEX, namely

$$\mu_{\text{Poisson}}^{\text{pt}}(d) = \frac{2(d-1) + \sqrt{d^2 - 4d + 8}}{3d + 2}.$$

It can be verified that this not only reduces to the known values $1/\sqrt{5}$ and $1/2$ for $d = 1$ and $d = 2$, respectively (Brandt, 1977) but also yields the exact expression

$$\mu_{\text{Poisson}}^{\text{pt}}(3) = \frac{4 + \sqrt{5}}{11} \approx 0.5669,$$

TABLE 1 *Smoothing factors of GS-LEX with point, line and plane relaxation for the Poisson problem in one, two and three dimensions. Moving from point to line or from line to plane relaxation is equivalent to reducing the dimension by one*

Relaxation/dimension	$d = 1$	$d = 2$	$d = 3$
Point relaxation	0.447	0.5	0.567
Line relaxation		0.447	0.5
Plane relaxation			0.447

which as far as we know has not appeared in the literature in closed form.

Similarly, Theorem 2.6 provides a general formula for smoothing factors of block GS-LEX applied to the d -dimensional Poisson problem. If each block is a k -dimensional subproblem, then we have

$$\mu_{\text{Poisson}}^{\text{block}}(d, k) = \begin{cases} \mu_{\text{Poisson}}^{\text{pt}}(d - k) & \text{if } d - k < 3, \\ \frac{d-k}{2+d-k} & \text{otherwise;} \end{cases}$$

see Table 1.

EXAMPLE 3.2 Suppose the anisotropic steady-state diffusion problem

$$-\rho_1 u_{x_1 x_1} - \rho_2 u_{x_2 x_2} - \dots - \rho_d u_{x_d x_d} = f \tag{3.1}$$

is discretized over \mathbb{R}^d with standard second-order centred differences. We then obtain a linear system with \mathcal{L}^h of the form (1.2) where $b_k^+ = b_k^- = \rho_k$ and $a = 2 \sum_{k=1}^d \rho_k$.

In particular, if $d = 3$ and $\rho_1 = \rho_2 = 1$ while $\rho_3 = \varepsilon \in (0, 1]$, then

$$\mu^{\text{pt}} = \frac{4 + \sqrt{5\varepsilon^2 - 4\varepsilon + 4}}{6 + 5\varepsilon}.$$

Note that $\mu^{\text{pt}} \rightarrow 1$ as $\varepsilon \rightarrow 0$. If line relaxation is performed in which unknowns along the x or y directions are relaxed simultaneously, one obtains

$$\mu^{\text{line}} = \frac{2 + \sqrt{5\varepsilon^2 - 2\varepsilon + 1}}{3 + 5\varepsilon}.$$

It is interesting to note that μ^{line} above is identical to μ^{pt} in the lower-dimensional case $d = 2$ and $\rho_1 = 1, \rho_2 = \varepsilon$. Figure 5 provides a comparison between the formulas for μ^{pt} and μ^{line} and measured asymptotic convergence rates of two-level multigrid on a $23 \times 23 \times 23$ grid, for both GS-LEX and GS-RB. The graphs illustrate that GS-RB is superior to GS-LEX in this symmetric case. We also consider multigrid V-cycles with one pre- and one post-GS-LEX smoothing step, applied to model problem (3.1) with $d = 2, \rho_1 = 1, \rho_2 = \varepsilon$ on a 1023×1023 grid. These are compared with theoretical smoothing factors in Table 2.

EXAMPLE 3.3 Suppose the constant coefficient convection–diffusion problem

$$-\Delta u + \vec{w} \cdot \nabla u = f$$

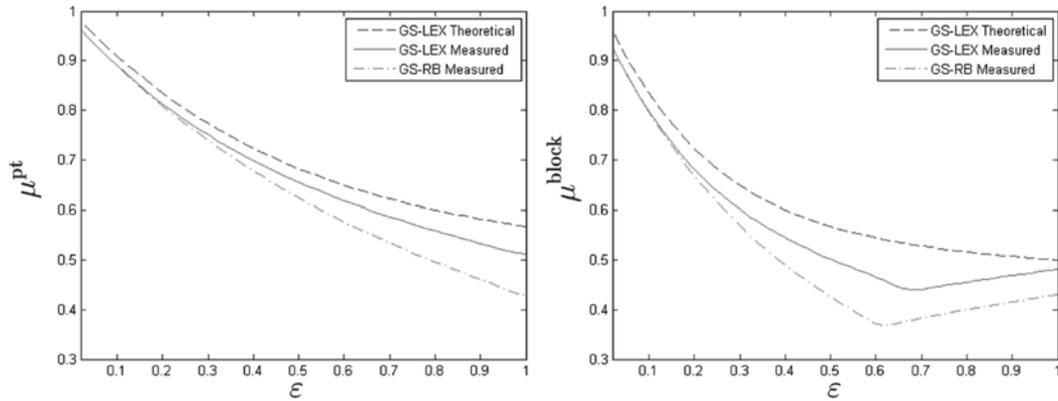


FIG. 5. Theoretical smoothing factors of GS-LEX versus experimental asymptotic convergence rates of two-level multigrid with GS-LEX and GS-RB smoothers, applied to the steady-state diffusion equation $-u_{xx} - u_{yy} - \epsilon u_{zz} = f$. Pointwise relaxation appears on the left, while x -oriented line relaxation is depicted on the right. The discretization is on a $23 \times 23 \times 23$ grid with centred differences.

TABLE 2 Comparison of predicted smoothing factors of GS-LEX with measured convergence rates of multigrid $V(1, 1)$ -cycles, for the PDE $-\epsilon u_{xx} - u_{yy} = f$. The finest grid is 1023×1023 , while the coarsest is 1×1 . Various values of ϵ are considered

ϵ	1.00	0.50	0.10	0.05
μ^2	0.25	0.32	0.70	0.83
$V(1, 1)$	0.12	0.27	0.68	0.81

is discretized on a uniform rectangular grid with mesh spacing h . We define the d mesh Reynolds numbers by $\gamma_k = w_k h/2$ and assume that they are all equal, that is,

$$\gamma_1 = \gamma_2 = \dots = \gamma_d = \gamma.$$

If we discretize this PDE using centred differences, we obtain $a = 2d$, $b_k^+ = 1 - \gamma$, $b_k^- = 1 + \gamma$ for all k . Provided $|\gamma| < 1$, equation (1.3) is satisfied and Theorem 2.5 gives

$$\mu^{\text{pt}} = (1 - |\gamma|) \left[\frac{(d - 1) + \sqrt{1 + (1 + |\gamma|)^2 (1 - \frac{d}{2})^2}}{2d + (1 + |\gamma|)^2 (1 - \frac{d}{2})} \right].$$

On the other hand, if we use first-order upwinding, then (assuming for simplicity that $\gamma \geq 0$) we obtain $a = 2d(1 + \gamma)$, $b_k^+ = 1$, $b_k^- = 1 + 2\gamma$ for all k . The constraints (1.3) are satisfied for all $\gamma \geq 0$ and

$$\mu^{\text{pt}} = \frac{1}{1 + \gamma} \left[\frac{(d - 1) + \sqrt{1 + (1 + \frac{\gamma}{1 + \gamma})^2 (1 - \frac{d}{2})^2}}{2d + (1 + \frac{\gamma}{1 + \gamma})^2 (1 - \frac{d}{2})} \right].$$

Table 3 lists the above smoothing factors for the cases of interest, $d = 1, 2, 3$.

TABLE 3 Smoothing factors of pointwise GS-LEX applied to two common discretizations of the convection–diffusion equation with all mesh Reynolds numbers equal to γ , for $d = 1, 2, 3$

	Centred differences, $\gamma \in (-1, 1)$	Upwinding, $\gamma \geq 0$
$d = 1$	$\frac{1- \gamma }{\sqrt{4+(1+ \gamma)^2}}$	$\frac{1}{\sqrt{8\gamma^2+12\gamma+5}}$
$d = 2$	$\frac{1- \gamma }{2}$	$\frac{1}{2(1+\gamma)}$
$d = 3$	$\frac{(1- \gamma)\left(2+\sqrt{1+\left(\frac{1+ \gamma }{2}\right)^2}\right)}{6-\frac{1}{2}(1+ \gamma)^2}$	$\frac{2+\sqrt{1+\frac{1}{4}\left(1+\frac{\gamma}{1+\gamma}\right)^2}}{(1+\gamma)\left(6-\frac{1}{2}\left(1+\frac{\gamma}{1+\gamma}\right)^2\right)}$

TABLE 4 Comparison of the smoothing factor μ of GS-LEX with the measured asymptotic convergence rate of multigrid applied to the PDE $-u_{xx} - u_{yy} + \sigma u_x + \sigma u_y = f$, discretized uniformly. The problem is discretized using upwinding on a 1023×1023 grid. The Galerkin coarse grid operator is used. $W(1, 0)$ -cycles are used, and various values of $\gamma = \sigma h/2$, where h is the grid spacing on the finest mesh, are considered. ‘NC’ stands for no convergence. ‘nL’ (with $n = 2, 3, 4$) signifies the number of levels

γ	0.00	0.33	0.66	1.00	3.00	5.00
μ	0.50	0.38	0.30	0.25	0.13	0.08
2L	0.39	0.36	0.30	0.25	0.13	0.08
3L	0.41	0.36	0.31	NC	NC	NC
4L	0.41	NC	NC	NC	NC	NC

For asymmetric problems such as convection–diffusion, Galerkin coarse grid operators obtained by linear interpolation and full weighting may cause unstable coarse grid discretizations, leading to multigrid convergence problems, especially as the number of levels increases (van Asselt & de Zeeuw, 1985). Indeed, in Table 4 we observe divergence for multigrid with three or more levels for upwinding in the convection-dominated regime; for two levels, however, we see a good agreement between measured convergence rates and the predicted smoothing factor. We note that there are ways of dealing with these instabilities within the Galerkin framework; see, for example, de Zeeuw (1990).

The coarse grid operator \mathcal{L}^{2h} may also be defined by direct discretization of the underlying PDE on the coarse mesh. For upwinding with constant coefficients, this yields a stable discretization on all grid levels, and we can expect multigrid methods to converge. However, it has been shown that in this setting the coarse grid correction becomes less effective as convection becomes more dominant. In particular, the reduction factor of certain smooth modes increases to a nonnegligible constant, which grows as the number of levels increases (Brandt & Yavneh, 1993). In the convection-dominated regime where the smoothing factor becomes smaller than this constant, it is these smooth modes, rather than the rough modes, that dominate the error asymptotically. Consequently, it is this constant, rather than the smoothing factor, that determines the convergence rate. Therefore, we expect that the asymptotic convergence rate of multigrid will follow the trend indicated by our smoothing analysis in the diffusion-dominated regime, while tending to a constant in the convection-dominated regime (see Table 5). We also include GS-RB W -cycles in the table to illustrate the superiority of GS-LEX in this case. For the centred-difference discretization of the convection–diffusion problem, our smoothing analysis applies to the case where the mesh Reynolds number γ is less than one in magnitude. But in a multigrid set-up,

TABLE 5 Comparison of the smoothing factor μ of GS-LEX with measured convergence rates of multi-grid $V(1, 0)$ - and $W(1, 0)$ -cycles, for the PDE $-u_{xx} - u_{yy} + \sigma(u_x + u_y) = f$, discretized uniformly. The finest grid is 1023×1023 , while the coarsest is 1×1 . The coarse grid operator is obtained by direct discretization of the PDE on the coarse mesh. Various values of $\gamma = \sigma h/2$ are considered, where h is the grid spacing on the finest mesh. '2L' stands for a two-level scheme, whereas $V(1, 0)$ and $W(1, 0)$ signify V - and W -cycles, respectively, with one pre-smoothing sweep and no post-smoothing

γ	0.00	1.00	2.00	3.00	4.00	5.00
μ	0.50	0.25	0.17	0.13	0.10	0.08
2L	0.37	0.25	0.24	0.27	0.29	0.30
$V(1, 0)$	0.42	0.56	0.54	0.52	0.50	0.48
$W(1, 0)_{\text{LEX}}$	0.37	0.29	0.34	0.35	0.36	0.36
$W(1, 0)_{\text{RB}}$	0.23	0.37	0.46	0.59	0.71	0.79

TABLE 6 Comparison of the smoothing factor μ of GS-LEX with the measured asymptotic convergence rate of two-level and multilevel multigrid applied to the PDE $-u_{xx} - u_{yy} + \sigma(u_x + u_y) = f$, discretized uniformly. The problem is discretized using centred differences on a 1023×1023 grid. The coarse grid operator is obtained by direct discretization of the PDE on the coarse mesh. $W(1, 0)$ -cycles are used, and various values of $\gamma = \sigma h/2$, where h is the grid spacing on the finest mesh, are considered. 'NC' stands for no convergence. 'nL' (with $n = 2, 3, 4$) signifies the number of levels

γ	0.00	0.20	0.40	0.60	0.80	0.99
μ	0.50	0.40	0.30	0.20	0.10	0.005
2L	0.37	0.36	0.30	0.21	0.10	0.005
3L	0.37	0.36	0.30	NC	NC	NC
4L	0.37	0.36	NC	NC	NC	NC
5L	0.37	NC	NC	NC	NC	NC

we have different mesh Reynolds numbers on different grids—for our analysis to apply, they must all obey this constraint. Therefore, if L denotes the number of levels in our algorithm and γ denotes the mesh Reynolds number on the finest grid, what we really require is $|\gamma| < 2^{2-L}$.

In Table 6 we compare our predictions with measured convergence rates for various values of L ; $W(1, 0)$ -cycles are applied. In practice, we can get away with a mesh Reynolds number moderately larger than 1 on the coarsest grid and still maintain expected convergence rates.

EXAMPLE 3.4 Suppose the time-dependent diffusion problem

$$u_t = \rho_1 u_{x_1 x_1} + \rho_2 u_{x_2 x_2} + \cdots + \rho_d u_{x_d x_d}$$

is discretized on a uniform mesh using backward Euler in time and centred differences in space, with multigrid used to solve the resulting linear system at each time step. If τ denotes the time step size, then μ^{pt} follows from Theorem 2.5 by setting

$$c_r = \frac{\rho - \rho_m}{2\rho + h^2/\tau}, \quad c_m = \frac{\rho_m}{2\rho + h^2/\tau}, \quad \alpha = 1,$$

where $\rho = \sum_{k=1}^d \rho_k$ and $\rho_m = \min(\{\rho_k\})$.

In particular, in the isotropic case $\rho_1 = \rho_2 = \dots = \rho_d = 1$, we obtain

$$\mu^{\text{pt}} = \frac{(d-1)(2d + h^2/\tau) + \sqrt{(2d + h^2/\tau)^2 + d^2(2-d)^2}}{(2d + h^2/\tau)^2 + d(2-d)}.$$

When $d = 2$ this reduces to the particularly simple expression

$$\mu^{\text{pt}} = \frac{1}{2 + \frac{h^2}{2\tau}}.$$

Note the (expected) behaviour of the smoothing factor as a function of τ : when h is fixed and τ gets smaller, the smoothing factor becomes smaller too.

4. Conclusions

Using the results from the complex analysis, primarily the maximum modulus principle and properties of Möbius transformations, we have derived closed-form expressions for the smoothing factors of lexicographic pointwise and block Gauss–Seidel (Theorems 2.5 and 2.6). An extension of Theorem 2.5 that incorporates a relaxation parameter is provided in (2.10). In the pointwise case our results are valid for general operators of the form (1.2) satisfying the constraints (1.3) and (2.2), whereas in the block case we require the additional assumption of symmetry. In some cases, block smoothing on a high-dimensional problem has the same smoothing factor as pointwise smoothing on a related lower-dimensional problem.

Our analysis provides smoothing factors for, among other equations, the following:

- Pointwise GS-LEX applied to the d -dimensional *anisotropic steady-state diffusion* equation $-\sum_{k=1}^d \rho_k u_{x_k x_k} = f$, discretized with centred differences.
- Pointwise and block GS-LEX applied to the d -dimensional *Poisson* equation $-\Delta u = f$, discretized with centred differences.
- Pointwise GS-LEX applied to the d -dimensional constant coefficient *convection–diffusion* equation $-\Delta u + \vec{w} \cdot \nabla u = f$, discretized with centred differences or upwinding, and all mesh Reynolds numbers equal.
- Pointwise GS-LEX applied to the linear systems arising in each time step of the solution of the d -dimensional *time-dependent diffusion* equation $u_t = \sum_{k=1}^d \rho_k u_{x_k x_k}$, discretized with centred differences in space and backward Euler in time.

We have also observed that GS-LEX smoothing is effective for equations with strong asymmetry. In particular, for the constant coefficient convection–diffusion equation with equal mesh Reynolds numbers we have shown for upwind discretizations that GS-LEX has a smaller smoothing factor than GS-RB in the convection-dominated regime.

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