Adaptive technique for Chebyshev-based solvers for three-dimensional elliptic equations

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Abstract. An adaptive technique for multigrid and Chebyshev iteration method is presented. These both solvers are intended for solving three dimensional elliptic partial differential equations. The key elements of the technique are self-adaptive procedures for improving the computational efficiency of these methods. The adaptation provides an estimation of needed unknown bounds of the spectrum of discrete operators. For Chebyshev method the self-adaptive algorithm is capable of evaluating an unknown lower bound of the discrete operator. For multigrid the adaptation adjusts smoothers for achieving the desired multigrid performance.

1. Introduction
We present an adaptive technique for three dimensional elliptic PDEs solvers, namely, for multigrid [1] and the Chebyshev iteration method [2]. The main features of the technique are self-adaptation in the iterative processes of both methods. The adaptation procedures provide the desired estimation of unknown bounds of the spectrum of discrete operators. An estimation of $\lambda_{\text{max}}$ is obtained by the Gershgorin theorem. For the Chebyshev method we develop the self-adaptive algorithm which is capable of evaluating an unknown lower bound of the discrete operator whenever the algorithm has not achieved an optimal convergence rate with the preceding estimate of the lower bound. For the multigrid such algorithm adjusts smoothers for achieving the prescribed rate of multigrid convergence and improves the multigrid efficiency. The numerical examples are presented to show that the self-adaptive algorithm is efficient.

In the process of geometric multigrid development [3–5], we have shown efficiency of applying the adaptation procedure when using polynomial smoothing based on the optimal properties of Chebyshev polynomials. Here we apply also the adaptive technique to the algebraic multigrid (AMG) [6].

2. Statement of the problem
In a bounded three-dimensional domain $\Omega$ with boundary $\partial\Omega$ we consider a boundary value problem

$$Lu = f \quad \text{in} \ \Omega,$$
$$-(\kappa \nabla u) \cdot n = \sigma u + \gamma \quad \text{on} \ \partial\Omega. \quad (1)$$

Here $L$ is a linear elliptic self-adjoint positive semi-definite operator

$$Lu = -\nabla \cdot (\kappa \nabla u) + a_0 \cdot u$$
with coefficients $\kappa = \text{diag}\{k_1, k_2, k_3\}$, $k_i \geq 0$, $a_0 \geq 0$. The boundary condition (Dirichlet, Neumann, or Robin) is set on $\partial \Omega$, $n$ is outward normal vector to $\partial \Omega$. The coefficients $\kappa(r)$, $f(r)$, $a_0(r) \geq 0$, $\sigma(r) \geq 0$, $\gamma(r)$ are given functions, and $u(r)$ is the sought function; $r = (x, y, z) \in \Omega$. The input data are assumed to ensure the existence and uniqueness of a solution of the required smoothness. Such problems usually arise in computations of the gravitational potential, diffusion, etc. The discretization of the problem (1) is not discussed here. Accordingly, for simplicity, we use $\Omega$ as a right parallelepiped, in which we introduce a Cartesian grid $\Omega_h = \{x \in \Omega, 0 \leq n \leq N\}$ with grid boundary $\Gamma_h$; the grid $\Omega_h$ is depends on a parameter $h$ (characteristic mesh size). The space $U_h$ of functions on $\Omega_h$ is defined in the standard manner (with the $L_2$-grid inner product and the corresponding norm). On the space $U_h$ we define a difference operator $L_h$ approximating the operator $L$ with the second order of accuracy. To be more specific, the grid functions are given at the grid nodes and operator $L_h$ arises from 7-point finite volume discretization of the problem. The operator $L_h$ is self-adjoint, and its eigenvalues are nonnegative and belong to the real interval $[\lambda_{\min}, \lambda_{\max}]$. For this consideration, we assume that $L_h$ is positive definite and estimates for the bounds $\lambda_{\min} > 0$ and $\lambda_{\max}$ of the spectrum are a priori unknown. An estimate for $\lambda_{\max}$ is fairly easy to obtain with the help of the Gershgorin theorem.

Therefore we demonstrate the main features of the adaptive technique of solving a large system of linear equations

$$ Au = f, $$  

where $u, f \in \mathbb{R}^n$ are vectors and $A \in \mathbb{R}^{n \times n}$ is a self-adjoint positive definite matrix with eigenvalues $\lambda \in [\lambda_{\min}, \lambda_{\max}]$, $0 < \lambda_{\min} < \lambda_{\max}$.

### 3. The adaptive Chebyshev method

The Chebyshev iterative method for solving the system (2) can be expressed as

$$ u_{k+1} = u_k + \tau (f - Au_k), \quad k = 0, \ldots, p - 1, $$  

where $u_0$ is an initial guess, $p$ is a number of iterations, $\{\tau\}$ is the optimal set of the parameters. The error propagation operator $F_p(A)$ of this method is defined by the optimal Chebyshev polynomial $F_p(\lambda)$ for the interval $[\lambda_{\min}, \lambda_{\max}]$. To achieve the specified accuracy $\varepsilon$, we need to know $\lambda_{\min}$, $\lambda_{\max}$. The operator $F_p(A)$ transfers an initial guess $u_0$ and error $z_0 = u - u_0$ into new approximation $u_p$ and new error $z_p = u - u_p$ correspondently due to formulas

$$ u_p = F_p(A) u_0 + \left[I - F_p(A)\right] A^{-1} f, \quad z_p = F_p(A) z_0, $$

here $I$ is the identity operator. Polynomial $F_p(A)$ is defined multiplication of $p$ linear multipliers

$$ F_p(A) = (I - \tau_p A)(I - \tau_{p-1} A) \cdots (I - \tau_2 A)(I - \tau_1 A). $$

A number $p$ of iterations is determined by the condition of achieving the prescribed accuracy $\varepsilon$ according the criterion $\|r_p\| < \varepsilon \|r_0\|$, where $r_0$ and $r_p = f - A \cdot y_p$ are the initial and final residuals. An estimate for $p$ has the form (see [2]):
\[ p = p(e, \eta) \approx \frac{\ln \left( e^{-1} + \sqrt{e^{-2} - 1} \right)}{\ln \rho}, \quad \rho = \frac{1 + \sqrt{\eta}}{1 - \sqrt{\eta}}, \quad \eta = \frac{\lambda_{\min}}{\lambda_{\max}}, \]

where \( \lambda_{\min} \) and \( \lambda_{\max} \) are minimal and maximal eigenvalues of the operator \( A \). Therefore the optimal iteration process is defined by the Chebyshev polynomial \( F_p \) of degree \( p \), which deviates least from zero on the interval \([\lambda_{\min}; \lambda_{\max}]\) and is normalized by the condition, see [2]. This polynomial \( F_p \) is expressed by the standard polynomial \( T_p \) with the linear mapping

\[ t = 0.5 \cdot ((\lambda_{\min} + \lambda_{\max}) - (\lambda_{\max} - \lambda_{\min}) \cdot x), \]

which maps the interval \([-1;1]\) into the interval \([\lambda_{\min}; \lambda_{\max}]\) and point \( x = 1 \) to the point \( t = \lambda_{\min} \), point \( \lambda_{0} = 0 \) maps to point \( x = x(\lambda_{0}) > 1 \), where \( x = x(\lambda) \) is the inverse to the above-mentioned mapping.

The polynomial \( T_p(x) \) is the first kind Chebyshev polynomial of degree \( p \) that deviates least from zero on the interval \([-1;1]\) (see [2]):

\[ T_p(x) = \cos(p \arccos x), \quad |x| \leq 1; \quad T_p(x) = \cosh(p \text{ Arch} x), \quad |x| > 1. \]

Denote

\[ q_p = \frac{1}{T_p(x_0)} = \frac{1}{\text{ch}(p \text{ Arch} x_0)}, \]

then \( F_p(\lambda) = q_p T_p(x) \) and of value \( q_p \) there is representation

\[ q_p = \frac{2\rho_p^p}{1 + \rho_p^p}, \quad \rho_p = \frac{1 + \sqrt{\eta}}{1 - \sqrt{\eta}}. \]

Optimal parameters \( \tau_i \) are defined by the set of zeros of \( T_p \):

\[ \beta_i \in K_p = \left\{ \cos \frac{2i - 1}{2p} \pi, \ i = 1, \ldots, p \right\}, \quad \tau_i^{-1} = \frac{\lambda_{\max} + \lambda_{\min} - \lambda_{\min}}{2}, \quad k = 1, \ldots, p, \]

where the set \( K_p \) is ordered to ensure computational stability. It is clear that \( |T_p(x)| \leq 1 \) when \( |x| \leq 1 \), and outside this interval (on hyperbolic branches) the function \( |T_p(x)| \) is strictly monotonic. The last property is important to justify the adaptation procedure.

For the successful application of the Chebyshev method we need to know the bounds of the spectral interval \([\lambda_{\min}; \lambda_{\max}]\). Usually a good estimate of the lower bound is missing. We suggest an iterative refinement procedure to find automatically appropriate lower bound. The algorithm [7] based on another principle. Further below \( \lambda_{\min} \) and \( \lambda_{\max} \) mean exact (usually unknown) lower and upper bounds of the spectrum and \( \lambda_{\min}^* \) and \( \lambda_{\max}^* \) their approximate evaluations. It is known that under the conditions

\[ 0 < \lambda_{\min}^* \leq \lambda_{\min} \leq \lambda_{\max} \leq \lambda_{\max}^*, \]

the Chebyshev method converges, but the convergence rate can be decreased. According to [2] for the convergence of the iterations with inexact bounds the necessary and sufficient conditions are
\[
\lambda_{\max} < \lambda_{\max}^* + \lambda_{\min}^*, \quad 0 < \lambda_{\min}^*.
\]

For construction the adaptive procedure we assume that
\[
0 < \lambda_{\min} \leq \lambda_{\min}^* \leq \lambda_{\max}^*.
\]

The upper estimate \(\lambda_{\max}^*\) obtains by the Gershgorin theorem. The conditions (5) guarantee convergence of the iterations (3), because it provides the fulfillment of the conditions (4). An estimate \(\lambda_{\min}^*\) will be updated during the outer iterative process (or adaptation cycle). Denote the current approximate value as \(\lambda_{\min}^*\), and as \(\lambda_{\min,\text{new}}^*\) a new approximation to the exact bound \(\lambda_{\min}^*\). For adaptation we need to set an initial approximation \(\lambda_{\min}^*\) is greater than the exact value \(\lambda_{\min}^*\), \(\lambda_{\min}^* \geq \lambda_{\min}^*\). Note that one can get \(\lambda_{\min}^*\) by applying the power method to the operator \(B = I - (1 / \lambda_{\max}^*) A\). Finding the maximal eigenvalue \(\mu_{\max}\) of this operator, we obtain \(\lambda_{\max}^* = (1 - \mu_{\max}) \lambda_{\max}^*\). We use another procedure, naturally integrated in the iterative process, without such a preliminary part. To avoid the empirical choice, we take as an initial guess Rayleigh-Ritz ratio: \(\lambda_{\min}^* = \lambda_{\text{RR}} = (A v, v) / (v, v)\) with any nonzero function \(v\). According to the known property of relations Rayleigh-Ritz the required inequality \(\lambda_{\min}^* \geq \lambda_{\min}^*\) is true.

The proposed procedure for refining the lower bound is based on two assumptions. Firstly, the bound \(\lambda_{\max}^*\) is an upper estimate of the maximal eigenvalue \(\lambda_{\max}\) of the operator \(A\). In the case of the definition \(\lambda_{\max}^*\) by the Gershgorin theorem this assumption is true. Then the conditions (5) and (4) are satisfied. Secondly, after application of \(F_p(A)\) to an initial residual \(r_0\) the final residual \(r_p\) contains a dominant eigenmode which corresponds to the exact eigenvalue \(\lambda_{\min}\).

Our adaptation algorithm is as follows. Let us have to solve a system (2) with the specified accuracy \(\varepsilon_{\text{tot}}\). To reach such accuracy, we specify an additional accuracy \(\varepsilon_i = \varepsilon_{\text{tot}}\). Some characteristic values are \(\varepsilon_i = 10^{-2}\), \(\varepsilon_{\text{tot}} = 10^{-10}\), for example. We implement one cycle of the Chebyshev algorithm with specified input \(\lambda_{\min}^*, \lambda_{\max}^*, \varepsilon_i\) and then compute
\[
\delta = \|r_{p}\| / \|r_{i}\|, \quad r_{p} = F_p(A)r_0.
\]

Here \(\delta\) is real accuracy achieved in the current cycle, \(r_0\) and \(r_p\) are initial and final residuals. Note, if \(\lambda_{\min}^* \leq \lambda_{\min}\) then prescribed accuracy \(\varepsilon_i\) is achieved in the current cycle.

Suppose that the value \(\delta\) exceeds the specified tolerance \(\varepsilon_i\). Then the maximal eigenvalue \(\lambda_{\max}(F_p)\) of the polynomial \(F_p(A)\) on the interval \([\lambda_{\min}, \lambda_{\max}]\) achieves at the point \(\lambda = \lambda_{\min}\): \(\lambda_{\max}(F_p) = F_p(\lambda_{\min})\). Therefore it can be found approximately by known power method. So we take as approximations to \(\lambda_{\max}(F_p)\) the resulting ration \(\delta = \|r_{p}\| / \|r_{i}\|\) of the norms of the residuals. Using the value \(\lambda_{\max}(F_p)\) we find a new approximation \(\lambda_{\text{new}}^*\) to \(\lambda_{\min}\) (see below) and set \(\lambda_{\min}^* = \lambda_{\text{new}}^*\). If the desired accuracy \(\varepsilon_{\text{tot}}\) is not achieved, then we implement next cycle of adaptation with the parameters \(\lambda_{\min}^*, \lambda_{\max}^*, \varepsilon_i\). In favor of this version of the power method, instead of applying it to the operator \(B = I - (1 / \lambda_{\max}^*) A\), provides the following important property of optimal Chebyshev polynomials: according to [8] outside the optimal segment Chebyshev polynomials have in some sense opposite extreme property, namely, they deviate most from zero outside the segment.
If on a cycle \( k \) the obtained accuracy \( \delta = \delta_i \) does not exceed the specified tolerance \( \varepsilon_i \), we implement next cycle of adaptation with the old data \( \lambda_{\min}^*, \lambda_{\max}^* , \varepsilon_i \) or change the accuracy, taking the new value \( \varepsilon_i = \varepsilon_{\text{int}} / (\delta_i \times \ldots \times \delta_i) \). Therefore, if the condition \( \delta_i \leq \varepsilon_i \) is satisfied, then the estimation of \( \lambda_{\min}^* \) is rather accurate and the desired accuracy \( \varepsilon_{\text{tot}} \) will be achieved in the next cycle of adaptation.

The new approximation \( \lambda_{\min}^{\text{new}} \) is evidently defined as a unique root of the algebraic equation \( F_p(\lambda) - \delta = 0 \) on the interval \([0; \lambda_{\min}^*] \). Finally, we get the following formulas to compute a new approximation to the \( \lambda_{\min} \) using the input parameters \( \lambda_{\min}^*, \lambda_{\max}^* , \varepsilon_i \) and the obtained accuracy \( \delta \):

1. \( \eta = \frac{\lambda_{\min}^*}{\lambda_{\max}^*} \), \( \rho_i = \frac{1+\sqrt{\eta}}{1-\sqrt{\eta}} \), \( q_p = \frac{2\rho_i}{1+\rho_i} \), 
2. \( y_i = \frac{\delta}{q_p} \), \( y_2 = \ln \left( y_1 + \sqrt{y_1^2 - 1} \right) \), \( x^* = ch \left( y_2 / p \right) \), 
3. \( \lambda_{\min}^{\text{new}} = \frac{1+\eta}{2} - \frac{1-\eta}{2} x^* \), \( \lambda_{\min}^{\text{new}} = \lambda_{\min}^* \).

In the calculations we confirmed the success of this algorithm.

4. The adaptive multigrid method

Multigrid methods are among the most efficient numerical methods for solving the large linear systems. We apply the adaptive technique for classical geometric multigrid (GMG) and the algebraic multigrid (AMG) to provide efficiency of the polynomial smoothing procedures based on optimal properties of the Chebyshev polynomials.

In AMG a set of «grid» levels is used based on the matrix arising from the approximation of PDEs on the initial grid. In the description of AMG the terminology of the geometric multigrid method is used. The construction of linear system at various levels can be interpreted as the generation of a sequence of coarse grid levels with the coarse grid correction equations on them. Each multigrid iteration of AMG consists of a transition from one grid level to another, till to the coarsest level and back using intergrid transfer operators. For a system of each level, except the coarsest one, smoothing procedures are constructed, providing a transfer from the current approximation to the more "smooth" one. Such a transfer is usually done using an iterative method. At the coarsest level, the linear system can be solved exactly or approximately. If the coarsest system is solved in parallel, we suggest to use the Chebyshev iterative method with the adaptation of the lower bound of the spectrum of the coarsest operator.

In [4] the efficiency of the geometric multigrid method with adaptive Chebyshev smoothers is shown with special attention to the problems with anisotropic and discontinuous coefficients. The great interest to the Chebyshev smoothers arises from their ability to efficiently run on parallel computers with potentially millions of processors. The development of smoothers in this case is challenging, because some the common smoothing procedures, such as the lexicographical Gauss-Seidel procedure, are intrinsically sequential and do not parallelize well.

The disadvantage of Chebyshev's smoothers is the need to know the bounds of discrete operators on subspaces generated in the multigrid method. At each level (except the coarsest one), a space of grid functions is represented by the orthogonal sum of two subspaces. This partition is generated by the conditional division of the eigenfunctions of a discrete elliptic operator into two parts: low-frequency and high-frequency functions, i.e. division of the operator spectrum into low and high frequencies. The notions of algebraically smooth (low) frequencies and algebraic high frequencies play an important role in AMG development. Chebyshev smoothers require estimates of the spectrum bounds of discrete operators on high-frequency subspaces. The upper bound of the spectrum is fairly
accurately estimated using Gershgorin’s theorem, but a priori information about the lower bound of the high-frequency interval of the spectrum is usually absent.

However, one can evaluate this lower bound of the high-frequency interval during the multigrid iterations, analyzing the convergence process and applying the procedure similar to (6). The reason is the following. At each multigrid iteration, as a result of applying the smoothing operator to the residual \( r \) at the current grid level, in the smooth residual an eigenmode corresponding to the eigenvalue at the frequency interface becomes the leading one. That is, in the smooth residual low-frequency components can be neglected. This condition can be performed, for example, including adaptation after two or three multigrid iterations.

5. Numerical experiments

Consider the anisotropic diffusion problem with discontinuous coefficients [9]. The equation (1) is solved in the region \( \Omega = [0; 1]^3 \). This region is divided into four sub-regions \( \Omega_i \), \( i = 1, \ldots, 4 \) by the following way:

\[
\begin{align*}
\Omega_1 &= \{(x, y, z) \in \Omega : y \leq 0.5, z \leq 0.5\}, \\
\Omega_2 &= \{(x, y, z) \in \Omega : y > 0.5, z \leq 0.5\}, \\
\Omega_3 &= \{(x, y, z) \in \Omega : y > 0.5, z > 0.5\}, \\
\Omega_4 &= \{(x, y, z) \in \Omega : y \leq 0.5, z > 0.5\}.
\end{align*}
\]

The diffusion tensor is diagonal, \( k(x, y, z) = \text{diag}(k_x, k_y, k_z) \). It has a discontinuity on the internal interfaces and is continuous each subregion \( i = 1, \ldots, 4 \):

\[
k_x^1 = k_y^2 = k_z^3 = k_z^4 = 1,
\]

\[
k_x^1 = 10, \quad k_y^2 = 0.1, \quad k_y^3 = 0.01, \quad k_y^4 = 100,
\]

\[
k_x^1 = 0.01, \quad k_y^2 = 100, \quad k_z^2 = 10, \quad k_z^4 = 0.1.
\]

The exact solution in each subregion has the form \( u(x, y, z) = \alpha_i \sin(2\pi x) \sin(2\pi y) \sin(2\pi z) \); the continuity of the solution and the flux provides a choice \( \alpha_1 = 0.1, \alpha_2 = 10, \alpha_3 = 100, \alpha_4 = 0.01 \). On the outer boundaries of the region, the Dirichlet boundary conditions are set. They and also right-hand side of the equation (1) (in this equation \( a = 0 \)) are determined from the exact solution. We use the Cartesian grid \( \Omega_N = \{(x, y, z) \in \Omega, 0 \leq n \leq N\} \) with the number of nodes \( N = N_x \times N_y \times N_z \).

**Chebyshev solver.** In table 1 we present the results of application of the Chebyshev solver without (first and second rows) adaptation and with adaptation (third row) on a sequence of grids. In the case of adaptation we use the total accuracy \( \varepsilon_{\text{tol}} = 10^{-12} \) and additional tolerance \( \varepsilon_i = 10^{-2} \) for adaptive process.

Note that value \( \lambda_{\min}^* = 140 \) is close to the exact minimal eigenvalue of the discrete operator.

| Сетка, \( N_x^3 \) | 16\(^3\) | 32\(^3\) | 64\(^3\) | 128\(^3\) |
|---------------------|---------|---------|---------|---------|
| \( \lambda_{\min}^* = 10 \), \( N_{\text{iter}}^{\text{total}} \) | 1422 | 2883 | 5766 | 11531 |
| \( \lambda_{\min}^* = 140 \), \( N_{\text{iter}}^{\text{total}} \) | 386 | 771 | 1541 | 3082 |
| Adaptation, \( N_{\text{iter}}^{\text{total}} \) | 481 | 926 | 1827 | 3561 |

**Algebraic multigrid solver.** The convergence of the algebraic multigrid method is estimated with the following parameters: the relative accuracy of the solution of the initial linear system \( \varepsilon_{\text{AMG}} = 10^{-10} \), the relative accuracy of smoothing iterations \( \varepsilon_{\text{smooth}} = 0.5 \). The number of grid levels is restricted by 6.
We construct the AMG structures follow the classic version of Ruge-Stuben [6] with $C_S$ splitting. In table 2 we represent the achieved convergence rate $q$ of AMG, the total number of the multigrid iterations $N_{AMG}$, the number of smoothing iterations $N_{smooth}^{total}$ on the sequence of the initial grids.

| Grid      | $q$ | $N_{AMG}$ | $N_{smooth}^{total}$ |
|-----------|-----|-----------|-----------------------|
| 16×16×16  | 0.28| 17        | 234                   |
| 32×32×32  | 0.34| 20        | 260                   |
| 64×64×64  | 0.31| 19        | 312                   |
| 128×128×128 | 0.18| 13        | 422                   |

Here $N_{smooth}^{total}$ is a number of iterations at the initial (most detailed) level, this number is the sum over all multigrid iterations $N_{AMG}$, and characterizes the main computing work. One can see that this parameter $N_{smooth}^{total}$ slightly depends on grid size.

The results of adaptation of smoothers on each grid level (level0, …, level5) indicate efficiency and stability of the adaptation procedure, see Figure 1, where in the computational grid 128×128×128 behavior of the adaptive process on each multigrid level is shown. Stabilization of value $\eta = \frac{\lambda_{min}}{\lambda_{max}}$ («cond» on Figure 1)) comes when this value reaches approximately $\eta = 0.01$ at all levels. It means that we find the lower bound of the high-frequency interval on each level rather well.

![Figure 1](image)

**Figure 1.** Adaptive value $cond = \frac{\lambda_{min}}{\lambda_{max}}$ with respect to number of AMG iteration.
6. Conclusions
We presented in details the algorithm of adaptation for the Chebyshev iterative method and adaptive polynomial smoothing within multigrid. We have shown that these adaptive algorithms may be preferable to traditional approaches. They are easy to implement and integrate within existing computer codes, perform identically on serial and parallel computers, and require only well-executed matrix-vector multiplications. Classical smoothers like Gauss-Seidel work with a fixed arithmetic intensity. Adaptive polynomial smoothers can be implemented with a variable arithmetic intensity. Numerical experiments were performed for verification of the adaptive technique and they confirmed the efficiency of the proposed adaptive approach.

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